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Nonlocal self-improving properties: a functional analytic approach

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A functional analytic approach to obtaining self-improving properties of solutions to linear nonlocal elliptic equations is presented. It yields conceptually simple and very short proofs of some previous results due to Kuusi–Mingione–Sire and Bass–Ren. Its flexibility is demonstrated by new applications to nonautonomous parabolic equations with nonlocal elliptic part and questions related to maximal regularity.

1. Introduction

Recently, there has been a particular interest in linear elliptic integrodifferential equations of type

$$\iint_{\mathbb{R}^n\times\mathbb{R}^n} A(x,y)\frac{(u(x)-u(y))\cdot\overline{(\phi(x)-\phi(y))}}{|x-y|^{n+2\alpha}}\,\mathrm{d}x\,\mathrm{d}y = \int_{\mathbb{R}^n} f(x)\cdot\overline{\phi(x)}\,\mathrm{d}x \quad (\phi\in \mathrm{C}_0^\infty(\mathbb{R}^n)),$$

where the kernel A is a measurable function on $\mathbb{R}^n\times\mathbb{R}^n$ with bounds

$$0<\lambda\le \operatorname{Re} A(x,y)\le |A(x,y)|\le \lambda^{-1} \quad (\text{a.e. } (x,y)\in\mathbb{R}^n\times\mathbb{R}^n) \tag{1-1}$$

and α is a number strictly between 0 and 1. See for example [Bass and Ren 2013; Biccari et al. 2017a; 2017b; Kuusi et al. 2015; Leonori et al. 2015; Schikorra 2016]. Such fractional equations of order 2α exhibit new phenomena that do not have any counterpart in the theory of second order elliptic equations in divergence form: In

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[Kuusi et al. 2015], building on earlier ideas in [Bass and Ren 2013], it has been shown that under appropriate integrability assumptions on f, weak solutions u in the corresponding fractional L^2-Sobolev space $\mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ self-improve in integrability *and* in differentiability. Whereas the former is also known for second-order equations under the name of “Meyers’ estimate” [Meyers 1963], the improvement in regularity without any further smoothness assumptions on the coefficients is a feature of nonlocal equations only [Kuusi et al. 2015, p. 59]. We mention that [Kuusi et al. 2015] also treats semilinear variants of the equation above, but already the linear case is of interest for further applications, for example to the stability of stable-like processes [Bass and Ren 2013].

Up to now, most approaches are guided by the classical strategy for the second-order case, that is, they employ fractional Caccioppoli inequalities to establish nonlocal reverse Hölder estimates and then prove a delicate self-improving property for such inequalities in the spirit of Gehring’s lemma. The purpose of this note is to present a functional analytic approach which we believe is of independent interest for several other applications related to partial differential equations of fractional order as it yields short and conceptually very simple proofs.

Let us outline our strategy that is concisely implemented in Section 3. Writing the fractional equation in operator form

$$\langle \mathcal{L}_{\alpha,A} u, \phi\rangle = \langle f, \phi\rangle, \quad (u, \phi \in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)), \tag{1-2}$$

the left-hand side is associated with a sesquilinear form on the Hilbert space $\mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ and thanks to ellipticity (1-1) the Lax–Milgram lemma applies and yields invertibility of $1+\mathcal{L}_{\alpha,A}$ onto the dual space. Now, the main difference compared with second order elliptic equations is that we can transfer regularity requirements between u and ϕ without interfering with the coefficients A: without making any further assumption we may write

$$\langle \mathcal{L}_{\alpha,A} u, \phi\rangle = \iint_{\mathbb{R}^n\times\mathbb{R}^n} A(x,y)\frac{u(x)-u(y)}{|x-y|^{n/2+\alpha+\varepsilon}}\cdot\frac{\overline{\phi(x)-\phi(y)}}{|x-y|^{n/2+\alpha-\varepsilon}}\,\mathrm{d}x\,\mathrm{d}y,$$

which yields boundedness $\mathcal{L}_{\alpha,A} : \mathrm{W}^{\alpha+\varepsilon,2}(\mathbb{R}^n) \to \mathrm{W}^{\alpha-\varepsilon,2}(\mathbb{R}^n)^*$. Then the ubiquitous analytic perturbation lemma of Shneiberg [1974] allows one to extrapolate invertibility to $\varepsilon > 0$ small enough. We can also work in an L^p-setting with hardly any additional difficulties. In this way, we shall recover some of the results from [Bass and Ren 2013; Kuusi et al. 2015] on global weak solutions in Section 4 and discuss some new and sharpened local self-improvement properties in Section 5.

Finally, in Section 6 we demonstrate the simplicity and flexibility of our approach by proving that for each $f \in \mathrm{L}^2(0,T;\mathrm{L}^2(\mathbb{R}^n))$ the unique solution

$$u \in \mathrm{H}^1(0,T;\mathrm{W}^{\alpha,2}(\mathbb{R}^n)^*) \cap \mathrm{L}^2(0,T;\mathrm{W}^{\alpha,2}(\mathbb{R}^n))$$

of the nonautonomous Cauchy problem

$$u'(t) + \mathcal{L}_{\alpha,A(t)}u(t) = f(t), \quad u(0) = 0,$$

self-improves to the class $\mathrm{H}^1(0, T; \mathrm{W}^{\alpha-\varepsilon,2}(\mathbb{R}^n)^*) \cap \mathrm{L}^2(0, T; \mathrm{W}^{\alpha+\varepsilon,2}(\mathbb{R}^n))$ for some $\varepsilon > 0$. Here, each $\mathcal{L}_{\alpha,A(t)}$ is a fractional elliptic operator as in (1-2) with uniform upper and lower bounds in t but again we do not assume any regularity on $A(t, x, y) := A(t)(x, y)$ besides measurability in all variables. We remark that $\varepsilon = \alpha$ and $\mathrm{W}^{0,2}(\mathbb{R}^n) := \mathrm{L}^2(\mathbb{R}^n)$ would mean maximal regularity, which in general requires some smoothness of the coefficients in the t-variable. See [Arendt et al. 2017] for a recent survey and the recent paper [Grubb 2018] for related results on regularity of solutions to such fractional heat equations with smooth coefficients. In this regard, our results reveal a novel phenomenon in the realm of nonautonomous maximal regularity. Let us remark that we have recently also explored related techniques for second-order parabolic systems [Auscher et al. 2017].

2. Notation

Any Banach space X under consideration is taken over the complex numbers and we shall denote by X^* the *antidual space* of conjugate linear functionals $X \to \mathbb{C}$. In particular, all function spaces are implicitly assumed to consist of complex valued functions. Throughout, we assume the dimension of the underlying Euclidean space to be $n \geq 2$.

Given $s \in (0, 1)$ and $p \in (1, \infty)$, the *fractional Sobolev space* $\mathrm{W}^{s,p}(\mathbb{R}^n)$ consists of all $u \in \mathrm{L}^p(\mathbb{R}^n)$ with finite seminorm

$$[u]_{s,p} := \left(\iint_{\mathbb{R}^n \times \mathbb{R}^n} \frac{|u(x) - u(y)|^p}{|x - y|^{n+sp}} \, \mathrm{d}x \, \mathrm{d}y \right)^{\frac{1}{p}} < \infty.$$

It becomes a Banach space for the norm $\| \cdot \|_{s,p} := (\| \cdot \|_p^p + [\,\cdot\,]_{s,p}^p)^{1/p}$, where here and throughout $\| \cdot \|_p$ denotes the norm on $\mathrm{L}^p(\mathbb{R}^n)$. Moreover, $\mathrm{W}^{s,2}(\mathbb{R}^n)$ is a Hilbert space for the inner product

$$\langle u, v \rangle := \int_{\mathbb{R}^n} u(x) \cdot \overline{v(x)} \, \mathrm{d}x + \iint_{\mathbb{R}^n \times \mathbb{R}^n} \frac{(u(x) - u(y)) \cdot \overline{(v(x) - v(y))}}{|x - y|^{n+2s}} \, \mathrm{d}x \, \mathrm{d}y.$$

Frequently it will be more convenient to view $\mathrm{W}^{s,p}(\mathbb{R}^n)$ within the scale of Besov spaces. More precisely, taking $\phi \in \mathcal{S}(\mathbb{R}^n)$ with Fourier transform $\mathcal{F}\phi : \mathbb{R}^n \to [0, 1]$ such that $\mathcal{F}\phi(\xi) = 1$ for $|\xi| \leq 1$ and $\mathcal{F}\phi(\xi) = 0$ for $|\xi| \geq 2$ and defining $\phi_0 := \phi$ and $(\mathcal{F}\phi_j)(\xi) := \mathcal{F}\phi(2^{-j}\xi) - \mathcal{F}\phi(2^{-j+1}\xi)$ for $\xi \in \mathbb{R}^n$ and $j \geq 1$, the *Besov space*

$\mathrm{B}^s_{p,p}(\mathbb{R}^n)$ is the collection of all $u \in \mathrm{L}^p(\mathbb{R}^n)$ with finite norm

$$\|u\|_{\mathrm{B}^s_{p,p}(\mathbb{R}^n)} := \Big(\sum_{j=0}^{\infty} 2^{jsp} \|\phi_j * u\|_p^p\Big)^{\frac{1}{p}} < \infty. \tag{2-1}$$

Different choices of ϕ yield equivalent norms on $\mathrm{B}^s_{p,p}(\mathbb{R}^n)$. Moreover, the Schwartz class $\mathcal{S}(\mathbb{R}^n)$, and thus also the space of smooth compactly supported functions $\mathrm{C}_0^\infty(\mathbb{R}^n)$, is dense in any of these spaces, see [Triebel 1983, Section 2.3.3]. Finally, $\mathrm{W}^{s,p}(\mathbb{R}^n) = \mathrm{B}^s_{p,p}(\mathbb{R}^n)$ up to equivalent norms [Triebel 1983, Section 2.5.12].

3. Analysis of the Dirichlet form

In this section, we carefully analyze the mapping properties of the *Dirichlet form*

$$\mathcal{E}_{\alpha,A}(u, v) := \iint_{\mathbb{R}^n \times \mathbb{R}^n} A(x, y) \frac{(u(x) - u(y)) \cdot \overline{(v(x) - v(y))}}{|x - y|^{n+2\alpha}} \, \mathrm{d}x \, \mathrm{d}y, \tag{3-1}$$

which we define here for $u, v \in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)$. Starting from now, $\alpha \in (0, 1)$ is fixed and $A : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{C}$ denotes a measurable kernel that satisfies the accretivity condition (1-1). This entails boundedness

$$|\mathcal{E}_{\alpha,A}(u, v)| \le \lambda^{-1} [u]_{\alpha,2} [v]_{\alpha,2} \le \lambda^{-1} \|u\|_{\alpha,2} \|v\|_{\alpha,2}$$

and quasicoercivity

$$\operatorname{Re} \mathcal{E}_{\alpha,A}(u, u) \ge \lambda [u]^2_{\alpha,2} \ge \lambda \|u\|^2_{\alpha,2} - \|u\|_2^2. \tag{3-2}$$

Together with the sesquilinear form $\mathcal{E}_{\alpha,A}$ comes the associated operator $\mathcal{L}_{\alpha,A} : \mathrm{W}^{\alpha,2}(\mathbb{R}^n) \to \mathrm{W}^{\alpha,2}(\mathbb{R}^n)^*$ defined through

$$\langle \mathcal{L}_{\alpha,A} u, v \rangle := \mathcal{E}_{\alpha,A}(u, v),$$

where $\langle \cdot\,, \cdot \rangle$ denotes the sesquilinear duality between $\mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ and its antidual, extending the inner product on $\mathrm{L}^2(\mathbb{R}^n)$.

As an immediate consequence of the Lax–Milgram lemma we can record:

Lemma 3.1. *The operator* $1 + \mathcal{L}_{\alpha,A} : \mathrm{W}^{\alpha,2}(\mathbb{R}^n) \to \mathrm{W}^{\alpha,2}(\mathbb{R}^n)^*$ *is bounded and invertible. Its norm and the norm of its inverse do not exceed* λ^{-1}.

The key step in our argument will be to obtain the analogous result on "nearby" fractional Sobolev spaces $\mathrm{W}^{s,p}(\mathbb{R}^n)$. We begin with boundedness, which of course is the easy part.

Lemma 3.2. *Let* $s, s' \in (0, 1)$ *and* $p, p' \in (1, \infty)$ *satisfy*

$$s + s' = 2\alpha \quad \textit{and} \quad \frac{1}{p} + \frac{1}{p'} = 1.$$

Then $1+\mathcal{L}_{\alpha,A}$ *extends from* $\mathrm{C}_0^\infty(\mathbb{R}^n)$ *by density to a bounded operator* $\mathrm{W}^{s,p}(\mathbb{R}^n) \to \mathrm{W}^{s',p'}(\mathbb{R}^n)^*$ *denoted also by* $1+\mathcal{L}_{\alpha,A}$, *and*

$$|\langle u+\mathcal{L}_{\alpha,A}u, v\rangle| \le \|u\|_p\|v\|_{p'} + \lambda^{-1}[u]_{s,p}[v]_{s',p'}$$

for all $u \in \mathrm{W}^{s,p}(\mathbb{R}^n)$ *and all* $v \in \mathrm{W}^{s',p'}(\mathbb{R}^n)$.

Proof. Given $u, v \in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ we split $n+2\alpha = (n/p+s)+(n/p'+s')$ and apply Hölder's inequality with exponents $1 = 1/\infty + 1/p + 1/p'$ to give

$$\begin{aligned}|\langle \mathcal{L}_{\alpha,A}u, v\rangle| &= \left| \iint_{\mathbb{R}^n\times\mathbb{R}^n} A(x,y)\frac{(u(x)-u(y))\cdot\overline{(v(x)-v(y))}}{|x-y|^{n+2\alpha}}\,\mathrm{d}x\,\mathrm{d}y\right| \\ &\le \lambda^{-1}[u]_{s,p}[v]_{s',p'}.\end{aligned}$$

Again by Hölder's inequality $|\langle u, v\rangle| \le \|u\|_p\|v\|_{p'}$, yielding the required estimate for $u, v \in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)$. Since $\mathrm{C}_0^\infty(\mathbb{R}^n)$ is a common dense subspace of all fractional Sobolev spaces under consideration here (see Section 2) this precisely means that $1+\mathcal{L}_{\alpha,A}$ extends to a bounded operator from $\mathrm{W}^{s,p}(\mathbb{R}^n)$ into the antidual space of $\mathrm{W}^{s',p'}(\mathbb{R}^n)$. □

Remark 3.3. It follows from Fatou's lemma that for u and v as in Lemma 3.2 we still have $\langle \mathcal{L}_{\alpha,A}u, v\rangle = \mathcal{E}_{\alpha,A}(u,v)$ with the right-hand side given by (3-1).

We turn to the study of invertibility by means of a powerful analytic perturbation argument going back to Shneiberg [1974]. In essence, the only supplementary piece of information needed for this approach is that the function spaces for boundedness obtained above form a complex interpolation scale.

We denote by $[X_0, X_1]_\theta$, $0<\theta<1$, the scale of *complex interpolation spaces* between two Banach spaces X_0, X_1 that are both included in the tempered distributions $\mathcal{S}'(\mathbb{R}^n)$. The reader may look up the Appendix for definitions and further references, but for the understanding of this paper we do not require any further knowledge on this theory except for the identity

$$\left[\mathrm{W}^{s_0,p_0}(\mathbb{R}^n), \mathrm{W}^{s_1,p_1}(\mathbb{R}^n)\right]_\theta = \mathrm{W}^{s,p}(\mathbb{R}^n) \tag{3-3}$$

for $p_0, p_1 \in (1,\infty)$, $s_0, s_1 \in (0,1)$, with p, s given by

$$\frac{1}{p} = \frac{1-\theta}{p_0} + \frac{\theta}{p_1}, \qquad s = (1-\theta)s_0 + \theta s_1,$$

and the analogous identity for the antidual spaces. Equality (3-3) is in the sense of Banach spaces with equivalent norms and the equivalence constants are uniform for s_i, p_i, θ within compact subsets of the respective parameter intervals. This uniformity is implicit in most proofs and we provide references where they are either stated or can be read off particularly easily: this is [Triebel 1983, Section 2.5.12] to identify $\mathrm{W}^{s,p}(\mathbb{R}^n) = \mathrm{B}^s_{p,p}(\mathbb{R}^n)$ up to equivalent norms, [Bergh and

Löfström 1976, Theorem 6.4.5(6)] for the interpolation and [Bergh and Löfström 1976, Corollary 4.5.2] for the (anti) dual spaces.

Proposition 3.4. *Let $s, s' \in (0,1)$ and $p, p' \in (1,\infty)$ satisfy $s + s' = 2\alpha$ and $1/p + 1/p' = 1$. There exists $\varepsilon > 0$, such that if $\left|\frac{1}{2} - \frac{1}{p}\right| < \varepsilon$ and $|s - \alpha| < \varepsilon$, then*

$$1 + \mathcal{L}_{\alpha,A} : \mathrm{W}^{s,p}(\mathbb{R}^n) \to \mathrm{W}^{s',p'}(\mathbb{R}^n)^*$$

is invertible and the inverse agrees with the one obtained for $s = \alpha$, $p = 2$ on their common domain of definition. Moreover, ε and the norms of the inverses depend only on λ, n, and α.

Proof. Consider the spaces $\mathrm{W}^{s,p}(\mathbb{R}^n)$ and $\mathrm{W}^{s',p'}(\mathbb{R}^n)^*$ as being arranged in the $(s, 1/p)$-plane, where $p \in (1,\infty)$ but to make sense of our assumption we only consider parameters s such that additionally $s' = 2\alpha - s \in (0,1)$. By Lemma 3.2 we have boundedness

$$1 + \mathcal{L}_{\alpha} : \mathrm{W}^{s,p}(\mathbb{R}^n) \to \mathrm{W}^{s',p'}(\mathbb{R}^n)^*$$

at every such $(s, 1/p)$ and Lemma 3.1 provides invertibility at $\left(\alpha, \frac{1}{2}\right)$.

Now, consider any line in the $(s, 1/p)$-plane passing through $\left(\alpha, \frac{1}{2}\right)$ and take $(s_0, 1/p_0)$, $(s_1, 1/p_1)$ on opposite sides of $\left(\alpha, \frac{1}{2}\right)$. Then (3-3) precisely says that the scale of complex interpolation spaces between $\mathrm{W}^{s_0,p_0}(\mathbb{R}^n)$ and $\mathrm{W}^{s_1,p_1}(\mathbb{R}^n)$ corresponds (up to uniformly controlled equivalence constants) to the connecting line segment. The same applies to $\mathrm{W}^{s_0',p_0'}(\mathbb{R}^n)^*$ and $\mathrm{W}^{s_1',p_1'}(\mathbb{R}^n)^*$ on the segment connecting $(s_0', 1/p_0')$ and $(s_1', 1/p_1')$ through $\left(\alpha, \frac{1}{2}\right)$.

According to the quantitative version of Shneiberg's result, Theorem A.1 of the Appendix, invertibility at the interior point $\left(\alpha, \frac{1}{2}\right)$ of this segment implies invertibility on an open surrounding interval. Its radius around $\left(\alpha, \frac{1}{2}\right)$ depends on an upper bound for the operator on nearby spaces, the lower bound at the center, and the constants of norm equivalence. Moreover, the inverses are compatible with the one computed at $\left(\alpha, \frac{1}{2}\right)$. In particular, since we can pick the same interval on every line segment, this sums up to a two-dimensional ε-neighborhood in the $(s, 1/p)$-plane as required. □

4. Weak solutions to elliptic nonlocal problems

We are ready to use the abstract results obtained so far, to establish higher differentiability and integrability results for weak solutions $u \in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ to elliptic nonlocal problems of the form

$$\mathcal{L}_{\alpha,A} u = \mathcal{L}_{\beta,B}\, g + f. \tag{4-1}$$

Here, $\mathcal{L}_{\alpha,A}$ is associated with the form $\mathcal{E}_{\alpha,A}$ in (3-1). In the same way, $\mathcal{L}_{\beta,B}$ is associated with

$$\mathcal{E}_{\beta,B}(g,v) := \iint_{\mathbb{R}^n\times\mathbb{R}^n} B(x,y)\frac{(g(x)-g(y))\cdot\overline{(v(x)-v(y))}}{|x-y|^{n+2\beta}}\,\mathrm{d}x\,\mathrm{d}y,$$

where starting from now, we fix $\beta\in(0,1)$ and $B\in \mathrm{L}^\infty(\mathbb{R}^n\times\mathbb{R}^n)$. Just like before, this guarantees that $\mathcal{E}_{\beta,B}$ is a bounded sesquilinear form on $\mathrm{W}^{\beta,2}(\mathbb{R}^n)$ and hence that $\mathcal{L}_{\beta,B}$ is bounded from $\mathrm{W}^{\beta,2}(\mathbb{R}^n)$ into its antidual. However, we carefully note that we do neither assume a lower bound on B nor any relation between α and β. In particular, $\beta>\alpha$ is allowed.

In the most general setup that is needed here, weak solutions are defined as follows.

Definition 4.1. Let $f\in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$ and $g\in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$ such that $\mathcal{E}_{\beta,B}(g,\phi)$ converges absolutely for every $\phi\in \mathrm{C}_0^\infty(\mathbb{R}^n)$. A function $u\in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ is called *weak solution* to (4-1) if

$$\mathcal{E}_{\alpha,A}(u,\phi)=\mathcal{E}_{\beta,B}(g,\phi)+\int_{\mathbb{R}^n} f\cdot\bar{\phi}\,\mathrm{d}x \quad (\phi\in \mathrm{C}_0^\infty(\mathbb{R}^n)).$$

Suppose now that we are given a weak solution $u\in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)$. In order to invoke Proposition 3.4, we write (4-1) in the form

$$(1+\mathcal{L}_{\alpha,A})u=\mathcal{L}_{\beta,B}g+f+u.$$

Hence, we see that higher differentiability and integrability for u, that is $u\in \mathrm{W}^{s,p}(\mathbb{R}^n)$ for some $s>\alpha$ and $p>2$, follows at once provided we can show $\mathcal{L}_{\beta,B}g+f+u\in \mathrm{W}^{s',p'}(\mathbb{R}^n)^*$ with $s'<\alpha$ and $p'<2$ as in Proposition 3.4. So, for the moment, our task is to work out the compatibility conditions on u, f, and g to run this argument.

4A. ***Compatibility conditions for the right-hand side.*** The standing assumptions for all results in this section are $s'\in(0,1)$, $p\in(1,\infty)$ and $1/p+1/p'=1$.

We begin by recalling the fractional Sobolev inequality, which will already take care of u and f.

Lemma 4.2 [Di Nezza et al. 2012, Theorem 6.5]. *Suppose $s'p'<n$ and put $1/p'^*:=1/p'-s'/n$. Then*

$$\|v\|_{p'^*}\lesssim [v]_{s',p'} \quad (v\in \mathrm{W}^{s',p'}(\mathbb{R}^n)).$$

In particular, $\mathrm{W}^{s',p'}(\mathbb{R}^n)\subset \mathrm{L}^{p'^*}(\mathbb{R}^n)$ and $\mathrm{L}^{p_*}(\mathbb{R}^n)\subset \mathrm{W}^{s',p'}(\mathbb{R}^n)^*$ with continuous inclusions, where $1/p_*:=1/p+s'/n$.

As for g, a dichotomy between the cases $2\beta \geq \alpha$ and $2\beta < \alpha$ occurs. This reflects a dichotomy for the parameter s', which typically is close to α. In the first case, $2\beta \geq \alpha$, we shall rely on

Lemma 4.3. *If* $2\beta - s' \in (0,1)$ *and* $g \in \mathrm{W}^{2\beta-s',p}(\mathbb{R}^n)$, *then*

$$|\langle \mathcal{L}_{\beta,B} g, v\rangle| \leq \|B\|_\infty [g]_{2\beta-s',p}[v]_{s',p'} \quad (v \in \mathrm{W}^{s',p'}(\mathbb{R}^n)).$$

Proof. Write $n+2\beta = (n/p+2\beta-s') + (n/p'+s')$ and note that

$$|\langle \mathcal{L}_{\beta,B} g, v\rangle| \leq \iint_{\mathbb{R}^n\times\mathbb{R}^n} \left|\frac{g(x)-g(y)}{|x-y|^{n/p+2\beta-s'}}\right| \left|\frac{v(x)-v(y)}{|x-y|^{n/p'+s'}}\right| |B(x,y)| \,\mathrm{d}x\,\mathrm{d}y.$$

The claim follows from Hölder's inequality. □

The second case, $2\beta < \alpha$, is slightly more complicated as we need the following embedding related to the fractional Laplacian $(-\Delta)^\beta$, compare with [Di Nezza et al. 2012, Section 3].

Lemma 4.4. *Suppose* $s' > 2\beta$, $s'p' < n$, *and put* $1/q' := 1/p' - (s'-2\beta)/n$. *Then*

$$\left(\int_{\mathbb{R}^n}\left(\int_{\mathbb{R}^n} \frac{|v(x)-v(y)|}{|x-y|^{n+2\beta}}\,\mathrm{d}y\right)^{q'}\mathrm{d}x\right)^{\frac{1}{q'}} \lesssim [v]_{s',p'} \quad (v \in \mathrm{W}^{s',p'}(\mathbb{R}^n)).$$

Proof. Let $v \in \mathrm{W}^{s',p'}(\mathbb{R}^n)$ and put $1/p'^* := 1/p' - s'/n$ as in Lemma 4.2, so that

$$\frac{1}{q'} = \frac{2\beta}{s'p'} + \frac{s'-2\beta}{s'}\frac{1}{p'^*} := \frac{1}{r_1} + \frac{1}{r_2}.$$

Note that our assumptions guarantee $p'^*, r_1, r_2 \in (1,\infty)$. Denote by M the Hardy–Littlewood maximal operator defined for $f \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^n)$ via

$$Mf(x) := \sup_{B \ni x} \frac{1}{|B|}\int_B |f(y)|\,\mathrm{d}y \quad (x \in \mathbb{R}^n),$$

where the supremum runs over all balls $B \subset \mathbb{R}^n$ that contain x. We claim that it suffices to prove

$$\int_{\mathbb{R}^n} \frac{|v(x)-v(y)|}{|x-y|^{n+2\beta}}\,\mathrm{d}y \lesssim \left(\int_{\mathbb{R}^n} \frac{|v(x)-v(y)|^{p'}}{|x-y|^{n+s'p'}}\,\mathrm{d}y\right)^{\frac{1}{r_1}} Mv(x)^{1-p'/r_1} \quad (\text{a.e. } x \in \mathbb{R}^n). \tag{4-2}$$

Indeed, temporarily assuming (4-2), we can take L^q-norms in the x-variable and apply Hölder's inequality on the integral in x with exponents $1/q' = 1/r_1 + 1/r_2$ to deduce

$$\left(\int_{\mathbb{R}^n}\left(\int_{\mathbb{R}^n} \frac{|v(x)-v(y)|}{|x-y|^{n+2\beta}}\,\mathrm{d}y\right)^{q'}\mathrm{d}x\right)^{\frac{1}{q'}} \lesssim [v]_{s',p'}^{p'/r_1} \|Mv\|_{p'^*}^{1-p'/r_1}.$$

The claim follows since we have $\|Mv\|_{p'^*} \lesssim \|v\|_{p'^*} \lesssim [v]_{s',p'}$ by the maximal theorem and Lemma 4.2.

Now, in order to establish (4-2) we split the integral at $|x-y| = h(x)$, with $h(x)$ to be chosen later. Since $2\beta - s' < 0$ by assumption, we can write $n+2\beta = n/p' + s' + n/p + (2\beta - s')$ and apply Hölder's inequality to give

$$\begin{aligned}\int_{|x-y|\le h(x)} \frac{|v(x)-v(y)|}{|x-y|^{n+2\beta}}\,\mathrm{d}y &\le h(x)^{s'-2\beta}\left(\int_{|x-y|\le h(x)} \frac{|v(x)-v(y)|^{p'}}{|x-y|^{n+s'p'}}\,\mathrm{d}y\right)^{\frac{1}{p'}} \\ &\le h(x)^{s'-2\beta}\left(\int_{\mathbb{R}^n} \frac{|v(x)-v(y)|^{p'}}{|x-y|^{n+s'p'}}\,\mathrm{d}y\right)^{\frac{1}{p'}}. \qquad (4\text{-}3)\end{aligned}$$

The remaining integral is bounded by

$$\begin{aligned}&\int_{|x-y|\ge h(x)} \frac{|v(x)-v(y)|}{|x-y|^{n+2\beta}}\,\mathrm{d}y \\ &\qquad \le \int_{|x-y|\ge h(x)} \frac{|v(x)|}{|x-y|^{n+2\beta}}\,\mathrm{d}y + \int_{|x-y|\ge h(x)} \frac{|v(y)|}{|x-y|^{n+2\beta}}\,\mathrm{d}y,\end{aligned}$$

where the first term equals $c|v(x)|h(x)^{-2\beta}$ for some dimensional constant c. Next, on writing

$$\frac{1}{|x-y|^{n+2\beta}} = \int_{|x-y|}^{\infty} \frac{n+2\beta}{r^n}\,\frac{\mathrm{d}r}{r^{1+2\beta}}$$

and changing the order of integration, the second term above becomes

$$(n+2\beta)\int_{h(x)}^{\infty}\left(\frac{1}{r^n}\int_{h(x)\le|x-y|\le r} |v(y)|\,\mathrm{d}y\right)\frac{\mathrm{d}r}{r^{1+2\beta}}$$

and thus can be controlled by $C_{n,\beta} Mv(x) h(x)^{-2\beta}$. Since $|v| \le Mv$ almost everywhere, we obtain in conclusion

$$\int_{|x-y|\ge h(x)} \frac{|v(x)-v(y)|}{|x-y|^{n+2\beta}}\,\mathrm{d}y \lesssim h(x)^{-2\beta} Mv(x) \quad (\text{a.e. } x \in \mathbb{R}^n). \qquad (4\text{-}4)$$

Finally, we pick $h(x)$ such that the right-hand sides of (4-3) and (4-4) are equal and obtain (4-2). □

As an easy consequence we obtain the required bounds for $\mathcal{L}_{\beta,B}$.

Corollary 4.5. *Suppose $s' > 2\beta$, $s'p' < n$, and put $1/q := 1/p + (s'-2\beta)/n$. For every $g \in \mathrm{L}^q(\mathbb{R}^n)$ there holds*

$$|\langle \mathcal{L}_{\beta,B} g, v\rangle| \lesssim \|B\|_\infty \|g\|_q [v]_{s',p'} \quad (v \in \mathrm{W}^{s',p'}(\mathbb{R}^n)).$$

Proof. We crudely bound $|g(x)-g(y)| \le |g(x)|+|g(y)|$ in the integral representation for $\langle \mathcal{L}_{\beta,B}g, v\rangle$ and apply Tonelli's theorem to give

$$\begin{aligned}|\langle \mathcal{L}_{\beta,B}g, v\rangle| &\le \int_{\mathbb{R}^n} |g(x)| \bigg(\int_{\mathbb{R}^n} \frac{|v(x)-v(y)|}{|x-y|^{n+2\beta}} \cdot \big(|B(x,y)|+|B(y,x)|\big)\,\mathrm{d}y \bigg)\,\mathrm{d}x \\ &\le 2\|B\|_\infty \|g\|_q \bigg(\int_{\mathbb{R}^n} \bigg(\int_{\mathbb{R}^n} \frac{|v(x)-v(y)|}{|x-y|^{n+2\beta}}\,\mathrm{d}y \bigg)^{q'} \mathrm{d}x \bigg)^{\frac{1}{q'}},\end{aligned}$$

the second step being due to Hölder's inequality. Since the Hölder conjugate of q is the exponent q' appearing in Lemma 4.4, the claimed inequality follows from that very lemma. □

4B. ***Proof of a global higher differentiability and integrability result.*** Combining Proposition 3.4 with the mapping properties found in the previous section, we can prove our main self-improvement property for weak solutions of (4-1) . As in [Kuusi et al. 2015], we impose the additional restriction $2\beta-\alpha<1$ in the case that $\beta>\alpha$.

Theorem 4.6. *There exists $\varepsilon>0$, depending only on $\lambda, n, \alpha, \beta$ with the following property. Suppose $s\in(\alpha,1)$ and $p\in[2,\infty)$ satisfy $|s-\alpha|, |p-2|<\varepsilon$. If $u\in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ is a weak solution to (4-1), then the following conditions guarantee $u\in \mathrm{W}^{s,p}(\mathbb{R}^n)$:*

$$f\in \mathrm{L}^r(\mathbb{R}^n), \qquad \frac{1}{r}=\frac{1}{p}+\frac{2\alpha-s}{n}$$

and

$$g\in \mathrm{L}^q(\mathbb{R}^n), \qquad \frac{1}{q}=\frac{1}{p}+\frac{2\alpha-2\beta-s}{n} \quad \text{if } 2\beta<\alpha,$$

or

$$g\in \mathrm{W}^{2\beta-2\alpha+s,p}(\mathbb{R}^n) \quad \text{if } 0\le 2\beta-\alpha<1.$$

Moreover, there is an estimate

$$\|u\|_{s,p} \lesssim \|u\|_{\alpha,2}+\|f\|+\|g\|,$$

where the norms of f and g are taken with respect to the function spaces specified above and the implicit constant depends on $\lambda, n, \alpha, \beta, s, p$ and $\|B\|_\infty$.

Proof. As usual we write $s+s'=2\alpha$ and $1/p+1/p'=1$. We let $\varepsilon>0$ as given by Proposition 3.4. If we can show $\mathcal{L}_{\beta,B}g+f+u\in \mathrm{W}^{s',p'}(\mathbb{R}^n)^*$, upon possibly forcing further restrictions on ε, then by density of $\mathrm{C}_0^\infty(\mathbb{R}^n)$ in the fractional Sobolev spaces we can write the equation for u in the form

$$(1+\mathcal{L}_{\alpha,A})u=\mathcal{L}_{\beta,B}g+f+u$$

and Proposition 3.4 yields $u\in \mathrm{W}^{s,p}(\mathbb{R}^n)$ with bound

$$\|u\|_{s,p} \lesssim \|\mathcal{L}_{\beta,B}g+f+u\|_{\mathrm{W}^{s',p'}(\mathbb{R}^n)^*}. \tag{4-5}$$

By assumption and Lemma 4.2 we have $u \in \mathrm{L}^p(\mathbb{R}^n)$ for all $p \in [2, 2^*]$ with $\frac{1}{2^*} = \frac{1}{2} - \frac{\alpha}{n}$. Note that here we used our assumption $n \geq 2$. For p in this range we write $1/p = (1-\theta)/2 + \theta/2^*$ with $\theta \in (0,1)$ and get for any $s' \in (0,1)$ the bound

$$\|u\|_{\mathrm{W}^{s',p'}(\mathbb{R}^n)^*} \leq \|u\|_p \leq \|u\|_2^{1-\theta} \|u\|_{2^*}^{\theta} \lesssim \|u\|_{\alpha,2}, \tag{4-6}$$

where the second step follows from Hölder's inequality. Next, we have $s'p' < 2\alpha < 2 \leq n$ (since $s' < \alpha$ and $p' < 2$) and hence Lemma 4.2 yields $\|f\|_{\mathrm{W}^{s',p'}(\mathbb{R}^n)^*} \lesssim \|f\|_r$. Finally, we consider $\mathcal{L}_{\beta,B}g$.

Suppose first that $2\beta < \alpha$. Upon taking ε smaller, we can assume $2\beta < s'$, in which case $\|\mathcal{L}_{\beta,B}g\|_{\mathrm{W}^{s',p'}(\mathbb{R}^n)^*} \lesssim \|g\|_q$ follows from Corollary 4.5. If, on the other hand, $2\beta - \alpha \in [0,1)$, then we can additionally assume $2\beta - s' \in (0,1)$ and apply Lemma 4.3 to give $\|\mathcal{L}_{\beta,B}g\|_{\mathrm{W}^{s',p'}(\mathbb{R}^n)^*} \lesssim \|g\|_{2\beta-2\alpha+s,p}$. Inserting these estimates on the right-hand side of (4-5) yields the desired bound for u. □

4C. *Comparison to earlier results.* As a consequence of our method, the exponents s and p for the higher differentiability and integrability of u in Theorem 4.6 are precisely related to the assumptions on f and g. As far as more qualitative results are concerned, this is by no means necessary since the following fractional Sobolev embedding allows for some play with the exponents.

Lemma 4.7 [Bergh and Löfström 1976, Theorems 6.2.4 and 6.5.1]. *Let $s_0, s_1, s_2 \in (0,1)$ and $1 < p_0 \leq p_1 < \infty$ satisfy $s_0 - n/p_0 = s_1 - n/p_1$ and $s_2 < s_1$. Then*

$$\mathrm{W}^{s_0,p_0}(\mathbb{R}^n) \subset \mathrm{W}^{s_1,p_1}(\mathbb{R}^n) \subset \mathrm{W}^{s_2,p_1}(\mathbb{R}^n)$$

with continuous inclusions.

As a particular example, we obtain a self-improving property more in the spirit of [Kuusi et al. 2015, Theorem 1.1]. For this we define the following exponents related to fractional Sobolev embeddings, see Lemma 4.2,

$$2_{*,\alpha} := \frac{2n}{n+2\alpha}, \quad 2_{*,\alpha-2\beta} := \frac{2n}{n+2(\alpha-2\beta)}, \tag{4-7}$$

where the second one will of course only be used when $2\beta < \alpha$.

Corollary 4.8. *Let $u \in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ be a weak solution to (4-1). Suppose for some $\delta > 0$ one has $f \in \mathrm{L}^{2_{*,\alpha}+\delta}(\mathbb{R}^n) \cap \mathrm{L}^{2_{*,\alpha}}(\mathbb{R}^n)$ and*

$$g \in \begin{cases} \mathrm{L}^{2_{*,\alpha-2\beta}+\delta}(\mathbb{R}^n) \cap \mathrm{L}^{2_{*,\alpha-2\beta}}(\mathbb{R}^n) & \text{if } 2\beta < \alpha, \\ \mathrm{W}^{2\beta-\alpha+\delta,2}(\mathbb{R}^n) & \text{if } 0 \leq 2\beta - \alpha < 1. \end{cases}$$

Then $u \in \mathrm{W}^{s,p}(\mathbb{R}^n)$ *for some* $s > \alpha$, $p > 2$. *Moreover*, s *and* p *depend only on* $\lambda, n, \alpha, \beta$.

Proof of Corollary 4.8. Throughout, we will have $s \in (\alpha, 1)$ and $p \in [2, \infty)$. We consider the case $2\beta < \alpha$ first. By the log-convexity of the Lebesgue space norms we may lower the value $\delta > 0$ as we please and still have the respective assumptions on f and g. On the other hand, the exponents in Theorem 4.6 satisfy $r > 2_{*,\alpha}$ and $q > 2_{*,\alpha-2\beta}$ and in the limits $s \to \alpha$ and $p \to 2$ we get equality. Hence, we can apply Theorem 4.6 with some choice of $s > \alpha$ and $p > 2$ and the claim follows.

It remains to deal with the assumption on g in the case $2\beta - \alpha \in [0, 1)$. But according to Lemma 4.7 we can find $s > \alpha$ and $p > 2$ arbitrarily close to α and 2, respectively, such that $\mathrm{W}^{2\beta-\alpha+\delta,2}(\mathbb{R}^n) \subset \mathrm{W}^{2\beta-2\alpha+s,p}(\mathbb{R}^n)$ holds with continuous inclusion and again $u \in \mathrm{W}^{s,p}(\mathbb{R}^n)$ follows by Theorem 4.6. □

As another application we reproduce the main result in [Bass and Ren 2013] concerning the nonlocal elliptic equation

$$\mathcal{L}_{\alpha,A} u = f$$

with $f \in \mathrm{L}^2(\mathbb{R}^n)$. We note that this corresponds to taking $g = 0$ in the general Equation (4-1). Hence, the entire Section 4A could be skipped except for the first lemma, thereby making the argument up to this stage particularly simple.

Corollary 4.9. *Let* $f \in \mathrm{L}^2(\mathbb{R}^n)$ *and let* $u \in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ *be a weak solution to* $\mathcal{L}_{\alpha,A} u = f$. *Then*

$$\Gamma u(x) := \left(\int_{\mathbb{R}^n} \frac{|u(x) - u(y)|^2}{|x-y|^{n+2\alpha}} \, \mathrm{d}y \right)^{\frac{1}{2}}$$

satisfies

$$\|\Gamma u\|_p \leq c(\|u\|_2 + \|f\|_2),$$

for some $p > 2$ *and a constant* c *both depending only on* λ, n, α.

Proof. We use the notation introduced in Theorem 4.6 and write as usual $s + s' = 2\alpha$, $1/p + 1/p' = 1$. According to Lemma 4.2 we have $\mathrm{L}^r(\mathbb{R}^n) \subset \mathrm{W}^{s',p'}(\mathbb{R}^n)^*$ with continuous inclusion and if s and p are sufficiently close to α and 2, respectively, then we have $r < 2$. Obviously, we also have $\mathrm{L}^p(\mathbb{R}^n) \subset \mathrm{W}^{s',p'}(\mathbb{R}^n)^*$ and $p > 2$. Hence, by virtue of the splitting

$$f = f \cdot \mathbf{1}_{\{|f| < \|f\|_2\}} + f \cdot \mathbf{1}_{\{|f| \geq \|f\|_2\}} \in \mathrm{L}^p(\mathbb{R}^n) + \mathrm{L}^r(\mathbb{R}^n)$$

we obtain $f \in \mathrm{W}^{s',p'}(\mathbb{R}^n)^*$ with bound $\|f\|_{\mathrm{W}^{s',p'}(\mathbb{R}^n)^*} \lesssim \|f\|_2$. Here $\mathbf{1}_E$ denotes the indicator function of the set $E \subset \mathbb{R}^n$. Moreover, $\|u\|_{\mathrm{W}^{s',p'}(\mathbb{R}^n)^*} \lesssim \|u\|_{\alpha,2}$, see (4-6), and thus we can follow the first part of the proof of Theorem 4.6 in order to find

$s > \alpha$, $p > 2$, and implicit constants depending only on the above mentioned parameters, such that

$$\|u\|_{s,p} \lesssim \|f\|_2 + \|u\|_{\alpha,2}.$$

The pair (s, p) could be chosen anywhere in the (s, p)-plane close to $(\alpha, 2)$ but for a reason that will become clear later on, we shall impose the relation

$$\frac{n}{2} - \frac{n}{p} = s - \alpha. \tag{4-8}$$

Quasicoercivity of the form associated with $\mathcal{L}_{\alpha,A}$ along with the equation for u yield

$$\lambda[u]_{\alpha,2}^2 \leq |\mathcal{E}_{\alpha,A}(u,u)| = \left| \int_{\mathbb{R}^n} f \cdot \bar{u} \, \mathrm{d}x \right| \leq \tfrac{1}{2}(\|u\|_2^2 + \|f\|_2^2),$$

and thus it suffices to prove the estimate $\|\Gamma u\|_p \lesssim \|u\|_{s,p}$ to conclude.

To this end, we split

$$\Gamma u(x) = \Gamma_1 u(x) + \Gamma_2 u(x)$$

according to whether or not $|x - y| > 1$ in the defining integral. Repeating the argument to deduce (4-4), we obtain

$$|\Gamma_1 u(x)| = \left(\int_{|x-y|>1} \frac{|u(x) - u(y)|^2}{|x-y|^{n+2\alpha}} \, \mathrm{d}y \right)^{\frac{1}{2}} \lesssim M(|u|^2)(x)^{\frac{1}{2}}$$

and as $p > 2$, we conclude $\|\Gamma_1 u\|_p \lesssim \|u\|_p$ from the boundedness of the maximal operator on $\mathrm{L}^{p/2}(\mathbb{R}^n)$. As for the other piece, we use Hölder's inequality with exponent $p/2$ on the integral in y, to give

$$\|\Gamma_2\|_p \lesssim \left(\int_{\mathbb{R}^n} \int_{|x-y|<1} \frac{|u(x) - u(y)|^p}{|x-y|^{np/2+p\alpha}} \, \mathrm{d}y \, \mathrm{d}x \right)^{\frac{1}{p}} \leq [u]_{s,p},$$

where in the final step we used that $np/2 + p\alpha = n + sp$ holds thanks to (4-8). □

5. Local results

In Theorem 4.6 and Corollary 4.8, we have obtained global improvements of regularity for solutions to (4-1) under global assumptions on the right-hand side. We now discuss some local analogs of this phenomenon. In order to formulate our main result in this direction, we define for balls $B \subset \mathbb{R}^n$ a local version of the fractional Sobolev norm by

$$\|u\|_{\mathrm{W}^{s,p}(B)} := \left(\int_B |u(x)|^p \, \mathrm{d}x \right)^{\frac{1}{p}} + \left(\iint_{B \times B} \frac{|u(x) - u(y)|^p}{|x-y|^{n+sp}} \, \mathrm{d}x \, \mathrm{d}y \right)^{\frac{1}{p}}$$

and write $u \in \mathrm{W}^{s,p}(B)$ provided this quantity is finite.

Theorem 5.1. *There exists $\varepsilon > 0$, depending only on $\lambda, n, \alpha, \beta$ with the following property. Suppose $s \in (\alpha, 1)$ and $p \in [2, \infty)$ satisfy $|s-\alpha|, |p-2| < \varepsilon$. Let $u \in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ be a weak solution to (4-1) and let $B \subset \mathbb{R}^n$ be a ball. Then the following conditions guarantee $u \in \mathrm{W}^{s,p}(B')$ for every ball $B' \Subset B$:*

$$f \in \mathrm{L}^r(B) \quad \text{for some } r \text{ with} \quad \frac{1}{r} \le \frac{1}{p} + \frac{2\alpha - s}{n}$$

and

$$g \in \mathrm{L}^q(B) \cap \mathrm{L}^t(\mathbb{R}^n) \quad \text{for some } q, t \text{ with}$$
$$\frac{1}{q} \le \frac{1}{p} + \frac{2\alpha - 2\beta - s}{n}, \qquad \frac{1}{p} \le \frac{1}{t} < \frac{1}{p} + \frac{2\alpha - s}{n} \qquad \text{if } 2\beta < \alpha,$$

or

$$g \in \mathrm{W}^{2\beta - 2\alpha + s, p}(\mathbb{R}^n) \qquad \text{if } 0 \le 2\beta - \alpha < 1.$$

Again, this gives a precise relation between the exponents, but we also state a more quantitative version. It follows by the exact same reasoning as Corollary 4.8 was obtained from Theorem 4.6 in the previous section and we shall not provide further details. We are using again the lower Sobolev conjugates defined in (4-7).

Corollary 5.2. *Let $u \in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ be a weak solution to (4-1) and let $B \subset \mathbb{R}^n$ be a ball. Suppose for some $\delta > 0$ it holds that $f \in \mathrm{L}^{2_{*,\alpha}+\delta}(B)$ and*

$$g \in \begin{cases} \mathrm{L}^{2_{*,\alpha-2\beta}+\delta}(B) \cap \mathrm{L}^t(\mathbb{R}^n) \quad \text{for some } t \in (2_{*,\alpha}, 2] & \text{if } 2\beta < \alpha, \\ \mathrm{W}^{2\beta-\alpha+\delta,2}(\mathbb{R}^n) & \text{if } 0 \le 2\beta - \alpha < 1. \end{cases}$$

Then there exist $s > \alpha$, $p > 2$, such that $u \in \mathrm{W}^{s,p}(B')$ for every ball $B' \Subset B$. Moreover, s and p depend only on $\lambda, n, \alpha, \beta$.

These statements are astonishingly local in that the assumption on f and part of that for g are only on the ball where we want to improve the regularity of u. To the best of our knowledge this has not been noted before. In particular, if f and g satisfy the assumption for every ball B, then the conclusion for u holds for every ball B'. This is the result in [Kuusi et al. 2015]. (Except that they suppose global integrability of exponent $t = 2_{*,\alpha-2\beta} + \delta$ instead, which for large δ is not comparable with the condition in Corollary 5.2. It is possible to modify our argument to work in the setting of [Kuusi et al. 2015] as well, but we leave this extension to interested readers, see Remark 5.4.)

For the proof of Theorem 5.1 it is instructive to recall a simple connection between the condition $\chi u \in \mathrm{W}^{s,p}(\mathbb{R}^n)$ for some $\chi \in \mathrm{C}_0^\infty(B)$ and the fractional Sobolev norm $\|\cdot\|_{\mathrm{W}^{s,p}(B)}$: On the one hand, denoting by $d > 0$ the distance between the support of χ and ${}^cB$ we obtain from the mean value theorem,

$$\left(\iint_{\mathbb{R}^n\times\mathbb{R}^n} \frac{|(\chi u)(x)-(\chi u)(y)|^p}{|x-y|^{n+sp}}\,\mathrm{d}x\,\mathrm{d}y\right)^{\frac{1}{p}} \le 2\|\chi\|_\infty\left(\iint_{B\times B} \frac{|u(x)-u(y)|^p}{|x-y|^{n+sp}}\,\mathrm{d}x\,\mathrm{d}y\right)^{\frac{1}{p}} + 4\|\chi\|_\infty\left(\int_B |u(x)|^p\left(\int_{|x-y|\ge d} \frac{1}{|x-y|^{n+sp}}\,\mathrm{d}y\right)\mathrm{d}x\right)^{\frac{1}{p}} + 2\|\nabla\chi\|_\infty\left(\int_B |u(x)|^p\left(\int_B \frac{1}{|x-y|^{n+(s-1)p}}\,\mathrm{d}y\right)\mathrm{d}x\right)^{\frac{1}{p}}, \tag{5-1}$$

where by symmetry and the fact that the integrand is zero when $x, y \notin \operatorname{supp}(\chi)$, we can assume $x \in \operatorname{supp}(\chi)$ and then distinguish whether or not $y \in B$. As $s > 0$ and $s-1 < 0$, the second and third terms are finite. Hence, we see that $u \in \mathrm{W}^{s,p}(B)$ implies $\chi u \in \mathrm{W}^{s,p}(\mathbb{R}^n)$. On the other hand, if $\chi = 1$ on a smaller ball $B' \Subset B$, then

$$\left(\int_{B'} |u(x)|^p\,\mathrm{d}x\right)^{\frac{1}{p}} + \left(\iint_{B'\times B'} \frac{|u(x)-u(y)|^p}{|x-y|^{n+sp}}\,\mathrm{d}x\,\mathrm{d}y\right)^{\frac{1}{p}} \le \|\chi u\|_{s,p}. \tag{5-2}$$

Due to these observations and the fact that Lebesgue spaces on a ball are ordered by inclusion, we see that Theorem 5.1 follows at once from:

Lemma 5.3. *There exists $\varepsilon > 0$, depending only on $\lambda, n, \alpha, \beta$ with the following property. Suppose $s \in (\alpha, 1)$ and $p \in [2, \infty)$ satisfy $|s-\alpha|, |p-2| < \varepsilon$. Let $u \in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ be a weak solution to (4-1) and let $\chi \in \mathrm{C}_0^\infty(\mathbb{R}^n)$. Assume*

$$\chi f \in \mathrm{L}^r(\mathbb{R}^n) \quad \text{with } \frac{1}{r} = \frac{1}{p} + \frac{2\alpha - s}{n}$$

and if $2\beta < \alpha$ assume

$$\chi g \in \mathrm{L}^q(\mathbb{R}^n), \qquad \frac{1}{q} = \frac{1}{p} + \frac{2\alpha-2\beta-s}{n},$$
$$g \in \mathrm{L}^t(\mathbb{R}^n), \qquad \frac{1}{p} \le \frac{1}{t} < \frac{1}{p} + \frac{2\alpha - s}{n},$$

whereas if $0 \le 2\beta - \alpha < 1$ assume $g \in \mathrm{W}^{2\beta-2\alpha+s,p}(\mathbb{R}^n)$. Then $\chi u \in \mathrm{W}^{s,p}(\mathbb{R}^n)$.

The strategy for the proof of this key lemma is as follows. We let $u \in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ be a weak solution to (4-1) and seek to write down a related fractional equation for χu in order to be able to apply Proposition 3.4. To this end, we note for three functions u, χ, ϕ and $x, y \in \mathbb{R}^n$ the factorization

$$\begin{aligned}(\chi_x u_x - \chi_y u_y)(\phi_x - \phi_y) &= (\chi_x\phi_x - \chi_y\phi_y)(u_x - u_y) + u_y(\chi_x - \chi_y)\phi_x + u_x(\chi_y - \chi_x)\phi_y \\ &= (\chi_x\phi_x - \chi_y\phi_y)(u_x - u_y) - (u_x - u_y)(\chi_x - \chi_y)\phi_y \\ &\qquad + u_y(\chi_x - \chi_y)(\phi_x - \phi_y), \qquad (5\text{-}3)\end{aligned}$$

where $u_x := u(x)$ and so on for the sake of readability. This identity plugged into the definition of $\mathcal{E}_{\alpha,A}$, see (3-1), yields

$$\langle \mathcal{L}_{\alpha,A}(\chi u), \phi\rangle = \langle \mathcal{L}_{\alpha,A}u, \chi\phi\rangle + \langle \mathcal{R}_{\alpha,A,\chi}u, \phi\rangle \quad (\phi \in \mathrm{C}_0^\infty(\mathbb{R}^n)),$$

where

$$\begin{aligned}\langle \mathcal{R}_{\alpha,A,\chi}u, \phi\rangle := &- \iint_{\mathbb{R}^n\times\mathbb{R}^n} A(x, y)\frac{(u(x)-u(y))\cdot(\chi(x)-\chi(y))}{|x-y|^{n+2\alpha}}\overline{\phi(y)}\,\mathrm{d}x\,\mathrm{d}y \\ &+ \iint_{\mathbb{R}^n\times\mathbb{R}^n} A(x, y)u(y)\frac{(\chi(x)-\chi(y))\cdot\overline{(\phi(x)-\phi(y))}}{|x-y|^{n+2\alpha}}\,\mathrm{d}x\,\mathrm{d}y\end{aligned}$$

provided all integrals are absolutely convergent. We shall check that in the proofs below. Of course, a similar calculation applies to $\mathcal{L}_{\beta,B}$. Therefore $\chi u \in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ solves the nonlocal elliptic equation

$$(1+\mathcal{L}_{\alpha,A})(\chi u) = \mathcal{R}_{\alpha,A,\chi}u - \mathcal{R}_{\beta,B,\chi}g + \chi u + \mathcal{L}_{\beta,B}(\chi g) + \chi f. \qquad (5\text{-}4)$$

Proof of Lemma 5.3. We start by taking $\varepsilon > 0$ as provided by Theorem 4.6 but for some steps we possibly need to impose additional smallness conditions that depend upon n, α, β through fractional Sobolev embeddings. As usual, we write $s + s' = 2\alpha$ and $1/p + 1/p' = 1$.

The claim is $\chi u \in \mathrm{W}^{s,p}(\mathbb{R}^n)$ and according to Proposition 3.4 we only need to make sure that the right-hand side in (5-4) belongs to $\mathrm{W}^{s',p'}(\mathbb{R}^n)^*$. But from the proof of Theorem 4.6 we know that this is the case for $\chi u \in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ and that the conditions on χf and χg are designed to make it work for the last two terms.

We are left with the error terms. We start with $\mathcal{R}_{\alpha,A,\chi}$, which as we recall is given for $\phi \in \mathrm{C}_0^\infty(\mathbb{R}^n)$ by

$$\begin{aligned}\langle \mathcal{R}_{\alpha,A,\chi}u, \phi\rangle := &- \iint_{\mathbb{R}^n\times\mathbb{R}^n} A(x, y)\frac{(u(x)-u(y))\cdot(\chi(x)-\chi(y))}{|x-y|^{n+2\alpha}}\overline{\phi(y)}\,\mathrm{d}x\,\mathrm{d}y \\ &+ \iint_{\mathbb{R}^n\times\mathbb{R}^n} A(x, y)u(y)\frac{(\chi(x)-\chi(y))\cdot\overline{(\phi(x)-\phi(y))}}{|x-y|^{n+2\alpha}}\,\mathrm{d}x\,\mathrm{d}y \\ := &\ \mathrm{I} + \mathrm{II}.\end{aligned}$$

Now,

$$\begin{aligned}\int_{\mathbb{R}^n} \frac{|\chi(x)-\chi(y)|^p}{|x-y|^{n+sp}}\,\mathrm{d}x &\leq \int_{|x-y|\geq 1} \frac{2^p\|\chi\|_\infty^p}{|x-y|^{n+sp}}\,\mathrm{d}x + \int_{|x-y|<1} \frac{\|\nabla\chi\|_\infty^p}{|x-y|^{n+(s-1)p}}\,\mathrm{d}x \\ &\lesssim 1 \end{aligned} \tag{5-5}$$

uniformly in $y \in \mathbb{R}^n$ since $s < 1$. Thus, applying Hölder's inequality first in x and then in y, we obtain

$$\begin{aligned}|\mathrm{II}| &\leq \lambda^{-1}\int_{\mathbb{R}^n} |u(y)|\Big(\int_{\mathbb{R}^n} \frac{|\chi(x)-\chi(y)|^p}{|x-y|^{n+sp}}\,\mathrm{d}x\Big)^{\frac{1}{p}}\Big(\int_{\mathbb{R}^n} \frac{|\phi(x)-\phi(y)|^{p'}}{|x-y|^{n+s'p'}}\,\mathrm{d}x\Big)^{\frac{1}{p}'}\,\mathrm{d}y \\ &\lesssim \|u\|_p[\phi]_{s',p'}.\end{aligned}$$

Similarly, but reversing the roles of ϕ and u, we get

$$\begin{aligned}|\mathrm{I}| &\leq \lambda^{-1}\int_{\mathbb{R}^n} |\phi(y)|\Big(\int_{\mathbb{R}^n} \frac{|\chi(x)-\chi(y)|^2}{|x-y|^{n+2\alpha}}\,\mathrm{d}x\Big)^{\frac{1}{2}}\Big(\int_{\mathbb{R}^n} \frac{|u(x)-u(y)|^2}{|x-y|^{n+2\alpha}}\,\mathrm{d}x\Big)^{\frac{1}{2}}\,\mathrm{d}y \\ &\lesssim [u]_{\alpha,2}\|\phi\|_2.\end{aligned}$$

By making $\varepsilon > 0$ smaller, we can assume $\frac{1}{2} - \alpha/n \leq 1/p$ and $1/p' - s'/n \leq \frac{1}{2}$, which pays for continuous inclusion

$$\mathrm{W}^{\alpha,2}(\mathbb{R}^n) \subset \mathrm{L}^p(\mathbb{R}^n) \quad \text{and} \quad \mathrm{W}^{s',p'}(\mathbb{R}^n) \subset \mathrm{L}^2(\mathbb{R}^n),$$

see Lemma 4.2. Thus,

$$|\langle \mathcal{R}_{\alpha,A,\chi}u, \phi\rangle| \lesssim \|u\|_{\alpha,2}\|\phi\|_{s',p'} \quad (\phi \in \mathrm{C}_0^\infty(\mathbb{R}^n))$$

and by density $\mathcal{R}_{\alpha,A,\chi}u$ extends to a functional on $\mathrm{W}^{s',p'}(\mathbb{R}^n)$ as required.

It remains to estimate $\mathcal{R}_{\beta,B,\chi}g$. In case $0 \leq 2\beta - \alpha < 1$ and $g \in \mathrm{W}^{2\beta-2\alpha+s,p}(\mathbb{R}^n)$, we can repeat the argument for bounding I and II by replacing u by g and changing the indices of integrability and smoothness in Hölder's inequality accordingly. In this manner,

$$\begin{aligned}|\langle \mathcal{R}_{\beta,B,\chi}g, \phi\rangle| &\lesssim \|g\|_p[\phi]_{s',p'} + [g]_{2\beta-2\alpha+s,p}\|\phi\|_{p'} \\ &\lesssim \|g\|_{2\beta-2\alpha+s,p}\|\phi\|_{s',p'} \qquad (\phi \in \mathrm{C}_0^\infty(\mathbb{R}^n)).\end{aligned}$$

In the complementary case $2\beta < \alpha$, there is no smoothness of g to be taken advantage of. This, however, can be compensated by the fact $\beta < \alpha/2 < \frac{1}{2}$. More precisely, we put $\tilde{B}(x,y) := B(x,y) + B(y,x)$ and use the first part of the factorization (5-3) to write the error term differently as

$$\begin{aligned}\langle \mathcal{R}_{\beta,B,\chi} g, \phi\rangle &= \iint_{\mathbb{R}^n\times\mathbb{R}^n} \tilde{B}(x,y) g(x) \frac{\chi(x)-\chi(y)}{|x-y|^{n+2\beta}} \overline{\phi(y)} \,\mathrm{d}x\,\mathrm{d}y \\ &:= \iint_{\mathbb{R}^n\times\mathbb{R}^n} \tilde{B}(x,y) g(y) \frac{(\chi(x)-\chi(y))\cdot\overline{(\phi(y)-\phi(x))}}{|x-y|^{n+2\beta}} \,\mathrm{d}x\,\mathrm{d}y \\ &\quad - \iint_{\mathbb{R}^n\times\mathbb{R}^n} \tilde{B}(x,y) g(y) \frac{\chi(x)-\chi(y)}{|x-y|^{n+2\beta}} \overline{\phi(y)} \,\mathrm{d}x\,\mathrm{d}y \\ &:= \mathrm{III} + \mathrm{IV},\end{aligned}$$

where we changed x and y in the second step. Now, our assumption is $g \in \mathrm{L}^t(\mathbb{R}^n)$ with $1/p \le 1/t < 1/p + s'/n$. We let $1/t + 1/t' = 1$ and obtain from Lemmas 4.2 and 4.7 that the condition on t is precisely to guarantee the continuous inclusions $\mathrm{W}^{s',p'}(\mathbb{R}^n) \subset \mathrm{W}^{\delta,t'}(\mathbb{R}^n) \subset \mathrm{L}^{t'}(\mathbb{R}^n)$ for at least some small $\delta \in (0,1)$. This being said, we use Hölder's inequality and (5-5) with (s,p) replaced by $(2\beta-\delta, t)$ to give

$$\begin{aligned}|\mathrm{III}| &\le \frac{2}{\lambda} \int_{\mathbb{R}^n} |g(y)| \biggl(\int_{\mathbb{R}^n} \frac{|\chi(x)-\chi(y)|^t}{|x-y|^{n+(2\beta-\delta)t}} \,\mathrm{d}x\biggr)^{\frac{1}{t}} \biggl(\int_{\mathbb{R}^n} \frac{|\phi(x)-\phi(y)|^{t'}}{|x-y|^{n+\delta t'}} \,\mathrm{d}x\biggr)^{\frac{1}{t'}} \,\mathrm{d}y \\ &\lesssim \|g\|_t \|\phi\|_{s',p'}.\end{aligned}$$

Likewise, for the term IV, we use the bound (5-5) with (s,p) replaced by $(2\beta,1)$ to conclude that

$$|\mathrm{IV}| \lesssim \int_{\mathbb{R}^n} |g(y)||\phi(y)| \,\mathrm{d}y \le \|g\|_t \|\phi\|_{t'} \lesssim \|g\|_t \|\phi\|_{s',p'}. \qquad \square$$

Remark 5.4. As we mentioned after stating Corollary 5.2, the assumption $g \in \mathrm{L}^{2_{*,\alpha-2\beta}}(B) \cap \mathrm{L}^t(\mathbb{R}^n)$ for $2\beta < \alpha$ can be replaced by one *global* assumption $g \in \mathrm{L}^{2_{*,\alpha-2\beta}+\delta}(\mathbb{R}^n)$ with $\delta > 0$ in accordance with the result in [Kuusi et al. 2015]. This follows from a simple modification of the argument above to give the required adaptation of Lemma 5.3. We sketch the main idea but leave the precise extensions to the interested reader. The difference arises from the term $\mathcal{L}_{\beta,B} g$ so it suffices to see that $\chi \mathcal{L}_{\beta,B} g$ and χf belong to the same $\mathrm{W}^{s',p'}(\mathbb{R}^n)^*$ so that one can apply Proposition 3.4.

If u is a weak solution to (4-1), then automatically

$$\chi \mathcal{L}_{\beta,B} g \in \mathrm{W}^{\alpha,2}(\mathbb{R}^n)^*$$

by the assumption on f, the mapping properties of $\mathcal{L}_{\alpha,A}$ and the error term considerations for $\mathcal{R}_{\alpha,A,\chi} u$. By Corollary 4.5,

$$\chi \mathcal{L}_{\beta,B} g \in \mathrm{W}^{\sigma',\tau'}(\mathbb{R}^n)^*$$

provided that $1/q = 1/\tau + (\sigma' - 2\beta)/n$. One can check that there is an admissible choice of $\sigma' < \alpha$ and $\tau' < 2$ when $q = 2_{*,\alpha-2\beta} + \delta$. By interpolation, we find a line segment ℓ connecting $(\sigma', 1/\tau')$ to $\left(\alpha, \frac{1}{2}\right)$ so that $\chi \mathcal{L}_{\beta,B} g \in \mathrm{W}^{s',p'}(\mathbb{R}^n)^*$ for all $(s', 1/p') \in \ell$. Finally, since $\chi f \in \mathrm{L}^t(\mathbb{R}^n)$ for all $t \in [1, 2_{*,\alpha}+\delta]$ with $\delta > 0$, there is at least one such t for which we can find $(s', 1/p') \in \ell$ with $1/t = 1/p + (2\alpha - s)/n$ so that Lemma 4.2 implies $f \in \mathrm{W}^{s',p'}(\mathbb{R}^n)^*$ with $(s', 1/p')$ as close to $\left(\alpha, \frac{1}{2}\right)$ as desired.

6. An application to fractional parabolic equations

We demonstrate the flexibility of our approach by a new application to fractional parabolic equations. We shall only treat a particularly interesting special case with connection to nonautonomous maximal regularity, leaving open the establishment of a suitable (full) parabolic analog of Theorem 4.6 and its local version, Theorem 5.1.

We are going to consider the Cauchy problem

$$\partial_t u(t) + \mathcal{L}_{\alpha,A(t)} u(t) = f(t), \quad u(0) = 0, \tag{6-1}$$

where $f \in \mathrm{L}^2(0, T; \mathrm{L}^2(\mathbb{R}^n))$, $\alpha \in (0, 1)$, and for each $t \in [0, T]$ we let $\mathcal{L}_{\alpha,A(t)} : \mathrm{W}^{\alpha,2}(\mathbb{R}^n) \to \mathrm{W}^{\alpha,2}(\mathbb{R}^n)^*$ be a fractional elliptic operator as in Section 3 satisfying the ellipticity condition (1-1) uniformly in t. We recall that the associated sesquilinear forms $\mathcal{E}_{\alpha,A(t)}$ were defined in (3-1). As for the coefficients

$$A(t, x, y) := A(t)(x, y)$$

we assume no regularity besides joint measurability in all variables.

Note that we formulated our parabolic problem on $[0, T) \times \mathbb{R}^n$ from the point of view of evolution equations using for, X, a Banach space, the space $\mathrm{L}^2(0, T; X)$ of X-valued square integrable functions on $(0, T)$ and the associated Sobolev space $\mathrm{H}^1(0, T; X)$ of all $u \in \mathrm{L}^2(0, T; X)$ with distributional derivative $\partial_t u \in \mathrm{L}^2(0, T; X)$.

Definition 6.1. Let $f \in \mathrm{L}^2(0, T; \mathrm{L}^2(\mathbb{R}^n))$. A function

$$u \in \mathrm{H}^1(0, T; \mathrm{W}^{\alpha,2}(\mathbb{R}^n)^*) \cap \mathrm{L}^2(0, T; \mathrm{W}^{\alpha,2}(\mathbb{R}^n))$$

is called weak solution to (6-1) if $u(0) = 0$ and

$$\int_0^T -\langle u, \partial_t \phi \rangle_2 + \mathcal{E}_{\alpha,A(t)}(u, \phi) \, \mathrm{d}t = \int_0^T \langle f, \phi \rangle_2 \, \mathrm{d}t \quad (\phi \in \mathrm{C}_0^\infty((0, T) \times \mathbb{R}^n)), \tag{6-2}$$

where $\langle \cdot, \cdot \rangle_2$ denotes the inner product on $\mathrm{L}^2(\mathbb{R}^n)$.

Remark 6.2. (i) Since $\mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ is a Hilbert space, the solution space for u above embeds into the continuous functions $\mathrm{C}([0,T];\mathrm{L}^2(\mathbb{R}^n))$ and hence the requirement $u(0)=0$ makes sense [Showalter 1997, Proposition III.1.2].

(ii) $\mathrm{C}_0^\infty((0,T)\times\mathbb{R}^n)$ is dense in $\mathrm{L}^2(0,T;\mathrm{W}^{\alpha,2}(\mathbb{R}^n))$, by smooth truncation and convolution. Thus, the integrated Equation (6-2) precisely means that u satisfies the parabolic equation in (6-1) almost everywhere on $(0,T)$ as an equality in $\mathrm{W}^{\alpha,2}(\mathbb{R}^n)^*$, which contains $\mathrm{L}^2(\mathbb{R}^n)$.

By a famous result of Lions, the Cauchy problem (6-1) has a unique weak solution u for every $f\in\mathrm{L}^2(0,T;\mathrm{L}^2(\mathbb{R}^n))$. See [Dautray and Lions 1992, p. 513; Dier and Zacher 2017, Theorem 6.1] for the case of function spaces over the complex numbers. The following self-improvement property is the main result of this section.

Theorem 6.3. *Let $f\in\mathrm{L}^2(0,T;\mathrm{L}^2(\mathbb{R}^n))$. Then there exists $\varepsilon>0$ such that the unique weak solution to (6-1) satisfies*

$$u\in\mathrm{H}^1(0,T;\mathrm{W}^{\alpha-\varepsilon,2}(\mathbb{R}^n)^*)\cap\mathrm{L}^2(0,T;\mathrm{W}^{\alpha+\varepsilon,2}(\mathbb{R}^n)).$$

Moreover, for some $s>\alpha$ and $p>2$ it holds that

$$u\in\mathrm{W}^{s/(2\alpha),p}(0,T;\mathrm{L}^p(\mathbb{R}^n))\cap\mathrm{L}^p(0,T;\mathrm{W}^{s,p}(\mathbb{R}^n)),$$

that is,

$$\begin{aligned}\Big(\int_0^T\int_{\mathbb{R}^n}|u(t,x)|^p\,\mathrm{d}x\,\mathrm{d}t\Big)^{\frac{1}{p}}+\Big(\int_{\mathbb{R}^n}\int_0^T\int_0^T\frac{|u(t,x)-u(s,x)|^p}{|t-s|^{1+sp/(2\alpha)}}\,\mathrm{d}s\,\mathrm{d}t\,\mathrm{d}x\Big)^{\frac{1}{p}}\\+\Big(\int_0^T\iint_{\mathbb{R}^n\times\mathbb{R}^n}\frac{|u(t,x)-u(t,y)|^p}{|x-y|^{n+sp}}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}t\Big)^{\frac{1}{p}}\\\lesssim\mathrm{e}^T\Big(\int_0^T\int_{\mathbb{R}^n}|f(t,x)|^2\,\mathrm{d}x\,\mathrm{d}t\Big)^{\frac{1}{2}}.\qquad(6\text{-}3)\end{aligned}$$

The values of ε, s, p and the implicit constant in (6-3) depend only on λ, n, α.

Remark 6.4. (i) Since $sp>2\alpha$, the boundedness of the second integral in (6-3) entails, in particular, $u\in\mathrm{C}^\gamma([0,T];\mathrm{L}^p(\mathbb{R}^n))$ with Hölder exponent $\gamma=\frac{sp}{2\alpha}-1$, see fore example [Simon 1990, Cor. 26].

(ii) The largest possible value $\varepsilon=\alpha$ with $\mathrm{W}^{0,2}(\mathbb{R}^n):=\mathrm{L}^2(\mathbb{R}^n)$ would mean *maximal regularity* because all three functions in the parabolic equation were in the same space $\mathrm{L}^2(0,T;\mathrm{L}^2(\mathbb{R}^n))$. See [Arendt et al. 2017] for further background and (counter-)examples.

For the proof, we shall apply the same scheme as in the stationary case, see Sections 3 and 4.

6A. ***Definition of the parabolic Dirichlet form.*** One of the immediate challenges in moving from the elliptic operator to the parabolic operator is the lack of coercivity of the operator $\partial_t + \mathcal{L}_{\alpha,A(t)}$. However, we can rely on the *hidden coercivity* introduced in this context in [Dier and Zacher 2017] (see also [Kaplan 1966]). This requires us to study the fractional parabolic equation for $t \in \mathbb{R}$ first, that is,

$$\partial_t u(t) + \mathcal{L}_{\alpha,A(t)} u(t) = f(t),$$

where weak solutions are in the sense of Definition 6.1, but by replacing $(0, T)$ with $\mathbb{R}$ and of course removing the initial condition. Note that we can simply extend the coefficients by $A(t, x, y) := 1$ if $t \notin [0, T]$ since we are not assuming any regularity.

For simplicity, put $H := \mathrm{L}^2(\mathbb{R}^n)$ and $V := \mathrm{W}^{\alpha,2}(\mathbb{R}^n)$. Let $\mathcal{F}$ be the Fourier transform in t on the vector-valued space $\mathrm{L}^2(\mathbb{R}; H)$ and define the *half-order time derivative* $D_t^{\frac{1}{2}}$ and the *Hilbert transform* H_t through the Fourier symbols $|\tau|^{\frac{1}{2}}$ and $-\mathrm{i}\,\mathrm{sgn}(\tau)$, respectively. They are crafted to factorize $\partial_t = D_t^{\frac{1}{2}} H_t D_t^{\frac{1}{2}}$. Next, we write $\mathrm{H}^{\frac{1}{2}}(\mathbb{R}; H)$ for the Hilbert space of all $u \in \mathrm{L}^2(\mathbb{R}; H)$ such that $D_t^{\frac{1}{2}} u \in \mathrm{L}^2(\mathbb{R}; H)$ and define the parabolic *energy space*

$$\mathbb{E} := \mathrm{H}^{\frac{1}{2}}(\mathbb{R}; H) \cap \mathrm{L}^2(\mathbb{R}; V)$$

equipped with the Hilbertian norm $\|u\|_{\mathbb{E}} := \big(\|u\|^2_{\mathrm{L}^2(\mathbb{R}; V)} + \|D_t^{\frac{1}{2}} u\|^2_{\mathrm{L}^2(\mathbb{R}; H)}\big)^{\frac{1}{2}}$. It allows one to define $1 + \partial_t + \mathcal{L}_{\alpha,A(t)}$ as a bounded operator $\mathbb{E} \to \mathbb{E}^*$ via

$$\langle (1 + \partial_t + \mathcal{L}_{\alpha,A(t)}) u, v \rangle := \int_{\mathbb{R}} \langle u, v \rangle_2 + \langle H_t D_t^{\frac{1}{2}} u, D_t^{\frac{1}{2}} v \rangle_2 + \mathcal{E}_{\alpha,A(t)}(u, v)\, \mathrm{d}t, \quad (6\text{-}4)$$

where $\langle \cdot\,, \cdot \rangle_2$ denotes the inner product on $H = \mathrm{L}^2(\mathbb{R}^n)$. We state our substitute for Lemma 3.1 in the parabolic case. It is an extension of Theorem 3.1 in [Dier and Zacher 2017].

Lemma 6.5. *The operator* $1 + \partial_t + \mathcal{L}_{\alpha,A(t)} : \mathbb{E} \to \mathbb{E}^*$ *is bounded and invertible. Its norm and the norm of its inverse can be bounded only in terms of* λ*. Moreover, given* $f \in \mathrm{L}^2(\mathbb{R}; H)$, $u := (1 + \partial_t + \mathcal{L}_{\alpha,A(t)})^{-1} f$ *is a weak solution to* $\partial_t u + \mathcal{L}_{\alpha,A(t)} u = f - u$ *on* $\mathbb{R}^{1+n}$.

Proof. The $\mathbb{E} \to \mathbb{E}^*$ boundedness of $1 + \partial_t + \mathcal{L}_{\alpha,A}$ is clear by definition. Next, for the invertibility, the form

$$a_\delta(u, v) := \int_{\mathbb{R}} \langle u, (1 + \delta H_t) v \rangle_2 + \langle H_t D_t^{\frac{1}{2}} u, D_t^{\frac{1}{2}} (1 + \delta H_t) v \rangle_2 + \mathcal{E}_{\alpha,A(t)}(u, (1 + \delta H_t) v)\, \mathrm{d}t$$

for $u, v \in \mathbb{E}$, is bounded and satisfies an accretivity bound for $\delta > 0$ sufficiently small, for example $\delta := \lambda^2/2$. Indeed, from boundedness and ellipticity of $\mathcal{E}_{\alpha,A(t)}$

uniformly in t (see Section 3) and the fact that the Hilbert transform is L^2-isometric and skew-adjoint,

$$\operatorname{Re} a_\delta(u,u) \geq \|u\|^2_{\mathrm{L}^2(\mathbb{R};H)} + \delta \|D_t^{\frac{1}{2}} u\|_2^2 + (\lambda - \lambda^{-1}\delta) \int_{\mathbb{R}} [u(t,\cdot)]^2_{\alpha,2} \,\mathrm{d}t \geq \frac{\lambda^2}{2} \|u\|^2_{\mathbb{E}}.$$

As

$$\big\langle (1 + \partial_t + \mathcal{L}_{\alpha,A(t)})u, (1+\delta H_t)v \big\rangle = a_\delta(u,v), \quad (u,v \in \mathbb{E}),$$

and since $(1+\delta^2)^{-\frac{1}{2}}(1+\delta H_t)$ is isometric on $\mathbb{E}$ as is seen using its symbol

$$(1+\delta^2)^{-\frac{1}{2}}(1 - \mathrm{i}\delta \operatorname{sgn} \tau),$$

it follows from the Lax–Milgram lemma that $1 + \partial_t + \mathcal{L}_{\alpha,A(t)}$ is invertible from $\mathbb{E}$ onto $\mathbb{E}^*$. Finally, given $f \in \mathrm{L}^2(\mathbb{R}; H) \subset \mathbb{E}$ we can define $u := (1+\partial_t + \mathcal{L}_{\alpha,A(t)})^{-1} f$ and have by definition

$$\int_{\mathbb{R}} \langle H_t D_t^{\frac{1}{2}} u, D_t^{\frac{1}{2}} v\rangle_2 + \mathcal{E}_{\alpha,A(t)}(u,v) \,\mathrm{d}t = \int_{\mathbb{R}} \langle f - u, v\rangle_2 \,\mathrm{d}t \quad (v \in \mathbb{E}).$$

Since for $v \in \mathrm{C}_0^\infty(\mathbb{R} \times \mathbb{R}^n)$ we can undo the factorization $\langle H_t D_t^{\frac{1}{2}} u, D_t^{\frac{1}{2}} v\rangle_2 = -\langle u, \partial_t v\rangle$, we see that u is a weak solution to $\partial_t u + \mathcal{L}_{\alpha,A(t)} u = f - u$. □

Remark 6.6. Skew-adjointness of the Hilbert transform and ellipticity of each sesquilinear form $\mathcal{E}_{\alpha,A(t)}$ yield $\operatorname{Re}\langle (\partial_t + \mathcal{L}_{\alpha,A(t)})u, u\rangle \geq 0$ for every $u \in \mathbb{E}$ and by the previous lemma $1 + (\partial_t + \mathcal{L}_{\alpha,A(t)}) : \mathbb{E} \to \mathbb{E}^*$ is invertible. By definition, this means that $\partial_t + \mathcal{L}_{\alpha,A(t)}$ can be defined as a *maximal accretive operator* in $\mathrm{L}^2(\mathbb{R}^{1+n})$ with maximal domain $\mathbb{D} := \{u \in \mathbb{E} : (\partial_t + \mathcal{L}_{\alpha,A(t)})u \in \mathrm{L}^2(\mathbb{R}^{1+n})\}$.

In order to proceed, we need to link the parabolic energy space $\mathbb{E}$ and the sesquilinear form on the right-hand side of (6-4) with a Dirichlet form on fractional Sobolev spaces as in Section 3. To this end, note that for $u, v \in \mathrm{L}^2(\mathbb{R}; H)$ we obtain from Plancherel's theorem applied to the integral in s,

$$\begin{aligned}&\iint_{\mathbb{R}\times\mathbb{R}} \frac{\langle u(s+h) - u(s), v(s+h) - v(s)\rangle_2}{|h|^2} \,\mathrm{d}s \,\mathrm{d}h \\ &\quad = \iint_{\mathbb{R}\times\mathbb{R}} \frac{|\mathrm{e}^{-\mathrm{i}h\tau} - 1|^2}{|h|^2} \langle \mathcal{F}u(\tau), \mathcal{F}v(\tau)\rangle_2 \,\mathrm{d}\tau \,\mathrm{d}h = 2\pi \int_{\mathbb{R}} \langle D_t^{\frac{1}{2}} u(t), D_t^{\frac{1}{2}} v(t)\rangle_2 \,\mathrm{d}t,\end{aligned}$$

where in the second step we evaluated the well-known integral in h to $2\pi|\tau|$. This calculation is understood in the sense that for $u = v$ the left-hand side is finite if and only if the right-hand side is defined and finite and if both u and v have this property, then equality above holds true. Consequently, $\partial_t + \mathcal{L}_{\alpha,A(t)}$ is the operator associated with the *parabolic Dirichlet form*

$$\begin{aligned}\mathcal{P}_{\alpha,A(t)}(u, v) \\ &:= \int_{\mathbb{R}} \langle H_t D_t^{\frac{1}{2}} u, D_t^{\frac{1}{2}} v\rangle_2 + \mathcal{E}_{\alpha,A(t)}(u, v)\,\mathrm{d}t \\ &= \frac{1}{2\pi} \int_{\mathbb{R}^n} \iint_{\mathbb{R}\times\mathbb{R}} \frac{(H_t u(t, x) - H_t u(s, x)) \cdot \overline{(v(t, x) - v(s, x))}}{|t - s|^2}\,\mathrm{d}s\,\mathrm{d}t\,\mathrm{d}x \\ &\quad + \int_{\mathbb{R}} \iint_{\mathbb{R}^n\times\mathbb{R}^n} A(t, x, y) \frac{(u(t, x) - u(t, y)) \cdot \overline{(v(t, x) - v(t, y))}}{|x - y|^{n+2\alpha}}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}t,\end{aligned}$$

defined so far for $u, v \in \mathbb{E}$. Here, $H_t u(\,\cdot\,, x)$ is understood as the Hilbert transform of $u(\,\cdot\,, x) \in \mathrm{L}^2(\mathbb{R})$ for almost every fixed $x \in \mathbb{R}^n$.

6B. ***Analysis of the parabolic Dirichlet form.*** The spaces “near” $\mathbb{E}$ to examine are determined by the definition of the parabolic Dirichlet form: For $p \in (1, \infty)$ and $s \in (0, 1) \cap (0, 2\alpha)$ we let $\mathbb{W}_\alpha^{s,p}(\mathbb{R}^{1+n})$ consist of all functions $u \in \mathrm{L}^p(\mathbb{R}^{1+n})$ with finite seminorm

$$[\![u]\!]_{s,p} := \Bigg(\int_{\mathbb{R}^n} \iint_{\mathbb{R}\times\mathbb{R}} \frac{|u(t, x) - u(s, x)|^p}{|t - s|^{1+sp/(2\alpha)}}\,\mathrm{d}s\,\mathrm{d}t\,\mathrm{d}x + \int_{\mathbb{R}} \iint_{\mathbb{R}^n\times\mathbb{R}^n} \frac{|u(t, x) - u(t, y)|^p}{|x - y|^{n+sp}}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}t \Bigg)^{\frac{1}{p}}$$

and put $\|\cdot\|_{\mathbb{W}_\alpha^{s,p}(\mathbb{R}^{1+n})} := \|\cdot\|_p + [\![\,\cdot\,]\!]_{s,p}$. Again, smooth truncation and convolution yields that $\mathrm{C}_0^\infty(\mathbb{R}^{1+n})$ is dense in any of these spaces. Often we shall write more suggestively

$$\mathbb{W}_\alpha^{s,p}(\mathbb{R}^{1+n}) = \mathrm{W}^{s/(2\alpha),p}(\mathbb{R}; \mathrm{L}^p(\mathbb{R}^n)) \cap \mathrm{L}^p(\mathbb{R}; \mathrm{W}^{s,p}(\mathbb{R}^n)),$$

where the vector-valued fractional Sobolev spaces are defined as their scalar-valued counterpart upon replacing absolute values by norms. But as

$$\mathrm{W}^{s/(2\alpha),p}(\mathbb{R}; \mathrm{L}^p(\mathbb{R}^n)) = \mathrm{L}^p(\mathbb{R}^n; \mathrm{W}^{s/(2\alpha),p}(\mathbb{R}))$$

in virtue of Tonelli’s theorem, all fractional Sobolev embeddings stated for the scalar-valued space $\mathrm{W}^{s/(2\alpha),p}(\mathbb{R})$ remain valid for $\mathrm{W}^{s/(2\alpha),p}(\mathbb{R}; \mathrm{L}^p(\mathbb{R}^n))$. Note the scaling in the spaces $\mathbb{W}_\alpha^{s,p}(\mathbb{R}^{1+n})$ adapted to the fractional parabolic equation: one time derivative accounts for 2α spatial derivatives.

By what we have seen before, $\mathbb{W}_\alpha^{\alpha,2}(\mathbb{R}^{1+n}) = \mathbb{E}$ up to equivalent norms and hence $1 + \partial_t + \mathcal{L}_{\alpha,A(t)}$ is invertible from that space onto its antidual by Lemma 6.5. The following mapping properties are then proved by Hölder’s inequality exactly as their elliptic counterpart, Lemma 3.2, on making the additional observation that $H_t : \mathrm{W}^{s,p}(\mathbb{R}) \to \mathrm{W}^{s,p}(\mathbb{R})$ is bounded. Indeed, this is immediate from the equivalent norm (2-1) on $\mathrm{W}^{s,p}(\mathbb{R})$ since the Hilbert transform commutes with convolutions and is bounded on $\mathrm{L}^p(\mathbb{R})$.

Lemma 6.7. *Let $s, s' \in (0,1)$ and $p, p' \in (1,\infty)$ satisfy*

$$s + s' = 2\alpha \quad \textit{and} \quad \frac{1}{p} + \frac{1}{p'} = 1.$$

Then $1 + \partial_t + \mathcal{L}_{\alpha,A(t)}$ extends from $\mathrm{C}_0^\infty(\mathbb{R}^n)$ by density to a bounded operator $\mathbb{W}_\alpha^{s,p}(\mathbb{R}^{1+n}) \to \mathbb{W}_\alpha^{s',p'}(\mathbb{R}^{1+n})^*$.

Remark 6.8. The extensions obtained above are also denoted by $1 + \partial_t + \mathcal{L}_{\alpha,A}$ and a comment analogous to Remark 3.3 applies.

Hence, the only ingredient missing in our recipe for self-improvement is the complex interpolation identity replacing (3-3). This can be obtained from [Dachkovski 2003] as follows. We define the vector of anisotropy $\boldsymbol{v}$ and the mean smoothness γ by

$$\boldsymbol{v} := \left(\tfrac{2\alpha(1+n)}{n+2\alpha}, \tfrac{1+n}{n+2\alpha}, \dots, \tfrac{1+n}{n+2\alpha}\right) \in \mathbb{R}^{1+n},$$
$$\gamma := \tfrac{(1+n)}{n+2\alpha} s \in (0,1) \quad \text{for } s \in (0,1) \cap (0, 2\alpha).$$

Then, [Dachkovski 2003, Theorem 6.2] identifies $\mathbb{W}_\alpha^{s,p}(\mathbb{R}^{1+n})$ up to equivalent norms with the *anisotropic Besov space* $\mathrm{B}_{p,p}^{\gamma,\boldsymbol{v}}(\mathbb{R}^{1+n})$. In turn, this space is defined in [Dachkovski 2003] exactly as the ordinary Besov space $\mathrm{B}_{p,p}^{\gamma}(\mathbb{R}^{1+n})$ in Section 2, upon replacing the scalar multiplication $2^j x = (2^j x_0, \dots, 2^j x_n)$ on $\mathbb{R}^{1+n}$ by the anisotropic multiplication $2^{\boldsymbol{v}j} x := (2^{\boldsymbol{v}_0 j} x_0, \dots, 2^{\boldsymbol{v}_n j} x_n)$, where $j \in \mathbb{R}$ and subscripts indicate coordinates of $(n+1)$-vectors, and the Euclidean norm $|x|$ by the anisotropic norm $|x|_{\boldsymbol{v}}$ defined as the unique positive number σ such that $\sum_j x_j^2/\sigma^{2\boldsymbol{v}_j} = 1$. With these modifications, $\mathrm{B}_{p,p}^{\gamma,\boldsymbol{v}}(\mathbb{R}^{1+n})$ is the collection of all $u \in \mathrm{L}^p(\mathbb{R}^{1+n})$ with finite norm

$$\|u\|_{\mathrm{B}_{p,p}^{\gamma,\boldsymbol{v}}(\mathbb{R}^{1+n})} := \left(\sum_{j=0}^{\infty} 2^{j\gamma p} \|\phi_j * u\|_p^p\right)^{\frac{1}{p}} < \infty.$$

Note that this norm now reads exactly as the one in (2-1) on the anisotropic space $\mathrm{B}_{p,p}^{\gamma}(\mathbb{R}^{1+n})$ because the anisotropy $\boldsymbol{v}$ is only present in the now anisotropic dyadic decomposition $1 = \sum_{j=0}^\infty \mathcal{F}(\phi_j)(\xi)$. With this particular structure of the norms, complex interpolation works by abstract results exactly as outlined before in Section 3, see again [Bergh and Löfström 1976, Theorem 6.4.5(6) and Corrolary 4.5.2]. Thus, we have

$$\left[\mathbb{W}_\alpha^{s_0,p_0}(\mathbb{R}^n), \mathbb{W}_\alpha^{s_1,p_1}(\mathbb{R}^{1+n})\right]_\theta = \mathbb{W}_\alpha^{s,p}(\mathbb{R}^n)$$

for $p_0, p_1 \in (1,\infty)$, $s_0, s_1 \in (0,1) \cap (0,2\alpha)$ and the analogous identity for the antidual spaces both up to equivalent norms with p, s given as before by $1/p =$

$(1-\theta)/p_0+\theta/p_1$ and $s=(1-\theta)s_0+\theta s_1$. We do not insist on uniformity of the equivalence constants as in Section 3 and leave the care of checking it to interested readers.

This interpolation identity and Lemma 6.7 set the stage to apply Shneiberg's result as in the proof of Proposition 3.4 to deduce

Proposition 6.9. *Fix any line ℓ passing through $\left(\alpha, \frac{1}{2}\right)$ in the $(s, 1/p)$-plane. There exists $\varepsilon > 0$ depending on ℓ, λ, n, such that for $(s, 1/p) \in \ell$ with $|s-\alpha|, |p-2| < \varepsilon$ and s', p' satisfying $s+s' = 2\alpha$ and $1/p+1/p' = 1$, the operator*

$$1+\partial_t+\mathcal{L}_{\alpha,A(t)} : \mathbb{W}^{s,p}_\alpha(\mathbb{R}^{1+n}) \to \mathbb{W}^{s',p'}_\alpha(\mathbb{R}^{1+n})^*$$

is invertible and the inverse agrees with the one obtained for $s=\alpha$, $p=2$ on their common domain of definition.

6C. *Higher differentiability and integrability result.* We still need a lemma making Proposition 6.9 applicable in the L^2-setting of our main result.

Lemma 6.10. *Suppose $s \in (\alpha, 2\alpha)$, $p \in [2, \infty)$ and let $s+s' = 2\alpha$, $1/p+1/p' = 1$. If $2/p \geq 1-s'/n$, then $\mathrm{L}^2(\mathbb{R}; \mathrm{L}^2(\mathbb{R}^n)) \subset \mathbb{W}^{s',p'}_\alpha(\mathbb{R}^{1+n})^*$ with continuous inclusion.*

Proof. Since $p's' < 2\alpha < 2 \leq n$ by assumption, we can infer from Lemma 4.2 the continuous embedding

$$\mathrm{W}^{s',p'}(\mathbb{R}^n) \subset \mathrm{L}^q(\mathbb{R}^n) \quad \left(\tfrac{1}{p'} - \tfrac{s'}{n} \leq \tfrac{1}{q} \leq \tfrac{1}{p'}\right).$$

Likewise, by the vector valued analog of Lemma 4.2 (see the beginning of Section 6B) we have

$$\mathrm{W}^{s'/(2\alpha),p'}(\mathbb{R}; \mathrm{L}^{p'}(\mathbb{R}^n)) \subset \mathrm{L}^r(\mathbb{R}; \mathrm{L}^{p'}(\mathbb{R}^n)) \quad \left(\tfrac{1}{p'} - \tfrac{s'}{2\alpha} \leq \tfrac{1}{r} \leq \tfrac{1}{p'}\right)$$

Now, the additional condition $2/p \geq 1-s'/n$ along with $2\alpha < n$ precisely guarantees that we can take $q = p = r$ and therefore

$$\begin{aligned}&\mathbb{W}^{s',p'}_\alpha(\mathbb{R}^{1+n})\\ &= \mathrm{W}^{s'/(2\alpha),p'}(\mathbb{R}; \mathrm{L}^{p'}(\mathbb{R}^n)) \cap \mathrm{L}^{p'}(\mathbb{R}; \mathrm{W}^{s',p'}(\mathbb{R}^n)) \subset \mathrm{L}^p(\mathbb{R}; \mathrm{L}^{p'}(\mathbb{R}^n)) \cap \mathrm{L}^{p'}(\mathbb{R}; \mathrm{L}^p(\mathbb{R}^n)).\end{aligned}$$

Taking into account the convex combinations $\frac{1}{2} = \frac{1-\theta}{p} + \frac{\theta}{p'} = \frac{1-\theta}{p'} + \frac{\theta}{p}$ for $\theta = \frac{1}{2}$, standard embeddings for mixed Lebesgue spaces imply that the right-hand space is continuously included in $\mathrm{L}^2(\mathbb{R}; \mathrm{L}^2(\mathbb{R}^n))$, see for example [Bergh and Löfström 1976, Theorems 5.1 and 5.2]. The claim follows by duality with respect to the inner product on $\mathrm{L}^2(\mathbb{R}; \mathrm{L}^2(\mathbb{R}^n))$. □

Proof of Theorem 6.3. Let $f \in \mathrm{L}^2(0, T; \mathrm{L}^2(\mathbb{R}^n))$. Since uniqueness is known, only existence of a weak solution to (6-1) with the stated properties is a concern. To this end, we shall argue as in [Dier and Zacher 2017] by restriction from the real line, where we know how to improve regularity.

We extend $A(t,x,y) := 1$ and $f(t) := 0$ for $t \notin [0,T]$. Then, $g(t) := \mathrm{e}^{-t} f(t) \in \mathrm{L}^2(\mathbb{R}; \mathrm{L}^2(\mathbb{R}^n))$ and thus Lemma 6.5 furnishes

$$v := (1 + \partial_t + \mathcal{L}_{\alpha,A})^{-1} g \in \mathbb{W}^{\alpha,2}_{\alpha}(\mathbb{R}^{1+n}),$$

which is a weak solution to

$$\partial_t v(t) + \mathcal{L}_{\alpha,A(t)} v(t) = e^{-t} f(t) - v(t) \quad (t \in \mathbb{R}).$$

In particular, v is a continuous function on $\mathbb{R}$ with values in $\mathrm{L}^2(\mathbb{R}^n)$ (see Remark 6.2(i)). We claim $v(0) = 0$. Indeed, $t \mapsto \|v(t)\|_2^2$ is absolutely continuous with derivative $\frac{\mathrm{d}}{\mathrm{d}t}\|v(t)\|_2^2 = 2\,\mathrm{Re}\langle \partial_t v(t), v(t)\rangle$, where $\langle \cdot\,, \cdot \rangle$ denotes the $\mathrm{W}^{\alpha,2}(\mathbb{R}^n)^*$–$\mathrm{W}^{\alpha,2}(\mathbb{R}^n)$ duality [Showalter 1997, Proposition 1.2]. By (3-2),

$$\lambda \int_{-\infty}^{0} \|v\|_{\alpha,2}^2 \mathrm{d}t \le \mathrm{Re} \int_{-\infty}^{0} \langle v + \mathcal{L}_{\alpha,A(t)} v, v\rangle \,\mathrm{d}t = -\,\mathrm{Re} \int_{-\infty}^{0} \langle \partial_t v, v\rangle \,\mathrm{d}t = -\tfrac{1}{2}\|v(0)\|_2^2,$$

where we have used the equation for v along with $f(t) = 0$ for $t \in (-\infty, 0)$ in the second step. Thus, $\|v(0)\|_2 = 0$. The upshot is that the restriction of $\mathrm{e}^t v(t)$ to $[0,T]$ is the unique weak solution u to the Cauchy problem (6-1) and it remains to prove the additional regularity.

Let $s > \alpha$, $p > 2$ sufficiently close to α, 2, so that we have both Lemma 6.10 and Proposition 6.9 at our disposal. Defining s' and p' as usual, the former guarantees $g \in \mathbb{W}^{s',p'}_{\alpha}(\mathbb{R}^{1+n})^*$ and thus the latter yields $v \in \mathbb{W}^{s,p}_{\alpha}(\mathbb{R}^{1+n})$. As we have $u(t) = \mathrm{e}^t v(t)$ for $t \in [0,T]$, restricting to $[0,T]$ readily yields that the left-hand side of (6-3) is controlled by

$$\mathrm{e}^T(\|v\|_p + [\![v]\!]_{s,p}) \lesssim \mathrm{e}^T \|g\|_{\mathbb{W}^{s',p'}_{\alpha}(\mathbb{R}^{1+n})^*} \lesssim \mathrm{e}^T \|g\|_{\mathrm{L}^2(\mathbb{R};\mathrm{L}^2(\mathbb{R}^n))} \lesssim \mathrm{e}^T \|f\|_{\mathrm{L}^2(0,T;\mathrm{L}^2(\mathbb{R}^n))}$$

as claimed.

Repeating the same argument with $s > \alpha$ and $p = 2$ reveals $v \in \mathbb{W}^{s,2}_{\alpha}(\mathbb{R}^{1+n})$ and in particular $u \in \mathrm{L}^2(0,T; \mathrm{W}^{\alpha+\varepsilon,2}(\mathbb{R}^n))$, where $\varepsilon := s - \alpha > 0$. By Hölder's inequality this also implies $u \in \mathrm{L}^2(0,T; \mathrm{W}^{\alpha-\varepsilon,2}(\mathbb{R}^n)^*)$. Moreover, from the equation for u since $\mathcal{L}_{\alpha,A(t)} : \mathrm{W}^{\alpha+\varepsilon,2}(\mathbb{R}^n) \to \mathrm{W}^{\alpha-\varepsilon,2}(\mathbb{R}^n)^*$ is bounded by λ^{-1} uniformly in t due to Lemma 3.2, we deduce

$$\left| \int_0^T -\langle u, \partial_t \phi\rangle_2 \,\mathrm{d}t \right| \le \int_0^T \|f(t)\|_2 \|\phi(t)\|_2 + \lambda^{-1}\|u(t)\|_{\alpha+\varepsilon,2}\|\phi(t)\|_{\alpha-\varepsilon,2}\,\mathrm{d}t$$

for all $\phi \in \mathrm{C}_0^\infty((0,T)\times\mathbb{R}^n)$. By density, see Remark 6.2, this remains true for $\phi \in \mathrm{H}^1(0,T; \mathrm{W}^{\alpha-\varepsilon,2}(\mathbb{R}^n))$ and we conclude $u \in \mathrm{H}^1(0,T; \mathrm{W}^{\alpha-\varepsilon,2}(\mathbb{R}^n)^*)$ as required.

□

Appendix: Shneiberg's stability theorem

We provide a self-contained proof of a *quantitative* version of Shneiberg's stability theorem. Quantitative bounds are often required in applications but up to now have not appeared explicitly in the literature. In principle, both the original proof [Shneiberg 1974] and the generalization to quasi-Banach spaces [Kalton and Mitrea 1998] allow one to track parameters.

We need to recall some essentials on complex interpolation theory beforehand. For general background we refer to [Bergh and Löfström 1976; Triebel 1983]. An *interpolation couple* $\overline{X} = (X_0, X_1)$ consists of two complex Banach spaces X_0, X_1 that both are included in the same linear Hausdorff space. In this case their sum $X_0 + X_1$ with norm

$$\|x\|_{X_0+X_1} = \inf\{\|x_0\|_{X_0} + \|x_1\|_{X_1} : x = x_0 + x_1\}$$

is a well-defined Banach space. Let now $S = \{z \in \mathbb{C} : 0 < \operatorname{Re} z < 1\}$ be the open unit strip in the complex plane. The space $\mathrm{F}(X_0, X_1)$ consists of all bounded continuous functions $f : \bar{S} \to X_0 + X_1$ that are holomorphic in S and whose restrictions to the boundary lines $\mathrm{i}\mathbb{R}$ and $1+\mathrm{i}\mathbb{R}$ are continuous functions with values in X_0 and X_1 that vanish at infinity, respectively. By the maximum principle, $\mathrm{F}(X_0, X_1)$ becomes a Banach space for the norm

$$\|f\|_{\mathrm{F}(X_0,X_1)} = \max\bigl\{\sup_{t\in\mathbb{R}}\|f(\mathrm{i}t)\|_{X_0},\ \sup_{t\in\mathbb{R}}\|f(1+\mathrm{i}t)\|_{X_1}\bigr\}.$$

Given $\theta \in (0, 1)$, the *complex interpolation space* $X_\theta = [X_0, X_1]_\theta$ consists of those $x \in X_0 + X_1$ that arise as $x = f(\theta)$ for some $f \in \mathrm{F}(X_0, X_1)$. It is complete for the norm

$$\|f\|_{X_\theta} = \inf\{\|f\|_{\mathrm{F}(X_0,X_1)} : f(\theta) = x\}.$$

These spaces have the following interpolation property. Suppose $\overline{X} = (X_0, X_1)$ and $\overline{Y} = (Y_0, Y_1)$ are interpolation couples and the same linear operator T is bounded $X_0 \to Y_0$ and $X_1 \to Y_1$ with norms M_0 and M_1, respectively. Then T can be viewed as an operator $X_0 + X_1 \to Y_0 + Y_1$ and it maps X_θ boundedly into Y_θ with norm at most $M_0^{1-\theta} M_1^\theta$. We shall write $T \in \mathcal{L}(\overline{X}, \overline{Y})$ in this situation.

Theorem A.1 (quantitative Shneiberg theorem). *Let $\overline{X} = (X_0, X_1)$ and $\overline{Y} = (Y_0, Y_1)$ be interpolation couples and $T \in \mathcal{L}(\overline{X}, \overline{Y})$. Suppose for some $\theta^* \in (0, 1)$ the lower bound*

$$\|Tx\|_{Y_{\theta^*}} \geq \kappa \|x\|_{X_{\theta^*}} \quad (x \in X_{\theta^*})$$

holds for some $\kappa > 0$. Then the following hold true:

(i) *Given $0 < \varepsilon < \frac{1}{4}$, the lower bound*

$$\|Tx\|_{Y_\theta} \geq \varepsilon\kappa \|x\|_{X_\theta} \quad (x \in X_\theta)$$

holds provided

$$|\theta-\theta^*| \le \frac{\kappa(1-4\varepsilon)\min\{\theta^*, 1-\theta^*\}}{3\kappa+6M},$$

where $M = \max_{j=0,1} \|T\|_{X_j\to Y_j}$.

(ii) *If* $T : X_{\theta^*} \to Y_{\theta^*}$ *is invertible, then the same is true for* $T : X_\theta \to Y_\theta$ *if* θ *is as in* (i). *The inverse mappings agree on* $X_\theta \cap X_{\theta^*}$ *and their norms are bounded by* $1/(\varepsilon\kappa)$.

Remark A.2. Qualitatively speaking, (ii) means that the set of parameters θ for which $T : X_\theta \to Y_\theta$ is an isomorphism is open in $(0, 1)$.

Consistency of the inverse as stated in part (ii) is a general feature of complex interpolation [Kalton et al. 2007, Theorem 8.1]. Here, we are only concerned with the other assertions. Strictly speaking, the latter article is limited to couples whose intersection is dense in both members but this becomes important only if one wishes to consider *quasi*-Banach spaces. For example, [Kalton et al. 2007, Theorem 8.1] needs that $X_0 \cap X_1$ is dense in all spaces $[X_0, X_1]_\theta$, $\theta \in (0, 1)$. In turn, this is holds for Banach spaces X_0, X_1 as above [Bergh and Löfström 1976, Theorem 4.2.2].

Reversing the order of statements, we begin with proving stability of ontoness with respect to the interpolation parameter θ.

Lemma A.3 (stability of ontoness). *Let* $\overline{X} = (X_0, X_1)$ *and* $\overline{Y} = (Y_0, Y_1)$ *be interpolation couples and let* $T \in \mathcal{L}(\overline{X}, \overline{Y})$. *Suppose that* $T : X_{\theta^*} \to Y_{\theta^*}$ *is invertible for some* $\theta^* \in (0, 1)$ *and let* $\kappa > 0$ *be such that* $\|T^{-1}\|_{Y_{\theta^*}\to X_{\theta^*}} \le 1/\kappa$. *If* $\theta \in (0, 1)$ *satisfies*

$$|\theta-\theta^*| < \frac{\kappa\min\{\theta^*, 1-\theta^*\}}{\kappa+\max_{j=0,1}\|T\|_{X_j\to Y_j}}, \tag{A-1}$$

then $T : X_\theta \to Y_\theta$ *is onto.*

For the proof we need:

Lemma A.4. *Let* $T : X \to Y$ *be a bounded linear operator between Banach spaces* X *and* Y. *If there are constants* $0 < c < 1$ *and* $C > 0$ *such that for every* y *in the unit sphere of* Y *there exists* $x \in X$ *with* $\|x\|_X \le C$ *and* $\|y - Tx\|_Y \le c$, *then* T *is onto.*

Proof. Given $y \in Y$, we apply the hypotheses inductively to construct a sequence $(x_n)_n$ such that for all $n = 0, 1, \dots$ we have

$$\|x_n\|_X \le Cc^{n-1}\|y\|_Y \quad \text{and} \quad \|y - \sum_{j=1}^{n} Tx_j\|_Y \le c^n\|y\|_Y.$$

By the first property $x = \sum_{n=1}^{\infty} x_n$ exists and by the second one $Tx = y$ as required. □

Proof of Lemma A.3. Pick $\varepsilon > 0$ such that $(1+\varepsilon)^2|\theta - \theta^*|$ is still smaller than the right-hand side of (A-1). Let us see how we can apply Lemma A.4 to $T : X_\theta \to Y_\theta$. We fix y in the unit sphere of Y_θ. By definition of complex interpolation we find $g \in \mathrm{F}(Y_0, Y_1)$ such that

$$g(\theta) = y, \quad \|g\|_{\mathrm{F}(Y_0,Y_1)} \le (1+\varepsilon). \tag{A-2}$$

Likewise, since $g(\theta^*) \in Y_{\theta^*}$ and $T^{-1}g(\theta^*) \in X_{\theta^*}$, there exists $f \in \mathrm{F}(X_0, X_1)$ such that

$$Tf(\theta^*) = g(\theta^*), \quad \|f\|_{\mathrm{F}(X_0,X_1)} \le (1+\varepsilon)\|T^{-1}g(\theta^*)\|_{X_{\theta^*}}. \tag{A-3}$$

We complete the proof by showing that $x = f(\theta) \in X_\theta$ fits the assumptions of Lemma A.4.

To this end, we first use (A-2) and (A-3) to give

$$\begin{aligned}\|x\|_{X_\theta} &\le \|f\|_{\mathrm{F}(X_0,X_1)} \le (1+\varepsilon)\|T^{-1}g(\theta^*)\|_{X_{\theta^*}} \\ &\le \frac{1+\varepsilon}{\kappa}\|g(\theta^*)\|_{Y_{\theta^*}} \le \frac{(1+\varepsilon)^2}{\kappa},\end{aligned} \tag{A-4}$$

independently of y. In order to estimate the norm of $y - Tx$, we use the auxiliary function

$$h(z) := \begin{cases} \dfrac{g(z)-Tf(z)}{z-\theta^*} & \text{for } z \neq \theta^*, \\ g'(\theta^*) - Tf'(\theta^*) & \text{for } z = \theta^*, \end{cases}$$

defined on the closure of the unit strip S. As we have $Tf(\theta^*) = g(\theta^*)$, we can conclude by Riemann's removable singularity theorem that h is holomorphic in S with values in $Y_0 + Y_1$. We even have $h \in \mathrm{F}(Y_0, Y_1)$ by the choices of f and g and since $T \in \mathcal{L}(\overline{X}, \overline{Y})$. From $y - Tx = (\theta - \theta^*)h(\theta)$ we obtain

$$\|y - Tx\|_{Y_\theta} \le |\theta - \theta^*|\|h\|_{\mathrm{F}(Y_0,Y_1)} \le \frac{|\theta - \theta^*|}{\min\{\theta^*, 1-\theta^*\}}\|g - Tf\|_{\mathrm{F}(Y_0,Y_1)}.$$

Abbreviating $M := \max_{j=0,1}\|T\|_{X_j \to Y_j}$, we have

$$\begin{aligned}\|g - Tf\|_{\mathrm{F}(Y_0,Y_1)} &\le \|g\|_{\mathrm{F}(Y_0,Y_1)} + M\|f\|_{\mathrm{F}(X_0,X_1)} \\ &\le (1+\varepsilon)^2\frac{\kappa + M}{\kappa},\end{aligned}$$

where the second step is due to (A-2) and the comparison between the second and the last term in (A-4). Combining the previous two estimates, we get a bound for $\|y - Tx\|_{Y_\theta}$ that is independent of y and strictly smaller than 1 precisely by the definition of ε at the beginning of the proof. □

Stability of the lower bound in part (i) of Theorem A.1 will follow from a variant of the Schwarz lemma from complex analysis.

Lemma A.5. *Let* (X_0, X_1) *be an interpolation couple and* $\theta^* \in (0,1)$. *Let* $r \leq \min\{\theta^*, 1-\theta^*\}/2$. *If* $|\theta - \theta^*| \leq r$, *then*

$$\|f(\theta)\|_{X_\theta} \geq \tfrac{1}{2}\|f(\theta^*)\|_{X_{\theta^*}} - \frac{|\theta-\theta^*|}{2r}\|f\|_{\mathrm{F}(X_0,X_1)}$$

for each $f \in \mathrm{F}(X_0, X_1)$.

Proof. Without loss of generality we may assume $\theta \neq \theta^*$. We fix $f \in \mathrm{F}(X_0, X_1)$. By definition of complex interpolation we have $f(\theta) \in X_\theta$. Let us consider any other $g \in \mathrm{F}(X_0, X_1)$ satisfying $g(\theta) = f(\theta)$. As in the proof of Lemma A.3 the function

$$h(z) := \begin{cases} \dfrac{f(z)-g(z)}{z-\theta} & \text{for } z \neq \theta, \\ f'(\theta) - g'(\theta) & \text{for } z = \theta, \end{cases}$$

turns out to belong to $\mathrm{F}(X_0, X_1)$. For $z \in \mathrm{i}\mathbb{R}$ we have $|z-\theta| \geq \theta \geq \theta^* - r \geq r$ by assumption. The same bound holds for $z \in 1 + \mathrm{i}\mathbb{R}$. By the definition of the norm on $\mathrm{F}(X_0, X_1)$ we obtain

$$\begin{aligned} \|h\|_{\mathrm{F}(X_0,X_1)} &\leq \frac{1}{r}\|f-g\|_{\mathrm{F}(X_0,X_1)} \\ &\leq \frac{1}{r}\|f\|_{\mathrm{F}(X_0,X_1)} + \frac{1}{r}\|g\|_{\mathrm{F}(X_0,X_1)}. \end{aligned}$$

The upshot is that the norm of $f(\theta^*)$ in X_{θ^*} can be estimated via h since we have $(\theta^* - \theta)h(\theta^*) = f(\theta^*) - g(\theta^*)$. Due to $|\theta - \theta^*| \leq r$ we get

$$\begin{aligned} \|f(\theta^*)\|_{X_{\theta^*}} &\leq \|g + (\theta^* - \theta)h\|_{\mathrm{F}(X_0,X_1)} \\ &\leq 2\|g\|_{\mathrm{F}(X_0,X_1)} + \frac{|\theta-\theta^*|}{r}\|f\|_{\mathrm{F}(X_0,X_1)}. \end{aligned}$$

This inequality has been established for every $g \in \mathrm{F}(X_0, X_1)$ satisfying $g(\theta) = f(\theta)$. On passing to the infimum we can replace $\|g\|_{\mathrm{F}(X_0,X_1)}$ by $\|f(\theta)\|_{X_\theta}$ on the right-hand side and the claim follows. □

Proof of Theorem A.1. Let $\theta \in (0,1)$ and assume $|\theta - \theta^*| \leq r$, where $r > 0$ will be subject to several restrictions culminating in the one alluded in the theorem. For brevity we put again $M := \max_{j=0,1}\|T\|_{X_j \to Y_j}$. The argument is in two steps: First we prove a lower bound for T on Y_θ and then we adjust parameters to prove the two assertions.

Step 1: *A lower bound for* T. Let $x \in X_\theta$ and pick $f \in \mathrm{F}(X_0, X_1)$ such that $f(\theta) = x$. Then $Tf \in \mathrm{F}(Y_0, Y_1)$ satisfies $Tf(\theta) = Tx \in Y_\theta$ and $\|Tf\|_{\mathrm{F}(Y_0,Y_1)} \leq M\|f\|_{\mathrm{F}(X_0,X_1)}$. We require $r \leq \min\{\theta^*, 1-\theta^*\}/2$ in order to bring into play Lemma A.5, which in turn provides the bound

$$\|Tx\|_{Y_\theta} = \|Tf(\theta)\|_{Y_\theta} \geq \tfrac{1}{2}\|Tf(\theta^*)\|_{Y_{\theta^*}} - \frac{M|\theta-\theta^*|}{2r}\|f\|_{\mathrm{F}(X_0,X_1)}.$$

As we have $f(\theta^*) \in X_{\theta^*}$, the assumption on T implies

$$\|Tx\|_{Y_\theta} \geq \frac{\kappa}{2}\|f(\theta^*)\|_{X_{\theta^*}} - \frac{M|\theta-\theta^*|}{2r}\|f\|_{\mathrm{F}(X_0,X_1)}.$$

In order to get rid of $f(\theta^*)$, let us require $r \leq \min\{\theta^*, 1-\theta^*\}/3$ because then we have $r \leq \min\{\theta, 1-\theta\}/2$. In turn, this allows us to reapply Lemma A.5 with the roles of θ and θ^* interchanged to the effect that

$$\|Tx\|_{Y_\theta} \geq \frac{\kappa}{2}\left(\tfrac{1}{2}\|f(\theta)\|_{X_\theta} - \frac{|\theta-\theta^*|}{2r}\|f\|_{\mathrm{F}(X_0,X_1)}\right) - \frac{M|\theta-\theta^*|}{2r}\|f\|_{\mathrm{F}(X_0,X_1)}.$$

Since we have obtained this estimate under the restriction $r \leq \min\{\theta^*, 1-\theta^*\}/3$ for every $f \in \mathrm{F}(X_0, X_1)$ satisfying $f(\theta) = x$, we can pass to the infimum and conclude

$$\|Tx\|_{Y_\theta} \geq \left(\frac{\kappa}{4} - |\theta-\theta^*|\frac{\kappa+2M}{4r}\right)\|x\|_{X_\theta}.$$

Step 2: *Adjusting parameters.* If $0 < \varepsilon < \frac{1}{4}$, then summa summarum Step 1 yields the required lower bound provided

$$|\theta-\theta^*| \leq r \leq \tfrac{1}{3}\min\{\theta^*, 1-\theta^*\}, \qquad \frac{\kappa}{4} - |\theta-\theta^*|\frac{\kappa+2M}{4r} \geq \varepsilon\kappa.$$

These conditions collapse to

$$|\theta-\theta^*| \leq r\frac{\kappa(1-4\varepsilon)}{\kappa+2M} \leq \min\{\theta^*, 1-\theta^*\}\frac{\kappa(1-4\varepsilon)}{3\kappa+6M}$$

as claimed in (i). Finally, if $T : X_{\theta^*} \to Y_{\theta^*}$ is an isomorphism, then

$$\|T^{-1}\|_{Y_{\theta^*}\to X_{\theta^*}} \leq \frac{1}{\kappa}.$$

Consequently, Lemma A.4 guarantees that $T : X_\theta \to Y_\theta$ remains onto provided

$$|\theta-\theta^*| < \min\{\theta^*, 1-\theta^*\}\frac{\kappa}{\kappa+M}$$

and this is a larger interval than the one obtained for the lower bound. □

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Saturated morphisms of logarithmic schemes

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The notion of universally saturated morphisms between saturated log schemes was introduced by Kazuya Kato. In this paper, we study universally saturated morphisms systematically by introducing the notion of saturated morphisms between integral log schemes as a relative analogue of saturated log structures. We eventually show that a morphism of saturated log schemes is universally saturated if and only if it is saturated. We prove some fundamental properties and characterizations of universally saturated morphisms via this interpretation.

Introduction

The notion of universally saturated morphisms between saturated log schemes was introduced by Kazuya Kato. The purpose of this paper is to study universally saturated morphisms systematically.

We define saturated morphisms not only for saturated log schemes but also for integral log schemes (Definitions I.3.5, I.3.7, I.3.12, II.2.10). They are stable under compositions and base changes (in the category of log schemes) (Proposition II.2.11). The first important property of saturated morphisms is the following (Propositions I.3.9, II.2.12):

> For a saturated morphism of integral log schemes $(X, M_X) \to (Y, M_Y)$, if M_Y is saturated, then M_X is also saturated.

This and the stability of saturated morphisms under base changes imply that saturated morphisms of saturated log schemes are universally saturated. In fact, we see that the converse is also true (Proposition II.2.13).

Our main results concerning saturated morphisms are the following:

This paper was written in 1997, and has been circulated among some experts since then. The author made very minor revisions to the original keeping the reference numbers of theorems, propositions, etc., unchanged because the original had already been cited in some published papers.

Some of the results of this paper will be absorbed into the book on foundation of logarithmic algebraic geometry which Arthur Ogus has been writing for years.

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(1) For a prime p and a morphism $f : (X, M_X) \to (Y, M_Y)$ of fine saturated log schemes over $\mathbb{F}_p$, f is of Cartier type if and only if f is saturated (Proposition II.2.14, Theorem II.3.1). (This is an unpublished result of K. Kato.)

(2) Let $f : (X, M_X) \to (Y, M_Y)$ be an integral morphism of fine saturated log schemes and assume that we are given a chart $Q_Y \to M_Y$ with Q saturated. We regard (Y, M_Y) as a log scheme over $(S, M_S) = (\mathrm{Spec}(\mathbb{Z}[Q]), \text{can. log})$ by the chart. If X is quasi-compact, then there exists a positive integer n such that the base change $f' : (X', M_{X'}) \to (Y', M_{Y'})$ of f in the category of fine saturated log schemes by the morphism $(S, M_S) \to (S, M_S)$ induced by the multiplication by n on Q, is saturated (Theorem II.3.4).

(3) For a smooth integral morphism $f : (X, M_X) \to (Y, M_Y)$ of fine saturated log schemes, f is saturated if and only if every fiber of the underlying morphism of schemes of f is reduced (Theorem II.4.2).

This paper consists of two chapters. The first chapter is devoted to the study of saturated morphisms of monoids. In the second chapter, we deduce some results on saturated morphisms of log schemes from the results in the first chapter. We use freely the terminology introduced in [Kato 1989].

I. Saturated morphisms of monoids

I.1. ***Prime ideals of monoids.*** Throughout this paper, a monoid means a commutative monoid with a unit element, and its monoid law is written multiplicatively except for the set of natural numbers $\mathbb{N} = \{0, 1, 2, \ldots\}$, which is regarded as a monoid by its additive law. A homomorphism of monoids always preserves the unit elements. For a monoid P, P^{gp} denotes the group associated to P (cf. [Kato 1989, §1]), and P^* denotes the group of invertible elements of P.

Definition I.1.1 [Kato 1994, (5.1) Definition]. A subset I of a monoid P is called an *ideal* of P if $PI \subset I$. An ideal I of P is called a *prime ideal* if its complement $P \backslash I$ is a submonoid of P. We denote by $\mathrm{Spec}(P)$ the set of all prime ideals of P.

A morphism of monoids $h : P \to Q$ induces a map

$$\mathrm{Spec}(Q) \to \mathrm{Spec}(P), \quad \mathfrak{q} \mapsto h^{-1}(\mathfrak{q}).$$

For a submonoid S of a monoid P, we define the monoid $S^{-1}P$ by $S^{-1}P = \{s^{-1}a \mid a \in P, s \in S\}/\sim$, where $s_1^{-1}a_1 \sim s_2^{-1}a_2$ if and only if there exists $t \in S$ such that $ts_1a_2 = ts_2a_1$ [Kato 1994, (5.2) Definition]. If P is integral (see [Kato 1989, (2.2)]), the last condition is equivalent to $s_1a_2 = s_2a_1$ and $S^{-1}P$ is canonically isomorphic to the submonoid of P^{gp} consisting of elements of the forms $s^{-1}a$ $(s \in S, a \in P)$.

For a prime ideal $\mathfrak{p}$ of P, we define $P_{\mathfrak{p}}$ to be $(P\backslash\mathfrak{p})^{-1}P$. If P is generated by $a_1, \dots, a_n \in P$, then $P\backslash\mathfrak{p}$ is generated by a_i contained in $P\backslash\mathfrak{p}$, and therefore $P_{\mathfrak{p}}$ is generated by $1^{-1}a_1, \dots, 1^{-1}a_n$ and $a_i^{-1}1$ ($a_i \in P\backslash\mathfrak{p}$). The set $\mathrm{Spec}(P_{\mathfrak{p}})$ is identified with the subset $\{\mathfrak{q} \in \mathrm{Spec}(P) \mid \mathfrak{q} \subset \mathfrak{p}\}$ of $\mathrm{Spec}(P)$ by the map $\mathrm{Spec}(P_{\mathfrak{p}}) \to \mathrm{Spec}(P)$ induced by the morphism $P \to P_{\mathfrak{p}},\ a \mapsto 1^{-1}a$. For $\mathfrak{r}, \mathfrak{r}' \in \mathrm{Spec}(P_{\mathfrak{p}})$, and the corresponding prime ideals $\mathfrak{q}, \mathfrak{q}' \in \mathrm{Spec}(P)$, we have $\mathfrak{r} \subset \mathfrak{r}'$ if and only if $\mathfrak{q} \subset \mathfrak{q}'$.

Definition I.1.2. (1) [Kato 1994, (5.4) Definition]. For a monoid P, we define the *dimension* $\dim(P)$ of P to be the maximal length of a sequence of prime ideals $\mathfrak{p}_0 \supsetneq \mathfrak{p}_1 \supsetneq \cdots \supsetneq \mathfrak{p}_r$ of P. If the maximum does not exist, we define $\dim(P) = \infty$.

(2) For a prime ideal $\mathfrak{p}$ of a monoid P, we define the *height* $\mathrm{ht}(\mathfrak{p})$ of $\mathfrak{p}$ to be the maximal length of a sequence of prime ideals $\mathfrak{p} = \mathfrak{p}_0 \supsetneq \mathfrak{p}_1 \supsetneq \cdots \supsetneq \mathfrak{p}_r$ of P. If the maximum does not exist, we define $\mathrm{ht}(\mathfrak{p}) = \infty$.

By the above identification of $\mathrm{Spec}(P_{\mathfrak{p}})$ with a subset of $\mathrm{Spec}(P)$, we have $\mathrm{ht}(\mathfrak{p}) = \dim(P_{\mathfrak{p}})$.

Proposition I.1.3 [Kato 1994, (5.5) Proposition]. *Let P be a finitely generated integral monoid. Then*:

(1) $\mathrm{Spec}(P)$ *is a finite set.*

(2) $\dim(P) = \mathrm{rank}_{\mathbb{Z}}(P^{\mathrm{gp}}/P^*)$.

(3) *For* $\mathfrak{p} \in \mathrm{Spec}(P)$, $\mathrm{ht}(\mathfrak{p}) + \dim(P\backslash\mathfrak{p}) = \dim(P)$.

Proposition I.1.4. *Let $f : P \to Q$ be a morphism of monoids and assume that there exists a positive integer n such that, for any $b \in Q$, $b^n \in f(P)$ and, for any $a_1, a_2 \in P$, $f(a_1) = f(a_2)$ implies $a_1^n = a_2^n$. Then, the morphism* $\mathrm{Spec}(Q) \to \mathrm{Spec}(P)$, $\mathfrak{q} \mapsto f^{-1}(\mathfrak{q})$ *is bijective and, for* $\mathfrak{q}_1, \mathfrak{q}_2 \in \mathrm{Spec}(Q)$, $\mathfrak{q}_1 \subset \mathfrak{q}_2$ *if and only if* $f^{-1}(\mathfrak{q}_1) \subset f^{-1}(\mathfrak{q}_2)$. *Especially* $\dim(P) = \dim(Q)$ *and* $\mathrm{ht}(\mathfrak{q}) = \mathrm{ht}(f^{-1}(\mathfrak{q}))$ *for* $\mathfrak{q} \in \mathrm{Spec}(Q)$.

Proof. For an element $b \in Q$, there exists $a \in P$ such that $b^n = f(a)$ and a^n is independent of the choice of a. Hence, we can define a map g from Q to P by associating a^n to b. We see easily that the map g is a morphism of monoids and $g \circ f = n^2$ and $f \circ g = n^2$. Now the claim follows from the fact that the multiplication by n^2 on P and on Q induces the identity maps on $\mathrm{Spec}(P)$ and on $\mathrm{Spec}(Q)$. □

Let P be a finitely generated saturated monoid (see [Kato 1994, (1.1)]) and let $\mathfrak{p}$ be a prime ideal of P of height 1. Then, since $\dim(P_{\mathfrak{p}}) = \mathrm{ht}(\mathfrak{p}) = 1$, we have $\mathrm{rank}_{\mathbb{Z}}(P_{\mathfrak{p}}^{\mathrm{gp}}/P_{\mathfrak{p}}^*) = 1$. Since P is saturated by assumption, $P_{\mathfrak{p}}$ and $P_{\mathfrak{p}}/P_{\mathfrak{p}}^*$ are saturated. Hence $P_{\mathfrak{p}}/P_{\mathfrak{p}}^* \cong \mathbb{N}$. By taking the associated abelian groups and using

$P_{\mathfrak{p}}^{\mathrm{gp}} \cong P^{\mathrm{gp}}$, we get an isomorphism $P^{\mathrm{gp}}/P_{\mathfrak{p}}^{*} \cong \mathbb{Z}$. We define the valuation $v_{\mathfrak{p}}$ associated to $\mathfrak{p}$ to be the homomorphism $P^{\mathrm{gp}} \to P^{\mathrm{gp}}/P_{\mathfrak{p}}^{*} \cong \mathbb{Z}$.

Lemma I.1.5. *Let P be a finitely generated saturated monoid and let $\mathfrak{p}$ be a prime ideal of P of height* 1. *Then, we have*

$$P_{\mathfrak{p}} = \{x \in P^{\mathrm{gp}} \mid v_{\mathfrak{p}}(x) \geq 0\}.$$

Proof. By definition, it is trivial that $v_{\mathfrak{p}}(x) \geq 0$ for $x \in P_{\mathfrak{p}}$. Conversely, if $v_{\mathfrak{p}}(x) \geq 0$ for $x \in P^{\mathrm{gp}}$, then there exist $y \in P_{\mathfrak{p}}$ and $z \in P_{\mathfrak{p}}^{*}$ such that $x = yz$. Hence $x \in P_{\mathfrak{p}}$. □

Proposition I.1.6 [Kato 1994, (5.8) Proposition (1)]. *Let P be a finitely generated saturated monoid. Then, we have $P = \bigcap_{\mathfrak{p}} P_{\mathfrak{p}}$, where $\mathfrak{p}$ ranges over all prime ideals of P of height* 1.

Lemma I.1.7. *Let $f : P \to Q$ be a morphism of finitely generated saturated monoids. Let $\mathfrak{q}$ be a prime ideal of Q of height* 1 *such that the prime ideal $\mathfrak{p} = f^{-1}(\mathfrak{q})$ of P is of height* 1. *Then, there exists a positive integer n such that $v_{\mathfrak{q}} \circ f^{\mathrm{gp}} = n v_{\mathfrak{p}}$. We call the integer n the* ramification index *of f at $\mathfrak{q}$.*

Proof. Since $f(P \backslash \mathfrak{p}) \subset Q \backslash \mathfrak{q}$, the morphism f induces a morphism $P_{\mathfrak{p}} \to Q_{\mathfrak{q}}$ and hence a morphism $P_{\mathfrak{p}}/P_{\mathfrak{p}}^{*} \to Q_{\mathfrak{q}}/Q_{\mathfrak{q}}^{*}$. Furthermore, if $f^{\mathrm{gp}}(s^{-1}a) \in Q_{\mathfrak{q}}^{*}$ for $s \in P \backslash \mathfrak{p}$ and $a \in P$, then $f(a) \in Q_{\mathfrak{q}}^{*}$. This implies $f(a) \in Q \backslash \mathfrak{q}$, that is, $a \in P \backslash \mathfrak{p}$. Hence $s^{-1}a \in P_{\mathfrak{p}}^{*}$. Now we see the lemma easily. □

I.2. *Integral morphisms.*

Proposition I.2.1 [Kato 1989, Proposition (4.1)(1)]. *Let $f : P \to Q$ be a morphism of integral monoids. Then in the following conditions,* (i) *and* (iv) *are equivalent, and* (ii), (iii), *and* (v) *are equivalent.*

(i) *For any integral monoid P' and for any morphism $g : P \to P'$, the pushout of $Q \leftarrow P \to P'$ in the category of monoids is integral.*

(ii) *The homomorphism $\mathbb{Z}[P] \to \mathbb{Z}[Q]$ induced by f is flat.*

(iii) *For any field k, the homomorphism $k[P] \to k[Q]$ induced by f is flat.*

(iv) *If $a_1, a_2 \in P$, $b_1, b_2 \in Q$ and $f(a_1)b_1 = f(a_2)b_2$, there exist $a_3, a_4 \in P$ and $b \in Q$ such that $b_1 = f(a_3)b$ and $a_1a_3 = a_2a_4$ (which implies $b_2 = f(a_4)b$).*

(v) *The condition* (iv) *is satisfied and f is injective.*

Definition I.2.2. We say a morphism $f : P \to Q$ of integral monoids is *integral* if it satisfies the equivalent conditions (i) and (iv) in Proposition I.2.1.

Using the condition (i), we can easily verify the following.

Proposition I.2.3. (1) *Let $f : P \to Q$ and $g : Q \to R$ be morphisms of integral monoids. If f and g are integral, then $g \circ f$ is integral.*

(2) *Let $f : P \to Q$ and $g : P \to P'$ be morphisms of integral monoids and let Q' be the pushout of $Q \leftarrow P \to P'$ in the category of monoids. If f is integral, then the canonical morphism $P' \to Q'$ is integral.*

Lemma I.2.4. *Let P be a monoid and let G be a subgroup of P. If P is integral, then P/G is integral.*

Proof. Straightforward. □

Proposition I.2.5. *Let $f : P \to Q$ be a morphism of integral monoids and let G and H be subgroups of P and Q respectively such that $f(G) \subset H$. Let $g : P/G \to Q/H$ be the morphism induced by f. Then, f is integral if and only if g is integral.*

Proof. Note first that P/G, Q/H and $Q/f(G)$ are integral by Lemma I.2.4. If f is integral, then the base change $P/G \to Q/f(G)$ is also integral. The morphism $Q/f(G) \to Q/H \cong (Q/f(G))/(H/f(G))$ is always integral by Lemma I.2.4 and the condition (i) of Proposition I.2.1 for integral morphisms. Hence g is integral. Conversely, suppose g is integral. Since $P \to P/G$ is always integral by the same reason as above, the composite h of $P \xrightarrow{f} Q$ with $Q \to Q/H$ is integral. We will prove that f satisfies the condition (iv) of Proposition I.2.1. Let $a_1, a_2 \in P$, $b_1, b_2 \in Q$ such that $f(a_1)b_1 = f(a_2)b_2$. Since h is integral, there exist $a_3, a_4 \in P$, $b \in Q$, and $c \in H$ such that $b_1 = f(a_3)bc$ and $a_1a_3 = a_2a_4$. This completes the proof. □

Lemma I.2.6. *Let P be a monoid and let S be a submonoid of P. If P is integral, then $S^{-1}P$ is integral.*

Proof. Straightforward. □

Proposition I.2.7. *Let $f : P \to Q$ be a morphism of integral monoids and let S and T be submonoids of P and Q respectively such that $f(S) \subset T$. If f is integral, then the morphism $S^{-1}P \to T^{-1}Q$ induced by f is integral.*

Proof. Note first that $S^{-1}P$, $T^{-1}Q$ and $f(S)^{-1}Q$ are integral by Lemma I.2.6. If f is integral, the base change $S^{-1}P \to f(S)^{-1}Q$ is integral. The morphism $f(S)^{-1}Q \to T^{-1}(f(S)^{-1}Q) \cong T^{-1}Q$ is integral by Lemma I.2.6 and the condition (i) of Proposition I.2.1 for integral morphisms. Hence the morphism $S^{-1}P \to T^{-1}Q$ is integral. □

Proposition I.2.8. *Let $f : P \to Q$ be an integral morphism of integral monoids such that $f^{-1}(Q^*) = P^*$. Then f is exact* (see Definition I.3.1). *Furthermore, if $P^* = \{1\}$, f^{gp} is injective.*

Proof. Take $a_1, a_2 \in P$ such that $f^{\mathrm{gp}}((a_1)^{-1}a_2) \in Q$. Then there exists $b_1 \in Q$ such that $f(a_1)b_1 = f(a_2)$ in Q. By the condition (iv) of Proposition I.2.1 for integral morphisms, there exist $a_3, a_4 \in P$ and $b \in Q$ such that $b_1 = f(a_3)b$, $1 = f(a_4)b$ and $a_1a_3 = a_2a_4$. Since $f^{-1}(Q^*) = P^*$, $a_4 \in P^*$ and hence $(a_1)^{-1}a_2 = (a_4)^{-1}a_3 \in P$.

The exactness of f implies that $\mathrm{Ker}(f^{\mathrm{gp}}) \subset P^*$. Hence, if $P^* = \{1\}$, f^{gp} is injective. □

Corollary I.2.9. *Let $f : P \to Q$ be an integral morphism of finitely generated integral monoids. Let $\mathfrak{q}$ be a prime ideal of Q and let $\mathfrak{p}$ be the prime ideal $f^{-1}(\mathfrak{q})$ of P. Then* $\mathrm{ht}(\mathfrak{p}) \leq \mathrm{ht}(\mathfrak{q})$.

Proof. The morphism $g : P_{\mathfrak{p}}/P_{\mathfrak{p}}^* \to Q_{\mathfrak{q}}/Q_{\mathfrak{q}}^*$ induced by f is integral by Propositions I.2.5 and I.2.7. By Proposition I.2.8, g^{gp} is injective. Hence $\mathrm{ht}(\mathfrak{q}) = \dim(Q_{\mathfrak{q}}) = \mathrm{rank}_{\mathbb{Z}}(Q_{\mathfrak{q}}^{\mathrm{gp}}/Q_{\mathfrak{q}}^*) \geq \mathrm{rank}_{\mathbb{Z}}(P_{\mathfrak{p}}^{\mathrm{gp}}/P_{\mathfrak{p}}^*) = \dim(P_{\mathfrak{p}}) = \mathrm{ht}(\mathfrak{p})$. □

Proposition I.2.10. *Let $f : P \to Q$ and $g : Q \to R$ be morphisms of integral monoids. If $g \circ f$ is integral and g is exact, then f is integral.*

Proof. We will prove that f satisfies the condition (iv) of Proposition I.2.1. Take $a_1, a_2 \in P$ and $b_1, b_2 \in Q$ such that $f(a_1)b_1 = f(a_2)b_2$. Then $(g \circ f)(a_1)g(b_1) = (g \circ f)(a_2)g(b_2)$ and, since $g \circ f$ is integral, there exist $a_3, a_4 \in P$ and $c \in R$ such that $g(b_1) = (g \circ f)(a_3)c$ and $a_1a_3 = a_2a_4$. Since g is exact, $b = b_1 f(a_3)^{-1}$ is contained in Q. This completes the proof. □

Proposition I.2.11. *Let $f : P \to Q$ be a morphism of finitely generated integral monoids. Then the following two conditions are equivalent*:

(i) *f is integral and $f^{-1}(Q^*) = P^*$.*

(ii) *f is exact and, for any $b \in Q$, there exists $b' \in Q$ such that*

$$f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q = f(P)b'.$$

Lemma I.2.12. *Let $f : P \to Q$ be an exact morphism of finitely generated integral monoids. Let $b \in Q$ and define a subset I of P^{gp} to be $\{a \in P^{\mathrm{gp}} \mid f^{\mathrm{gp}}(a)b \in Q\}$. Then, there exists $c \in P$ such that $cI \subset P$.*

Proof. First we will prove the lemma assuming P and Q are saturated. For a prime ideal $\mathfrak{q}$ of Q of height 1, we define $c_{\mathfrak{q}} \in P$ as follows. If $v_{\mathfrak{q}}(f(P)) = 0$, we define $c_{\mathfrak{q}} = 1$. If $v_{\mathfrak{q}}(f(P)) \neq 0$, we define $c_{\mathfrak{q}}$ to be an element of P such that $v_{\mathfrak{q}}(f(c_{\mathfrak{q}})) \geq v_{\mathfrak{q}}(b)$. Set $c = \prod_{\mathfrak{q}} c_{\mathfrak{q}}$, where $\mathfrak{q}$ ranges over all prime ideals of Q of height 1. We assert $cI \subset P$. Since f is exact, it suffices to prove $f^{\mathrm{gp}}(cI) \subset Q$. Let $a \in P^{\mathrm{gp}}$ such that $f^{\mathrm{gp}}(a)b \in Q$. Let $\mathfrak{q}$ be a prime ideal of Q of height 1. By Lemma I.1.5 and Proposition I.1.6, it is enough to prove $v_{\mathfrak{q}}(f^{\mathrm{gp}}(ac)) \geq 0$. If $v_{\mathfrak{q}}(f(P)) = 0$, then $v_{\mathfrak{q}}(f^{\mathrm{gp}}(P^{\mathrm{gp}})) = 0$ and hence $v_{\mathfrak{q}}(f^{\mathrm{gp}}(ac)) = 0$. If $v_{\mathfrak{q}}(f(P)) \neq 0$, then

$$\begin{aligned} v_{\mathfrak{q}}(f^{\mathrm{gp}}(ac)) = v_{\mathfrak{q}}(f^{\mathrm{gp}}(a)) + v_{\mathfrak{q}}(f(c)) &\geq v_{\mathfrak{q}}(f^{\mathrm{gp}}(a)) + v_{\mathfrak{q}}(f(c_{\mathfrak{q}})) \\ &\geq v_{\mathfrak{q}}(f^{\mathrm{gp}}(a)) + v_{\mathfrak{q}}(b) = v_{\mathfrak{q}}(f^{\mathrm{gp}}(a)b) \geq 0. \end{aligned}$$

Next we will reduce the general case to the case where P and Q are saturated. Let P^{sat} and Q^{sat} be the saturated monoids associated to P and Q (see

Definition II.2.2), which are finitely generated by Proposition II.2.4, and let $f^{\mathrm{sat}}: P^{\mathrm{sat}} \to Q^{\mathrm{sat}}$ be the morphism induced by f. Then the morphism f^{sat} is exact. Define a subset J of $(P^{\mathrm{sat}})^{\mathrm{gp}} = P^{\mathrm{gp}}$ to be $\{a \in (P^{\mathrm{sat}})^{\mathrm{gp}} \mid f^{\mathrm{gp}}(a)b \in Q^{\mathrm{sat}}\}$. Then we have proven that there exists $c \in P^{\mathrm{sat}}$ such that $cJ \subset P^{\mathrm{sat}}$. By multiplying c by some element of P, we may assume $c \in P$. Let $a_1, \dots, a_r \in P^{\mathrm{sat}}$ be a system of generators and choose a positive integer n such that $a_i^n \in P$ for all $1 \le i \le r$. Then

$$P^{\mathrm{sat}} = \bigcup_{0 \le n_i \le n-1} P \cdot \prod_{1 \le i \le r} a_i^{n_i}.$$

Choose $d \in P$ such that $da_i \in P$ for all $1 \le i \le r$. Then $d^{r(n-1)} P^{\mathrm{sat}} \subset P$. Hence $d^{r(n-1)} cI \subset d^{r(n-1)} cJ \subset d^{r(n-1)} P^{\mathrm{sat}} \subset P$. □

Proof of Proposition I.2.11. (i) ⇒ (ii). By Proposition I.2.8, f is exact. Let I be the set $\{a \in P^{\mathrm{gp}} \mid f^{\mathrm{gp}}(a)b \in Q\}$. We have $PI \subset I$. By Lemma I.2.12, there exists $c \in P$ such that $cI \subset P$. By [Kato 1994, (5.6) Lemma], there exist $a_1, \dots, a_r \in I$ such that $I = \bigcup_{1 \le i \le r} Pa_i$. Set $b_i = f^{\mathrm{gp}}(a_i)b \in f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q$. Then $f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q = f^{\mathrm{gp}}(I)b = \bigcup_{1 \le i \le r} f(P)b_i$. If $r = 1$, we are done. Suppose $r \ge 2$. Since $b_1 b_2^{-1} \in f^{\mathrm{gp}}(P^{\mathrm{gp}})$ and $b_1, b_2 \in Q$, by the condition (iv) of Proposition I.2.1 for integral morphisms, there exist $d_1, d_2 \in P$, $b_1' \in Q$ such that $b_1 = f(d_1)b_1'$ and $b_2 = f(d_2)b_1'$. Then $b_1' \in f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q$ and we have

$$f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q \supset f(P)b_1' \cup \Big(\bigcup_{3 \le i \le r} f(P)b_i\Big) \supset \bigcup_{1 \le i \le r} f(P)b_i = f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q.$$

Hence $f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q = f(P)b_1' \cup \big(\bigcup_{3 \le i \le r} f(P)b_i\big)$. Repeating this procedure, we are reduced to the case $r = 1$.

(ii) ⇒ (i). It is trivial that the exactness of f implies $f^{-1}(Q^*) = P^*$. We will prove that f satisfies the condition (iv) of Proposition I.2.1. Take $a_1, a_2 \in P$ and $b_1, b_2 \in Q$ such that $f(a_1)b_1 = f(a_2)b_2$. Then, by assumption, there exists $b \in Q$ such that $f^{\mathrm{gp}}(P^{\mathrm{gp}})b_1 \cap Q = f^{\mathrm{gp}}(P^{\mathrm{gp}})b_2 \cap Q = f(P)b$. Choose $a_3, a_4 \in P$ such that $b_1 = f(a_3)b$ and $b_2 = f(a_4)b$. Then, by $f(a_1)b_1 = f(a_2)b_2$, we have $f(a_1a_3) = f(a_2a_4)$. The element $a := (a_1a_3)^{-1}a_2a_4$ belongs to $\mathrm{Ker}(f^{\mathrm{gp}})$, which is contained in P since f is exact. By replacing a_3 by aa_3, we obtain the desired elements $a_1, a_3 \in P$ and $b \in Q$. □

I.3. *p-saturated monoids and p-saturated morphisms.*

Definition I.3.1 [Kato 1989, Definition (4.6)(1)]. We say a morphism of integral monoids $f: P \to Q$ is *exact* if $(f^{\mathrm{gp}})^{-1}(Q) = P$.

Proposition I.3.2. (1) *Let $f: P \to Q$ and $g: Q \to R$ be morphisms of integral monoids. If f and g are exact, then $g \circ f$ is exact. If $g \circ f$ is exact, then f is exact.*

(2) *Let $f: P \to Q$ and $g: P \to P'$ be morphisms of integral monoids and define a morphism of integral monoids $f': P' \to Q'$ by the following cocartesian*

diagram in the category of integral monoids.

$$\begin{array}{ccc} Q' & \xleftarrow{h} & Q \\ {\scriptstyle f'}\uparrow & & \uparrow{\scriptstyle f} \\ P' & \xleftarrow{g} & P \end{array}$$

If f is exact, then f' is exact.

Proof. The claim (1) is trivial. We prove (2). Let a be an element of $(P')^{\mathrm{gp}}$ such that $(f')^{\mathrm{gp}}(a) \in Q'$. Since the diagram of abelian groups

$$\begin{array}{ccc} (Q')^{\mathrm{gp}} & \xleftarrow{h^{\mathrm{gp}}} & Q^{\mathrm{gp}} \\ {\scriptstyle (f')^{\mathrm{gp}}}\uparrow & & \uparrow{\scriptstyle f^{\mathrm{gp}}} \\ (P')^{\mathrm{gp}} & \xleftarrow{g^{\mathrm{gp}}} & P^{\mathrm{gp}} \end{array}$$

is cocartesian and $Q' = (f')^{\mathrm{gp}}(P')h^{\mathrm{gp}}(Q)$ in $(Q')^{\mathrm{gp}}$, there exist $b \in P'$, $c \in Q$ and $d \in P^{\mathrm{gp}}$ such that $a = b \cdot g^{\mathrm{gp}}(d)$ and $c = f^{\mathrm{gp}}(d)$. Since f is exact by assumption, $d \in P$ and hence $a \in P'$. □

Definition I.3.3. Let p be a prime. We say an integral monoid P is *p-saturated* if the multiplication by p on P is exact (or equivalently, for any $a \in P^{\mathrm{gp}}$, $a^p \in P$ implies $a \in P$).

It is easy to see that an integral monoid P is saturated if and only if P is p-saturated for every prime p.

Example I.3.4. Let n be a positive integer and let P be the submonoid $(\mathbb{N} \times \mathbb{N}_{>0}) \cup n\mathbb{N} \times \{0\}$ of $\mathbb{N} \oplus \mathbb{N}$, which is generated by $(n, 0)$ and $(m, 1)$ $(m \in \mathbb{N}, 0 \leq m \leq n-1)$. Then, for a prime p, P is p-saturated if and only if $p \nmid n$.

Definition I.3.5. Let p be a prime and let $f : P \to Q$ be a morphism of integral monoids. Define Q', f' and g by the following cocartesian diagram in the category of integral monoids:

$$\begin{array}{ccc} Q' & \xleftarrow{g} & Q \\ {\scriptstyle f'}\uparrow & & \uparrow{\scriptstyle f} \\ P & \xleftarrow{p} & P \end{array}$$

Let h be the unique morphism $Q' \to Q$ such that $h \circ g = p$ and $h \circ f' = f$. We say the morphism f is *p-quasi-saturated* if h is exact.

Proposition I.3.6. *Let p be a prime.*

(1) *Let $f : P \to Q$ and $g : Q \to R$ be morphisms of integral monoids. If f and g are p-quasi-saturated, then $g \circ f$ is p-quasi-saturated.*

(2) *Let $f : P \to Q$ and $g : P \to R$ be morphisms of integral monoids and define a morphism of integral monoids $h : R \to S$ by the following cocartesian diagram in the category of integral monoids*:

$$\begin{array}{ccc} S & \xleftarrow{\;i\;} & Q \\ {\scriptstyle h}\uparrow & & \uparrow{\scriptstyle f} \\ R & \xleftarrow{\;g\;} & P \end{array}$$

If f is p-quasi-saturated, then h is p-quasi-saturated.

Proof. (1) We have the following commutative diagram of integral monoids in which the composite of each line is the multiplication by p, $j \circ g' = g$, $h \circ f' = f$ and each square is cocartesian in the category of integral monoids:

$$\begin{array}{ccccccc} R & \xleftarrow{\;j\;} & R' & \xleftarrow{\;i\;} & R'' & \longleftarrow & R \\ & & {\scriptstyle g'}\uparrow & & \uparrow & & \uparrow{\scriptstyle g} \\ & & Q & \xleftarrow{\;h\;} & Q' & \longleftarrow & Q \\ & & & & {\scriptstyle f'}\uparrow & & \uparrow{\scriptstyle f} \\ & & & & P & \xleftarrow{\;p\;} & P \end{array}$$

If f and g are p-quasi-saturated, h and j are exact. By Proposition I.3.2 (2), i is exact. Hence $j \circ i$ is exact and $g \circ f$ is p-quasi-saturated.

(2) Define morphisms $f' : P \to Q'$ and $j : Q' \to Q$ (resp. $h' : R \to S'$ and $k : S' \to S$) using $f : P \to Q$ (resp. $h : R \to S$) as in Definition I.3.5. Let $i' : Q' \to S'$ be the morphism induced by $g : P \to R$ and $i : Q \to S$. Then, we have a commutative diagram

$$\begin{array}{ccc} S & \xleftarrow{\;i\;} & Q \\ {\scriptstyle k}\uparrow & & \uparrow{\scriptstyle j} \\ S' & \xleftarrow{\;i'\;} & Q' \\ {\scriptstyle h'}\uparrow & & \uparrow{\scriptstyle f'} \\ R & \xleftarrow{\;g\;} & P. \end{array}$$

The outer big square and the lower square are cocartesian in the category of integral monoids. (For the first one, note $k \circ h' = h$ and $j \circ f' = f$.) Hence the upper square is also cocartesian. Therefore, by Proposition I.3.2 (2), if j is exact, then k is exact. $\square$

Definition I.3.7. We say a morphism of integral monoids $f : P \to Q$ is *quasi-saturated* if it is p-quasi-saturated for every prime p.

Proposition I.3.8. *Let n be an integer ≥ 2. Let $f : P \to Q$ be a quasi-saturated morphism of integral monoids and define an integral monoid Q' by the cocartesian diagram in the category of integral monoids*

$$\begin{array}{ccc} Q' & \xleftarrow{g} & Q \\ {\scriptstyle f'}\uparrow & & \uparrow{\scriptstyle f} \\ P & \xleftarrow{n} & P. \end{array}$$

Let h be the unique morphism $Q' \to Q$ such that $h \circ g = n$ and $h \circ f' = f$. Then h is exact.

Proof. It suffices to prove that, if the proposition is true for integers $n_1 \geq 2$ and $n_2 \geq 2$, then it is true also for $n_3 = n_1 n_2$. Consider the following cocartesian diagrams in the category of integral monoids:

$$\begin{array}{ccccc} Q_2 & \xleftarrow{g_2} & Q_1 & \xleftarrow{g_1} & Q \\ {\scriptstyle f_2}\uparrow & & {\scriptstyle f_1}\uparrow & & \uparrow{\scriptstyle f} \\ P & \xleftarrow{n_2} & P & \xleftarrow{n_1} & P \end{array}$$

Let $h_1 : Q_1 \to Q$ (resp. $h_2 : Q_2 \to Q_1$) be the unique morphism such that $h_1 \circ f_1 = f$ and $h_1 \circ g_1 = n_1$ (resp. $h_2 \circ f_2 = f_1$ and $h_2 \circ g_2 = n_2$). Then $h_3 := h_1 \circ h_2 : Q_2 \to Q$ is the unique morphism such that $h_3 \circ f_2 = f$ and $h_3 \circ g_2 \circ g_1 = n_1 n_2$. Since f is quasi-saturated, h_1 is exact by assumption. Since f_1 is quasi-saturated by Proposition I.3.6 (2), h_2 is also exact by assumption. Hence h_3 is exact. □

Proposition I.3.9. *Let p be a prime and let $f : P \to Q$ be a morphism of integral monoids. If P is p-saturated* (*resp. saturated*) *and f is p-quasi-saturated* (*resp. quasi-saturated*), *then Q is p-saturated* (*resp. saturated*).

Proof. Define an integral monoid Q' and morphisms of monoids $f' : P \to Q'$, $g : Q \to Q'$ and $h : Q' \to Q$ as in Definition I.3.5 using p and $f : P \to Q$. If P is p-saturated, g is exact by Proposition I.3.2 (2). If f is p-quasi-saturated, h is exact. Hence $h \circ g = p : Q \to Q$ is exact, that is, Q is p-saturated. By considering all p, we obtain the claim in the case when P is saturated. □

Proposition I.3.10. *Let p be a prime and let $f : P \to Q$ be a morphism of p-saturated monoids. Then, the following three conditions are equivalent*:

(1) *The morphism f is p-quasi-saturated.*

(2) *For any p-saturated monoid P' and any morphism $g : P \to P'$, the pushout of the diagram $Q \xleftarrow{f} P \xrightarrow{g} P'$ in the category of integral monoids, is p-saturated.*

(3) *The pushout of the diagram $Q \xleftarrow{f} P \xrightarrow{p} P$ in the category of integral monoids, is p-saturated.*

Proof. The implication (1) ⇒ (2) follows from Propositions I.3.6 (2) and I.3.9 and (2) ⇒ (3) is trivial. We prove (3) ⇒ (1). Define an integral monoid Q' and a morphism of integral monoids $g : Q \to Q'$ and $h : Q' \to Q$ as in Definition I.3.5. Then, we see that $g \circ h : Q' \to Q'$ is the multiplication by p and hence it is exact by assumption. By Proposition I.3.2 (1), h is exact. □

Corollary I.3.11. *Let $f : P \to Q$ be a morphism of saturated monoids. Then, the following three conditions are equivalent*:

(1) *The morphism f is quasi-saturated.*

(2) *For any saturated monoid P' and any morphism $g : P \to P'$, the pushout of the diagram $Q \xleftarrow{f} P \xrightarrow{g} P'$ in the category of integral monoids, is saturated.*

(3) *For every prime p, the pushout of the diagram $Q \xleftarrow{f} P \xrightarrow{p} P$ in the category of integral monoids, is saturated.*

Definition I.3.12. Let p be a prime. We say a morphism of integral monoids $f : P \to Q$ is *p-saturated* (resp. *saturated*) if f is integral and p-quasi-saturated (resp. quasi-saturated).

Proposition I.3.13. *Let p be a prime and let $f : P \to Q$ be an integral morphism of p-saturated monoids. Then, the following three conditions are equivalent*:

(1) *The morphism f is p-saturated.*

(2) *For any p-saturated monoid P' and any morphism $g : P \to P'$, the pushout of the diagram $Q \xleftarrow{f} P \xrightarrow{g} P'$ in the category of monoids, is p-saturated.*

(3) *The pushout of the diagram $Q \xleftarrow{f} P \xrightarrow{p} P$ in the category of monoids, is p-saturated.*

Proposition I.3.14. *Let $f : P \to Q$ be an integral morphism of saturated monoids. Then, the following three conditions are equivalent*:

(1) *The morphism f is saturated.*

(2) *For any saturated monoid P' and any morphism $g : P \to P'$, the pushout of the diagram $Q \xleftarrow{f} P \xrightarrow{g} P'$ in the category of monoids, is saturated.*

(3) *For every prime p, the pushout of the diagram $Q \xleftarrow{f} P \xrightarrow{p} P$ in the category of monoids, is saturated.*

Lemma I.3.15. *Let P be an integral monoid and let G be a subgroup of P.*

(1) *The monoid P is saturated if and only if P/G is saturated.*

(2) *The morphism $P \to P/G$ is saturated.*

Proof. (1) Straightforward.

(2) The morphism $P \to P/G$ is integral by Proposition I.2.5. For any prime p, the base change of $P \to P/G$ by $p : P \to P$ in the category of monoids is given by the quotient $P \to P/G^p$. Hence $P \to P/G$ is p-quasi-saturated because the projection map $P/G^p \to P/G$ is exact. □

Proposition I.3.16. *Let $f : P \to Q$ be a morphism of integral monoids and let G and H be subgroups of P and Q respectively such that $f(G) \subset H$. Let $g : P/G \to Q/H$ be the morphism induced by f. Let p be a prime. Then f is p-saturated if and only if g is p-saturated. In particular, f is saturated if and only if g is saturated.*

Proof. By Proposition I.2.5, we may assume that f and g are integral. If f is p-saturated, the base change $P/G \to Q/f(G)$ of f by $P \to P/G$ in the category of monoids is p-saturated by Propositions I.2.3 (2) and I.3.6 (2). The morphism $Q/f(G) \to (Q/f(G))/(H/f(G)) \cong Q/H$ is p-saturated by Lemma I.3.15 (2). Hence $P/G \to Q/H$ is p-saturated by Propositions I.2.3 (1) and I.3.6 (1). Conversely, suppose that $P/G \to Q/H$ is p-saturated. Since $P \to P/G$ is p-saturated, $P \to Q/H$ is p-saturated. Put $\bar{Q} := Q/H$. Define a monoid Q' (resp. $\bar{Q}'$) and morphisms of monoids $k : Q \to Q'$ and $h : Q' \to Q$ (resp. $\bar{k} : \bar{Q} \to \bar{Q}'$ and $\bar{h} : \bar{Q}' \to \bar{Q}$) as in Definition I.3.5 using p and $f : P \to Q$ (resp. $P \xrightarrow{f} Q \to \bar{Q}$). Then the natural map $Q' \to \bar{Q}'$ is the quotient by $k(H)$. Therefore the morphisms $Q' \to \bar{Q}'$ and $Q \to \bar{Q}$ are exact. Since $\bar{h}$ is exact, we see that h is also exact by using Proposition I.3.2 (1). □

Lemma I.3.17. *Let P be an integral monoid and let S be a submonoid of P.*

(1) *If P is saturated, then $S^{-1}P$ is saturated.*

(2) *The morphism $P \to S^{-1}P$ is saturated.*

Proof. (1) Straightforward.

(2) The morphism $P \to S^{-1}P$ is integral by Proposition I.2.7. For a prime p, the following diagram is cocartesian in the category of monoids:

$$\begin{array}{ccc} S^{-1}P & \xleftarrow{\;p\;} & S^{-1}P \\ \uparrow & & \uparrow \\ P & \xleftarrow{\;p\;} & P \end{array}$$

Hence $P \to S^{-1}P$ is p-quasi-saturated. □

Proposition I.3.18. *Let $f : P \to Q$ be a morphism of integral monoids and let S and T be submonoids of P and Q respectively such that $f(S) \subset T$. Let p be a prime. If f is p-saturated* (*resp. saturated*), *then the morphism $S^{-1}P \to T^{-1}Q$ induced by f is p-saturated* (*resp. saturated*).

Proof. If f is p-saturated, then the base change $S^{-1}P \to f(S)^{-1}Q$ of f by $P \to S^{-1}P$ in the category of monoids is p-saturated by Propositions I.2.3 (2) and I.3.6 (2). The morphism $f(S)^{-1}Q \to T^{-1}(f(S)^{-1}Q) \cong T^{-1}Q$ is p-saturated by Lemma I.3.17 (2). Hence, the morphism $S^{-1}P \to T^{-1}Q$ is p-saturated by Propositions I.2.3 (1) and I.3.6 (1). □

Remark I.3.19. For an integral monoid P and a submonoid S of P, the natural morphism $P \to S^{-1}P$ induces an isomorphism $P/S \xrightarrow{\cong} S^{-1}P/S^{\mathrm{gp}}$. Therefore, Propositions I.2.5, I.2.7, I.3.16, and I.3.18 immediately imply the following claim: Let $f : P \to Q$ be a morphism of integral monoids, and let S and T be submonoids of P and Q respectively such that $f(S) \subset T$. Let p be a prime. If f is integral (resp. p-saturated, resp. saturated), then so is the morphism $P/S \to Q/T$ induced by f.

I.4. ***A criterion of p-saturated morphisms.*** In this section, we give a criterion for an integral morphism of finitely generated integral monoids to be p-saturated (Theorem I.4.2). As corollaries, we prove that, under certain conditions, p-saturated morphisms are always saturated (Corollaries I.4.5 and I.4.7).

Proposition I.4.1. *Let p be a prime and let $f : P \to Q$ be a morphism of integral monoids. We consider the following condition on f.*

- (∗) *For any $a \in P$ and $b \in Q$ such that $f(a) \mid b^p$, there exists $c \in P$ such that $a \mid c^p$ and $f(c) \mid b$.*
- (1) *If P is p-saturated and f is p-quasi-saturated, then f satisfies* (∗).
- (2) *If Q is p-saturated and f satisfies* (∗), *then f is p-quasi-saturated.*

In particular, *if P and Q are p-saturated*, *f is p-quasi-saturated if and only if f satisfies* (∗).

Proof. Consider the following cocartesian diagram in the category of integral monoids:

$$\begin{array}{ccc} Q' & \xleftarrow{\;g\;} & Q \\ {\scriptstyle f'}\uparrow & & \uparrow{\scriptstyle f} \\ P & \xleftarrow{\;p\;} & P \end{array}$$

Let $h : Q' \to Q$ be the unique morphism such that $h \circ g = p$ and $h \circ f' = f$. Then $(Q')^{\mathrm{gp}}$ is canonically identified with

$$(P^{\mathrm{gp}} \oplus Q^{\mathrm{gp}})/\{(a^p, f^{\mathrm{gp}}(a)^{-1}) \mid a \in P^{\mathrm{gp}}\}$$

and Q' corresponds to the image of $P \oplus Q$. For $(a, b) \in P^{\mathrm{gp}} \oplus Q^{\mathrm{gp}}$, we denote by $\overline{(a, b)}$ its image in $(Q')^{\mathrm{gp}}$. We have $h^{\mathrm{gp}}(\overline{(a, b)}) = f^{\mathrm{gp}}(a)b^p$.

(1) Suppose that P is p-saturated and that f is p-quasi-saturated, that is, h is exact. Let $a \in P$ and $b \in Q$ such that $f(a) \mid b^p$. Then $h^{\mathrm{gp}}(\overline{(a^{-1}, b)}) = f(a)^{-1}b^p \in Q$. Hence $\overline{(a^{-1}, b)} \in Q'$, that is, there exists $c \in P^{\mathrm{gp}}$ such that $a^{-1}c^p \in P$ and $bf^{\mathrm{gp}}(c)^{-1} \in Q$. Since P is p-saturated, $a^{-1}c^p \in P$ implies $c \in P$. Now we have $a \mid c^p$ and $f(c) \mid b$.

(2) Suppose that Q is p-saturated and that f satisfies $(*)$. Let $a \in P^{\mathrm{gp}}$ and $b \in Q^{\mathrm{gp}}$ be elements satisfying $h^{\mathrm{gp}}(\overline{(a, b)}) = f^{\mathrm{gp}}(a)b^p \in Q$. If a is of the form $a_2a_1^{-1}$ $(a_1, a_2 \in P)$, then $\overline{(a, b)} = \overline{((a_1a_2^{p-1})^{-1}, bf(a_2))}$. Hence we may assume that a is of the form a_2^{-1} $(a_2 \in P)$. Then, since Q is p-saturated, $f^{\mathrm{gp}}(a)b^p \in Q$ implies $b \in Q$ and $f(a_2) \mid b^p$. Hence, by $(*)$, there exists $c \in P$ such that $a_2 \mid c^p$ and $f(c) \mid b$, which implies $\overline{(a, b)} = \overline{((a_2)^{-1}c^p, f(c)^{-1}b)} \in Q'$. □

Theorem I.4.2. *Let p be a prime. Let $f : P \to Q$ be an integral morphism of finitely generated integral monoids such that $f^{-1}(Q^*) = P^*$. Then f is p-saturated if and only if f satisfies the following two conditions*:

(i) *For $b \in Q^{\mathrm{gp}}$, if there exists $a \in P$ such that $f(a)b^p \in Q$, then there exists $a' \in P$ such that $f(a')b \in Q$.*

(ii) *For $b \in Q$, if there exists $a \in P \backslash P^*$ such that $f(a) \mid b^p$, then there exists $a' \in P \backslash P^*$ such that $f(a') \mid b$.*

Lemma I.4.3. *Let $f : P \to Q$ be an integral morphism of finitely generated integral monoids such that $f^{-1}(Q^*) = P^*$. Then, for any $b \in Q$ and $b' \in f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q$, $f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q = f(P)b'$ if and only if $f(a) \nmid b'$ for all $a \in P \backslash P^*$.*

Proof. By Proposition I.2.11, there exists $b'' \in Q$ such that $f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q = f(P)b''$. Take $c \in P$ such that $b' = f(c)b''$. If $f(a) \nmid b'$ for all $a \in P \backslash P^*$, then $c \in P^*$ and hence $f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q = f(P)b'$. Conversely, assume $f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q = f(P)b'$. Then, for any $a \in P$ such that $f(a) \mid b'$, there exists $a' \in P$ such that $f(a)^{-1}b' = f(a')b'$ because $f(a)^{-1}b' \in f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q = f(P)b'$. Hence $f(a) \in Q^*$ and $a \in P^*$. □

Proof of Theorem I.4.2. We use the same notation as in the first paragraph of the proof of Proposition I.4.1.

First assume that f is p-saturated, that is, the morphism $h : Q' \to Q$ is exact. Take $b \in Q^{\mathrm{gp}}$ and $a \in P$ such that $f(a)b^p \in Q$. Then $h^{\mathrm{gp}}(\overline{(a, b)}) = f(a)b^p \in Q$. Since h is exact, $\overline{(a, b)} \in Q'$, that is, there exists $c \in P^{\mathrm{gp}}$ such that $ac^{-p} \in P$ and $bf^{\mathrm{gp}}(c) \in Q$. Hence f satisfies the condition (i). Take $b \in Q$ such that $f(a) \nmid b$ for all $a \in P \backslash P^*$. To prove that f satisfies the condition (ii), it suffices to prove that $f(a) \nmid b^p$ for all $a \in P \backslash P^*$. By Lemma I.4.3, $f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q = f(P)b$ and it is enough to prove $f^{\mathrm{gp}}(P^{\mathrm{gp}})b^p \cap Q = f(P)b^p$. Let $a \in P^{\mathrm{gp}}$ and suppose $f^{\mathrm{gp}}(a)b^p \in Q$.

Then $h^{\mathrm{gp}}(\overline{(a,b)}) = f^{\mathrm{gp}}(a)b^p \in Q$. Since h is exact, $\overline{(a,b)} \in Q'$, that is, there exists $c \in P^{\mathrm{gp}}$ such that $ac^{-p} \in P$ and $bf^{\mathrm{gp}}(c) \in Q$. By $f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q = f(P)b$, there exists $d \in P$ such that $f^{\mathrm{gp}}(c)b = f(d)b$, i.e., $f^{\mathrm{gp}}(c) = f(d)\,(\in Q)$. Since f is exact by Proposition I.2.8, $c \in P$ and hence $a \in c^pP \subset P$.

Next assume that f satisfies the conditions (i) and (ii). It suffices to prove that h is exact. Let $a \in P^{\mathrm{gp}}$, $b \in Q^{\mathrm{gp}}$ and suppose $h^{\mathrm{gp}}(\overline{(a,b)}) = f^{\mathrm{gp}}(a)b^p \in Q$. We will prove $\overline{(a,b)} \in Q'$. By the condition (i), there exists $c \in P$ such that $f(c)b \in Q$, and we have $\overline{(a,b)} = \overline{(ac^{-p}, f(c)b)}$. Hence we may assume $b \in Q$. By Proposition I.2.11, there exists $b' \in Q$ such that $f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q = f(P)b'$. Take $c \in P$ such that $b = f(c)b'$. Since $\overline{(a,b)} = \overline{(ac^p, b')}$, it is enough to prove $ac^p \in P$. By the condition (ii) and Lemma I.4.3, $f^{\mathrm{gp}}(P^{\mathrm{gp}})(b')^p \cap Q = f(P)(b')^p$. Since $f^{\mathrm{gp}}(ac^p)(b')^p = f^{\mathrm{gp}}(a)b^p \in Q$, we obtain $f^{\mathrm{gp}}(ac^p) \in f(P) \subset Q$. Since f is exact by Proposition I.2.8, $ac^p \in P$. □

Remark I.4.4. Let $f : P \to Q$ be an integral morphism of finitely generated integral monoids such that $f^{-1}(Q^*) = P^*$. Then, using Lemma I.4.3, we see easily that the condition (i) (resp. (ii)) in Theorem I.4.2 is equivalent to the condition (i′) (resp. (ii′)) below:

(i′) The image of Q in $Q^{\mathrm{gp}}/f^{\mathrm{gp}}(P^{\mathrm{gp}})$ is p-saturated.

(ii′) For $b \in Q$, if $f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q = f(P)b$, then $f^{\mathrm{gp}}(P^{\mathrm{gp}})b^p \cap Q = f(P)b^p$.

Corollary I.4.5. *Let p and q be two different primes and let $f : P \to Q$ be a morphism of finitely generated integral monoids. If Q is q-saturated and f is p-saturated, then f is q-saturated.* (*Thus, if Q is saturated and f is p-saturated, then f is saturated.*)

Proof. Let S be the submonoid $f^{-1}(Q^*)$ of P, which is the complement of the prime ideal $f^{-1}(Q \backslash Q^*)$ of P. Then the morphism f uniquely factors as $P \xrightarrow{g} S^{-1}P \xrightarrow{h} Q$. The monoid $S^{-1}P$ is finitely generated and integral. The morphism g is q-saturated by Lemma I.3.17 (2). Since $h : S^{-1}P \to Q$ is the base change of $f : P \to Q$ by $g : P \to S^{-1}P$, h is p-saturated. Thus, we are reduced to the case $f^{-1}(Q^*) = P^*$. By Theorem I.4.2, it suffices to prove that f satisfies the conditions (i) and (ii) in Theorem I.4.2 for the prime q. The condition (i) follows from the fact that Q is q-saturated. Indeed, if $f(a)b^q \in Q$ for $a \in P$ and $b \in Q^{\mathrm{gp}}$, then $(f(a)b)^q \in Q$ and hence $f(a)b \in Q$. Let $b \in Q$ and suppose that there exists $a \in P \backslash P^*$ such that $f(a) \mid b^q$. Choose a positive integer m such that $q \le p^m$. Then, $f(a) \mid b^{p^m}$ and, by Theorem I.4.2, there exists $a' \in P \backslash P^*$ such that $f(a') \mid b$. □

Definition I.4.6. Let $f : P \to Q$ be a morphism of monoids. We say the morphism f is *vertical* if, for any $b \in Q$, there exists $a \in P$ such that $b \mid f(a)$, that is, $f(a) \in bQ$.

Corollary I.4.7. *Let p be a prime and let $f : P \to Q$ be a morphism of finitely generated integral monoids. If f is vertical and p-saturated, then f is saturated.*

Proof. Let q be any prime different from p. We prove that f is q-saturated. By the same argument as in the proof of Corollary I.4.5, we may assume $f^{-1}(Q^*) = P^*$. Then, it suffices to prove that f satisfies the conditions (i) and (ii) in Theorem I.4.2 for the prime q. The assumption that f is vertical implies that, for any $b \in Q^{\mathrm{gp}}$, there exists $a \in P$ such that $f(a)b \in Q$. Hence f satisfies the condition (i). We can prove that f satisfies the condition (ii) exactly in the same way as in the proof of Corollary I.4.5. □

Remark I.4.8. (1) If P and Q are not finitely generated, Corollaries I.4.5 and I.4.7 are not true. We have the following counterexample. Let p be a prime and set $P = \{np^{-m} \mid n \in \mathbb{N}, m \in \mathbb{N}\} \subset \mathbb{Q}$. Let n be an integer≥ 2 prime to p and let $f : P \to P$ be the morphism defined by the multiplication by n. It is easy to see that P is saturated and the morphism f is integral and vertical. However, for a prime q, f is q-saturated if and only if q is prime to n. We prove it. If q is prime to n, then the following diagram is cocartesian in the category of monoids:

$$\begin{array}{ccc} P & \xleftarrow{\;q\;} & P \\ {\scriptstyle f}\uparrow & & {\scriptstyle f}\uparrow \\ P & \xleftarrow{\;q\;} & P \end{array}$$

Indeed, it is easy to see that this becomes cocartesian after taking the associated groups. On the other hand, we have $f(P)P^q = P$ because, for a sufficiently large integer m, there exist positive integers r and s such that $rn + sq = p^m$. Hence, by definition, f is q-saturated. If n is divisible by q, set

$$m = nq^{-1}, \quad G = P^{\mathrm{gp}}/(P^{\mathrm{gp}})^q \ (\cong \mathbb{Z}/q\mathbb{Z})$$

and define morphisms of monoids $g, h : P^{\mathrm{gp}} \to G \oplus P^{\mathrm{gp}}$ by

$$g(a) = (a \bmod (P^{\mathrm{gp}})^q, a^m), \quad h(a) = (0, a).$$

Then the following diagram is cocartesian:

$$\begin{array}{ccc} G \oplus P^{\mathrm{gp}} & \xleftarrow{\;h\;} & P^{\mathrm{gp}} \\ {\scriptstyle g}\uparrow & & \uparrow{\scriptstyle f^{\mathrm{gp}}} \\ P^{\mathrm{gp}} & \xleftarrow{\;q\;} & P^{\mathrm{gp}} \end{array}$$

The pushout of the diagram $P \xleftarrow{f} P \xrightarrow{q} P$ is $g(P)h(P)$. On the other hand, we see easily that $g(P)h(P) \cap G = \{1\}$ and $G^q = \{1\}$. Hence $g(P)h(P)$ is not q-saturated. By Proposition I.3.13, f is not q-saturated.

(2) If f is not vertical, Corollary I.4.7 is not true. Indeed, for two integral monoids P and Q and a prime p, the morphism $P \to P \oplus Q$, $a \mapsto (a, 1)$ is integral and it is p-saturated if and only if Q is p-saturated. By taking the monoid in Example I.3.4 as Q, we obtain a counterexample.

I.5. ***A criterion of saturated morphisms, I.*** The purpose of this section is to prove Theorem I.5.1 below. This is an unpublished result of K. Kato. As a corollary, we will prove that every integral morphism of finitely generated saturated monoids is "potentially" saturated (Corollary I.5.4).

Theorem I.5.1. *Let $f : P \to Q$ be an integral morphism of finitely generated saturated monoids. Then, the morphism f is saturated if and only if, for every prime ideal $\mathfrak{q}$ of Q of height* 1 *such that the prime ideal $f^{-1}(\mathfrak{q})$ of P is of height* 1, *the ramification index of f at $\mathfrak{q}$* (Lemma I.1.7) *is* 1.

Lemma I.5.2. *Let n be a positive integer. Then the morphism $n : \mathbb{N} \to \mathbb{N}$ is saturated if and only if $n = 1$.*

Proof. Suppose $n \geq 2$. First note that the morphism $n : \mathbb{N} \to \mathbb{N}$ is integral. Let m be an integer ≥ 2 and set $d = \gcd(n, m)$, $m_0 = md^{-1}$ and $n_0 = nd^{-1}$. Choose integers r and s such that $s \cdot m_0 + r \cdot n_0 = 1$ and define morphisms $f, g : \mathbb{N} \to \mathbb{N} \oplus \mathbb{Z}/d\mathbb{Z}$ by $f(1) = (n_0, s)$ and $g(1) = (m_0, -r)$. Then, the diagram

$$\begin{array}{ccc} \mathbb{N} \oplus \mathbb{Z}/d\mathbb{Z} & \xleftarrow{\;g\;} & \mathbb{N} \\ {\scriptstyle f}\uparrow & & \uparrow{\scriptstyle n} \\ \mathbb{N} & \xleftarrow{\;m\;} & \mathbb{N} \end{array}$$

is cocartesian in the category of saturated monoids. Indeed, we see easily that the diagram becomes cocartesian in the category of abelian groups after taking the associated groups and that $\mathbb{N} \oplus \mathbb{Z}/d\mathbb{Z}$ is the saturation of $f(\mathbb{N}) + g(\mathbb{N})$. If $n_0 \geq 2$ and $m_0 \geq 2$, $\mathbb{N} \oplus \mathbb{Z}/d\mathbb{Z} \supsetneq f(\mathbb{N}) + g(\mathbb{N})$ because $(1, 0) \notin f(\mathbb{N}) + g(\mathbb{N})$. Otherwise, $d \geq 2$ and again $\mathbb{N} \oplus \mathbb{Z}/d\mathbb{Z} \supsetneq f(\mathbb{N}) + g(\mathbb{N})$ because $(0, 1 \bmod d) \notin f(\mathbb{N}) + g(\mathbb{N})$. Hence the pushout of $\mathbb{N} \xleftarrow{m} \mathbb{N} \xrightarrow{n} \mathbb{N}$ in the category of monoids is not saturated for integers $n, m \geq 2$. □

Proof of Theorem I.5.1. First let us prove the necessity. Let $\mathfrak{q}$ be a prime ideal of height 1 of Q such that $\mathfrak{p} = f^{-1}(\mathfrak{q})$ is a prime ideal of height 1 of P. Then, by Propositions I.3.16 and I.3.18, the morphism $\mathbb{N} \cong P_{\mathfrak{p}}/P^*_{\mathfrak{p}} \to Q_{\mathfrak{q}}/Q^*_{\mathfrak{q}} \cong \mathbb{N}$ induced by f is saturated. Hence, by Lemma I.5.2, the ramification index of f at $\mathfrak{q}$ is 1.

Next let us prove the sufficiency. First we prove it in the case $\dim(P) = 1$ and $f^{-1}(Q^*) = P^*$. The set $\mathrm{Spec}(P)$ consists of two elements $\varnothing$ and $P \backslash P^*$, and we have $P/P^* \cong \mathbb{N}$. If we choose a lifting $e \in P$ of the generator of P/P^*, the maximal ideal $P \backslash P^*$ is generated by e. Let p be a prime. We will prove that

f satisfies the conditions (i) and (ii) in Theorem I.4.2. The condition (i) follows from the fact that Q is saturated. Let $b \in Q$ and suppose that there exists $a \in P\backslash P^*$ such that $f(a) \mid b^p$, or equivalently, $f(e) \mid b^p$. Then, for any prime ideal $\mathfrak{q}$ of Q of height 1, $v_{\mathfrak{q}}(b^p) \geq v_{\mathfrak{q}}(f(e))$. By the assumption on f, $v_{\mathfrak{q}}(f(e)) = 1$ or 0. If $v_{\mathfrak{q}}(f(e)) = 1$, then $v_{\mathfrak{q}}(b) \geq 1$ and hence $v_{\mathfrak{q}}(bf(e)^{-1}) \geq 0$. If $v_{\mathfrak{q}}(f(e)) = 0$, then $v_{\mathfrak{q}}(bf(e)^{-1}) = v_{\mathfrak{q}}(b) \geq 0$. By Lemma I.1.5 and Proposition I.1.6, we see $bf(e)^{-1} \in Q$, that is, $f(e) \mid b$.

Now let us consider the general case. Let $\mathfrak{p}$ be the prime ideal $f^{-1}(Q\backslash Q^*)$ of P. Then the morphism f factors as $P \to P_{\mathfrak{p}} \to Q$. The first morphism is saturated and the second morphism is integral by Propositions I.3.18 and I.2.7. Hence we may assume $f^{-1}(Q^*) = P^*$. Let p be a prime. Since Q is saturated, f satisfies the condition (i) in Theorem I.4.2. It remains to prove that f satisfies the condition (ii$'$) in Remark I.4.4. Let $b \in Q$ and assume $f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q = f(P)b$. We will prove $f^{\mathrm{gp}}(P^{\mathrm{gp}})b^p \cap Q = f(P)b^p$. By Proposition I.2.11, there exists $b' \in Q$ such that $f^{\mathrm{gp}}(P^{\mathrm{gp}})b^p \cap Q = f(P)b'$. Choose $a \in P$ such that $b^p = f(a)b'$. By Proposition I.1.6, it suffices to prove $a \in P^*_{\mathfrak{p}}$ for all prime ideals $\mathfrak{p}$ of P of height 1. Let $\mathfrak{p}$ be a prime ideal of height 1 of P and define an integral morphism of finitely generated saturated monoids $f_{\mathfrak{p}} : P_{\mathfrak{p}} \to Q_{\mathfrak{p}}$ by the following cocartesian diagram in the category of monoids:

$$\begin{array}{ccc} Q_{\mathfrak{p}} & \longleftarrow & Q \\ {\scriptstyle f_{\mathfrak{p}}}\uparrow & & {\scriptstyle f}\uparrow \\ P_{\mathfrak{p}} & \longleftarrow & P \end{array}$$

By Propositions I.2.11 and I.3.2 (2), $f_{\mathfrak{p}}$ is exact, and therefore $f_{\mathfrak{p}}^{-1}(Q^*_{\mathfrak{p}}) = P^*_{\mathfrak{p}}$. Using $Q_{\mathfrak{p}} = f(P\backslash\mathfrak{p})^{-1}Q$, we see that, for every prime ideal $\mathfrak{s}$ of $Q_{\mathfrak{p}}$ of height 1 such that the prime ideal $f_{\mathfrak{p}}^{-1}(\mathfrak{s})$ of $P_{\mathfrak{p}}$ is of height 1, the ramification index of $f_{\mathfrak{p}}$ at $\mathfrak{s}$ is 1. So, as we have proven above, the morphism $f_{\mathfrak{p}}$ is p-saturated. On the other hand, $f^{\mathrm{gp}}(P^{\mathrm{gp}})b \cap Q = f(P)b$ implies $(f_{\mathfrak{p}})^{\mathrm{gp}}((P_{\mathfrak{p}})^{\mathrm{gp}})b \cap Q_{\mathfrak{p}} = f_{\mathfrak{p}}(P_{\mathfrak{p}})b$. Hence, by Theorem I.4.2 and Remark I.4.4, we have $(f_{\mathfrak{p}})^{\mathrm{gp}}((P_{\mathfrak{p}})^{\mathrm{gp}})b^p \cap Q_{\mathfrak{p}} = f_{\mathfrak{p}}(P_{\mathfrak{p}})b^p$. Choose $c \in P_{\mathfrak{p}}$ such that $b' = f_{\mathfrak{p}}(c)b^p$ (in $(Q_{\mathfrak{p}})^{\mathrm{gp}} = Q^{\mathrm{gp}}$). Then $f_{\mathfrak{p}}(c)f(a) = 1$ and hence $f(a) \in Q^*_{\mathfrak{q}}$, which implies $a \in P^*_{\mathfrak{p}}$. □

Proposition I.5.3. *Let $f : P \to Q$ be an integral morphism of finitely generated saturated monoids. Let n be a positive integer and consider the following cocartesian diagram in the category of* saturated *monoids*:

$$\begin{array}{ccc} Q' & \xleftarrow{\ g\ } & Q \\ {\scriptstyle f'}\uparrow & & {\scriptstyle f}\uparrow \\ P & \xleftarrow{\ n\ } & P \end{array}$$

Then:

(1) *f' is integral.*

Let $\mathfrak{q}'$ be a prime ideal of height 1 *of Q' and let $\mathfrak{p}$ (resp. $\mathfrak{q}$) be the prime ideal $(f')^{-1}(\mathfrak{q}')$ (resp. $g^{-1}(\mathfrak{q}')$) of P (resp. Q). Then:*

(2) $\mathrm{ht}(\mathfrak{q}) = 1$ *and* $f^{-1}(\mathfrak{q}) = \mathfrak{p}$.

Let $n_{\mathfrak{q}'}$ be the ramification index of g at $\mathfrak{q}'$.

(3) *If* $\mathrm{ht}(\mathfrak{p}) = 0$, *then* $n_{\mathfrak{q}'} = 1$.

(4) *Suppose* $\mathrm{ht}(\mathfrak{p}) = 1$. *If we denote by $m_{\mathfrak{q}'}$ (resp. $m_{\mathfrak{q}}$) the ramification index of f' (resp. f) at $\mathfrak{q}'$ (resp. $\mathfrak{q}$), we have* $m_{\mathfrak{q}'} = m_{\mathfrak{q}} \gcd(n, m_{\mathfrak{q}})^{-1}$ *and* $n_{\mathfrak{q}'} = n \gcd(n, m_{\mathfrak{q}})^{-1}$.

Proof. (1) There exists a unique morphism $h : Q' \to Q$ such that $h \circ f' = f$ and $h \circ g = n$. The morphism $g \circ h$ is the multiplication by n on Q', which is exact. Hence h is exact, and the claim follows from Proposition I.2.10.

(2) The second claim follows from the fact that the inverse image of $\mathfrak{p}$ under $n : P \to P$ is $\mathfrak{p}$. For any $b \in Q'$, $b^n = g(h(b))$ and, for any $a_1, a_2 \in Q$, $g(a_1) = g(a_2)$ implies $a_1^n = h(g(a_1)) = h(g(a_2)) = a_2^n$. Hence, the first claim follows from Proposition I.1.4.

(3) The assumption $\mathrm{ht}(\mathfrak{p}) = 0$ implies $v_{\mathfrak{q}'}((f')^{\mathrm{gp}}(P^{\mathrm{gp}})) = 0$. Since Q'^{gp} is generated by $(f')^{\mathrm{gp}}(P^{\mathrm{gp}})$ and $g^{\mathrm{gp}}(Q^{\mathrm{gp}})$, we have

$$\mathbb{Z} = v_{\mathfrak{q}'}((Q')^{\mathrm{gp}}) = v_{\mathfrak{q}'}((f')^{\mathrm{gp}}(P^{\mathrm{gp}})) + v_{\mathfrak{q}'}(g^{\mathrm{gp}}(Q^{\mathrm{gp}})) = n_{\mathfrak{q}'} v_{\mathfrak{q}}(Q^{\mathrm{gp}}) = n_{\mathfrak{q}'}\mathbb{Z}.$$

Hence $n_{\mathfrak{q}'} = 1$.

(4) Since $(Q')^{\mathrm{gp}} = (f')^{\mathrm{gp}}(P^{\mathrm{gp}}) g^{\mathrm{gp}}(Q^{\mathrm{gp}})$, we have

$$\begin{aligned}\mathbb{Z} = v_{\mathfrak{q}'}((Q')^{\mathrm{gp}}) &= v_{\mathfrak{q}'}((f')^{\mathrm{gp}}(P^{\mathrm{gp}})) + v_{\mathfrak{q}'}(g^{\mathrm{gp}}(Q^{\mathrm{gp}})) \\ &= m_{\mathfrak{q}'} v_{\mathfrak{p}}(P^{\mathrm{gp}}) + n_{\mathfrak{q}'} v_{\mathfrak{q}}(Q^{\mathrm{gp}}) = m_{\mathfrak{q}'}\mathbb{Z} + n_{\mathfrak{q}'}\mathbb{Z}.\end{aligned}$$

Hence $(m_{\mathfrak{q}'}, n_{\mathfrak{q}'}) = 1$. On the other hand, since the ramification index of $n : P \to P$ at $\mathfrak{p}$ is n, we have $n_{\mathfrak{q}'} m_{\mathfrak{q}} = m_{\mathfrak{q}'} n$. The two equalities in (4) follow from these two facts. □

Corollary I.5.4. *Let $f : P \to Q$, n and $f' : P \to Q'$ be as in Proposition I.5.3. Then f' is saturated if and only if n is divisible by the least common multiple of the ramification indices of f at all prime ideals $\mathfrak{q}$ of Q of height* 1 *such that* $\mathrm{ht}(f^{-1}(\mathfrak{q})) = 1$.

Proof. This follows from Proposition I.5.3 and Theorem I.5.1. □

I.6. ***A criterion of saturated morphisms, II.*** In this section, we give several characterizations of saturated morphisms of finitely generated saturated monoids; see Theorem I.6.3.

Proposition I.6.1. *Let $f : P \to Q$ be a morphism of finitely generated saturated monoids. If f is saturated, $P^* = \{1\}$, $Q^* = \{1\}$, $f^{-1}(\{1\}) = \{1\}$ and $\dim(P) = \dim(Q)$, then f is an isomorphism.*

Proof. By Proposition I.2.8, the morphism $f^{\mathrm{gp}} : P^{\mathrm{gp}} \to Q^{\mathrm{gp}}$ is injective. On the other hand, $\mathrm{rank}_{\mathbb{Z}}(P^{\mathrm{gp}}) = \dim(P) = \dim(Q) = \mathrm{rank}_{\mathbb{Z}}(Q^{\mathrm{gp}})$ by assumption. Hence $Q^{\mathrm{gp}}/f^{\mathrm{gp}}(P^{\mathrm{gp}})$ is a finite group. Set $G = Q^{\mathrm{gp}}/f^{\mathrm{gp}}(P^{\mathrm{gp}})$ and define morphisms of monoids $g, h : Q \to Q \oplus G$ by $g(b) = (b, 0)$ and $h(b) = (b, b \bmod f^{\mathrm{gp}}(P^{\mathrm{gp}}))$. Then the diagram of saturated monoids

$$\begin{array}{ccc} Q \oplus G & \xleftarrow{\;h\;} & Q \\ {\scriptstyle g}\uparrow & & \uparrow{\scriptstyle f} \\ Q & \xleftarrow{\;f\;} & P \end{array}$$

is cocartesian in the category of saturated monoids. Indeed, we see easily that the diagram becomes cocartesian after taking the associated abelian groups and that $Q \oplus G$ is the saturated monoid associated to its submonoid $h(Q)g(Q)$ (see Definition II.2.2). Using $Q^* = \{1\}$, we see $h(Q)g(Q) \cap G = \{1\}$. On the other hand, since f is saturated, $h(Q)g(Q) = Q \oplus G$. Hence $G = \{1\}$ and $P^{\mathrm{gp}} = Q^{\mathrm{gp}}$. Since f is exact by Proposition I.2.8, $P = Q$. □

Corollary I.6.2. *Let $f : P \to Q$ be a saturated morphism of finitely generated saturated monoids. Let $\mathfrak{q}$ be a prime ideal of Q and let $\mathfrak{p}$ be the prime ideal $f^{-1}(\mathfrak{q})$ of P. If $\mathrm{ht}(\mathfrak{q}) = \mathrm{ht}(\mathfrak{p})$, then the morphism $P_{\mathfrak{p}}/P_{\mathfrak{p}}^* \to Q_{\mathfrak{q}}/Q_{\mathfrak{q}}^*$ induced by f is an isomorphism.*

Proof. By Propositions I.3.16 and I.3.18, the morphism $P_{\mathfrak{p}}/P_{\mathfrak{p}}^* \to Q_{\mathfrak{q}}/Q_{\mathfrak{q}}^*$ is saturated. On the other hand, $\dim(P_{\mathfrak{p}}/P_{\mathfrak{p}}^*) = \mathrm{ht}(\mathfrak{p}) = \mathrm{ht}(\mathfrak{q}) = \dim(Q_{\mathfrak{q}}/Q_{\mathfrak{q}}^*)$. Hence the claim follows from Proposition I.6.1. □

Theorem I.6.3. *Let $f : P \to Q$ be an integral morphism of finitely generated saturated monoids such that $f^{-1}(Q^*) = P^*$. Set $\mathfrak{m}_P = P \backslash P^*$. Then the following conditions are equivalent*:

(1) *f is saturated.*

(2) *There exists a prime p such that f is p-saturated.*

(3) *For any $b \in Q$, if there exist a positive integer n and $a \in \mathfrak{m}_P$ such that $f(a) \mid b^n$, then there exists $a' \in \mathfrak{m}_P$ such that $f(a') \mid b$.*

(4) *For any $\mathfrak{q} \in \mathrm{Spec}(Q)$ and $\mathfrak{p} = f^{-1}(\mathfrak{q}) \in \mathrm{Spec}(P)$ such that $\mathrm{ht}(\mathfrak{q}) = \mathrm{ht}(\mathfrak{p})$, the morphism $P_{\mathfrak{p}}/P_{\mathfrak{p}}^* \to Q_{\mathfrak{q}}/Q_{\mathfrak{q}}^*$ induced by f is an isomorphism.*

(5) *For any* $\mathfrak{q} \in \mathrm{Spec}(Q)$ *and* $\mathfrak{p} = f^{-1}(\mathfrak{q}) \in \mathrm{Spec}(P)$ *such that* $\mathrm{ht}(\mathfrak{q}) = \mathrm{ht}(\mathfrak{p}) = 1$, *the morphism* $P_{\mathfrak{p}}/P^*_{\mathfrak{p}} \to Q_{\mathfrak{q}}/Q^*_{\mathfrak{q}}$ *induced by* f *is an isomorphism.*

(6) *For any* $\mathfrak{q} \in \mathrm{Spec}(Q)$ *such that* $f^{-1}(\mathfrak{q}) = \mathfrak{m}_P$ *and* $\mathrm{ht}(\mathfrak{q}) = \mathrm{ht}(\mathfrak{m}_P)$ $(= \dim(P))$, *the morphism* $P/P^* \to Q_{\mathfrak{q}}/Q^*_{\mathfrak{q}}$ *induced by* f *is an isomorphism.*

(7) *For any* $\mathfrak{q} \in \mathrm{Spec}(Q)$ *such that* $f^{-1}(\mathfrak{q}) = \mathfrak{m}_P$ *and* $\mathrm{ht}(\mathfrak{q}) = \mathrm{ht}(\mathfrak{m}_P)$ $(= \dim(P))$, $\mathfrak{q}(Q_{\mathfrak{q}}/Q^*_{\mathfrak{q}}) = f(\mathfrak{m}_P)(Q_{\mathfrak{q}}/Q^*_{\mathfrak{q}})$.

(8) *For any field* k *on which the order of the torsion part of* $Q^{\mathrm{gp}}/f(P^*)$ *is invertible*, $k[Q/f(P^*)]/f(\mathfrak{m}_P)k[Q/f(P^*)]$ *is reduced.*

(9) *There exists a field* k *such that* $k[Q/f(P^*)]/f(\mathfrak{m}_P)k[Q/f(P^*)]$ *satisfies* (R_0).

Theorem I.6.4 [Hochster 1972]. *For any finitely generated saturated monoid* P *and any field* k, *the ring* $k[P]$ *is Cohen–Macaulay.*

Proposition I.6.5 (A part of [EGA IV$_2$ 1965, Corollaire (6.3.5)]). *Let* $f : X \to Y$ *be a flat morphism of locally noetherian schemes. Let* $x \in X$ *and* $y = f(x)$. *If* $\mathcal{O}_{X,x}$ *is Cohen–Macaulay, then* $\mathcal{O}_{X,x} \otimes_{\mathcal{O}_{Y,y}} k(y)$ *and* $\mathcal{O}_{Y,y}$ *are Cohen–Macaulay.*

Corollary I.6.6. *Let* $f : P \to Q$ *be an integral morphism of finitely generated saturated monoids such that* $f^{-1}(Q^*) = P^* = \{1\}$. *Then, for any field* k, *the ring* $k[Q]/f(P\backslash\{1\})k[Q]$ *is Cohen–Macaulay.*

Proof. By Propositions I.2.8 and I.2.1, the homomorphism $k[P] \to k[Q]$ induced by f is flat. Hence, the claim follows from Theorem I.6.4 and Proposition I.6.5. □

Lemma I.6.7. *Let* P *be a finitely generated saturated monoid. Then, the surjective morphism* $P \to P/P^*$ *has a section* $s : P/P^* \to P$, *which induces an isomorphism* $(s, \iota) : P/P^* \oplus P^* \cong P$, *where* ι *is the inclusion* $P^* \hookrightarrow P$.

Proof. Since P is saturated, P^{gp}/P^* is torsion-free and the surjective homomorphism $P^{\mathrm{gp}} \to P^{\mathrm{gp}}/P^*$ has a section $t : P^{\mathrm{gp}}/P^* \to P^{\mathrm{gp}}$. It is easy to see that $t(P/P^*) \subset P$ and the restriction of t on P/P^* gives a desired morphism. □

Lemma I.6.8. *Let* P *be a finitely generated integral monoid. Then, for any field* k, *the dimension of every irreducible component of* $\mathrm{Spec}(k[P])$ *is* $\mathrm{rank}_{\mathbb{Z}}(P^{\mathrm{gp}})$.

Proof. Let $a_1, a_2, \ldots, a_n$ be a set of generators of P. Then $\mathrm{Spec}(k[P^{\mathrm{gp}}]) = \mathrm{Spec}(k[P]_{a_1\cdots a_n})$. Since P is integral, $a_1 \cdots a_n$ is a nonzero divisor in $k[P]$. Hence the generic point of every irreducible component of $\mathrm{Spec}(k[P])$ is contained in $\mathrm{Spec}(k[P^{\mathrm{gp}}])$. Therefore we may assume $P = P^{\mathrm{gp}}$. Then $P \cong \mathbb{Z}^r \oplus C$ with C a finite group and $k[P]$ is isomorphic to $k[T_1^{\pm 1}, \ldots, T_r^{\pm 1}] \otimes_k k[C]$, where $r = \mathrm{rank}_{\mathbb{Z}} P^{\mathrm{gp}}$. Hence $\mathrm{Spec}(k[P])_{\mathrm{red}}$ is a finite disjoint union of schemes of the form $\mathrm{Spec}(k'[T_1^{\pm 1}, \ldots, T_r^{\pm 1}])$ with k' finite extensions of k. □

Proposition I.6.9. *Let* P *be a finitely generated saturated monoid and let* k *be a field. Set* $X = \mathrm{Spec}(k[P])$. *Let* $x \in X$ *and let* $\mathfrak{p}$ *be the inverse image of the* *maximal ideal of* $\mathcal{O}_{X,x}$ *in* P (*which is a prime ideal of* P). *Then* $\mathrm{ht}(\mathfrak{p}) \le \dim(\mathcal{O}_{X,x})$. *The equality holds if and only if* x *is of codimension* 0 *in the closed subscheme* $Y = \mathrm{Spec}(k[P]/\mathfrak{p}k[P])$ *of* X. *Furthermore*, *if the order of the torsion part of* P^{gp} *is invertible in* k *and* $\mathrm{ht}(\mathfrak{p}) = \dim(\mathcal{O}_{X,x})$, *then the maximal ideal of* $\mathcal{O}_{X,x}$ *is generated by the image of* $\mathfrak{p}$.

Proof. Let U be the open subscheme $\mathrm{Spec}(k[P_{\mathfrak{p}}])$ of X. Then, the point x is contained in the closed subscheme $V = \mathrm{Spec}(k[P_{\mathfrak{p}}]/\mathfrak{p}k[P_{\mathfrak{p}}])$ of U. Note that the scheme V is an open subscheme of Y. By Lemma I.6.7, $P_{\mathfrak{p}} \cong P_{\mathfrak{p}}/P_{\mathfrak{p}}^* \oplus P_{\mathfrak{p}}^*$ and $\mathfrak{p}P_{\mathfrak{p}}$ corresponds to $\{(a,b) \in P_{\mathfrak{p}}/P_{\mathfrak{p}}^* \oplus P_{\mathfrak{p}}^* \mid a \ne 1\}$. Hence $V \cong \mathrm{Spec}(k[P_{\mathfrak{p}}^*])$. By Lemma I.6.8, $\dim(\mathcal{O}_{X,x}) \ge \mathrm{rank}_{\mathbb{Z}}(P^{\mathrm{gp}}) - \mathrm{rank}_{\mathbb{Z}}(P_{\mathfrak{p}}^*) = \mathrm{rank}_{\mathbb{Z}}(P_{\mathfrak{p}}^{\mathrm{gp}}/P_{\mathfrak{p}}^*) = \dim(P_{\mathfrak{p}}) = \mathrm{ht}(\mathfrak{p})$, and the equality holds if and only if x is of codimension 0 in V, or, equivalently in Y. Suppose that the order of the torsion part of P^{gp} is invertible in k. Then V is a finite disjoint union of regular schemes. Hence, if x is of codimension 0 in V, the maximal ideal of $\mathcal{O}_{X,x}$ is generated by the image of $\mathfrak{p}$. □

Proof of Theorem I.6.3. The implications (1) ⇒ (2), (4) ⇒ (5), (4) ⇒ (6), (6) ⇒ (7) and (8) ⇒ (9) are trivial. It follows from Corollary I.4.5 that (2) ⇒ (1). Since Q is saturated, f satisfies the condition (i) in Theorem I.4.2. Hence the equivalence between (2) and (3) follows from Theorem I.4.2. It follows from Corollary I.6.2 that (1) ⇒ (4) and from Theorem I.5.1 that (5) ⇒ (1). Now it suffices to prove (7) ⇒ (8) and (9) ⇒ (3).

(7) ⇒ (8): Let k be a field satisfying the assumption in (8). The morphism $g : P/P^* \to Q/f(P^*)$ induced by f is integral,

$$g^{-1}((Q/f(P^*))^*) = g^{-1}(Q^*/f(P^*)) = \{1\} = (P/P^*)^*$$

and $Q^{\mathrm{gp}}/f(P^*) \cong (Q/f(P^*))^{\mathrm{gp}}$. Furthermore, if f satisfies (7), then g also satisfies (7). Hence, we may assume $P^* = \{1\}$. By Corollary I.6.6, the ring $k[Q]/f(\mathfrak{m}_P)k[Q]$ is Cohen–Macaulay, in particular, it satisfies (S_1). Hence it suffices to prove that the ring $k[Q]/f(\mathfrak{m}_P)k[Q]$ satisfies (R_0). Set $Y = \mathrm{Spec}(k[Q])$, $X = \mathrm{Spec}(k[P])$, and $Z = \mathrm{Spec}(k[Q]/f(\mathfrak{m}_P)k[Q])$. By Propositions I.2.8 and I.2.1, the morphism $Y \to X$ induced by f is flat. Let y be a point of Z of codimension 0 and let x be the image of y in X, which is the closed point defined by the maximal ideal $\mathfrak{m}_P k[P]$ of $k[P]$. Since Y is flat over X and Z is the fiber over x, we have $\dim(\mathcal{O}_{X,x}) = \dim(\mathcal{O}_{Y,y})$. Let $\mathfrak{q}$ be the inverse image of the maximal ideal of $\mathcal{O}_{Y,y}$ in Q. Since the inverse image of the maximal ideal of $\mathcal{O}_{X,x}$ in P is $\mathfrak{m}_P$, we have $f^{-1}(\mathfrak{q}) = \mathfrak{m}_P$. By Proposition I.6.9, we have $\mathrm{ht}(\mathfrak{q}) \le \dim(\mathcal{O}_{Y,y})$ and $\mathrm{ht}(\mathfrak{m}_P) = \dim(\mathcal{O}_{X,x})$. On the other hand, by Corollary I.2.9, we have $\mathrm{ht}(\mathfrak{m}_P) \le \mathrm{ht}(\mathfrak{q})$. Hence $\mathrm{ht}(\mathfrak{m}_P) = \mathrm{ht}(\mathfrak{q}) = \dim(\mathcal{O}_{X,x}) = \dim(\mathcal{O}_{Y,y})$. Since the order of the torsion part of Q^{gp} is invertible in k, the maximal ideal of $\mathcal{O}_{Y,y}$ is generated by the image of $\mathfrak{q}$ by Proposition I.6.9. Therefore, if f satisfies the condition (7), then $\mathfrak{q}Q_{\mathfrak{q}} = f(\mathfrak{m}_P)Q_{\mathfrak{q}}$ and hence the maximal ideal of $\mathcal{O}_{Y,y}$ is generated by the image of $f(\mathfrak{m}_P)$, that is, Z is regular at y.

(9) $\Rightarrow$ (3): Let g be as in the proof of (7) $\Rightarrow$ (8). By Proposition I.3.16 and (1) $\Leftrightarrow$ (3), we may replace f by g and assume $P^* = \{1\}$. Then, by Corollary I.6.6, $k[Q]/f(\mathfrak{m}_P)k[Q]$ is Cohen–Macaulay, so it satisfies (S_1). Hence, if f satisfies (9), then $k[Q]/f(\mathfrak{m}_P)k[Q]$ is reduced. Let $b \in Q$, let n be a positive integer, and suppose that there exists $a \in \mathfrak{m}_P$ such that $f(a) \mid b^n$. Then $b^n \in f(\mathfrak{m}_P)k[Q]$. If $k[Q]/f(\mathfrak{m}_P)k[Q]$ is reduced, then $b \in f(\mathfrak{m}_P)k[Q]$. Hence, $b \in f(\mathfrak{m}_P)Q$. In other words, there exists $a' \in \mathfrak{m}_P$ such that $f(a') \mid b$. □

II. Saturated morphisms of log schemes

II.1. ***Preliminaries on log schemes.*** In this section, we prove some fundamental properties on log schemes.

Lemma II.1.1. *Let $f_1 : M_0 \to M_1$ and $f_2 : M_0 \to M_2$ be morphisms of log structures on a scheme X and let M_3 be the pushout of the diagram $M_1 \xleftarrow{f_1} M_0 \xrightarrow{f_2} M_2$ as sheaves of monoids.*

(1) *The sheaf of monoids M_3 endowed with the morphism $M_3 \to \mathcal{O}_X$ induced by the structure morphisms $M_0, M_1, M_2 \to \mathcal{O}_X$, is a log structure on X.*

(2) *The following diagram of sheaves of monoids is cocartesian*:

$$\begin{array}{ccc} M_3/\mathcal{O}_X^* & \longleftarrow & M_1/\mathcal{O}_X^* \\ \uparrow & & \uparrow \\ M_2/\mathcal{O}_X^* & \longleftarrow & M_0/\mathcal{O}_X^* \end{array}$$

Proof. Let α_i denote the structure morphism $M_i \to \mathcal{O}_X$ for $i = 0, 1, 2, 3$ and let g_1 and g_2 denote the canonical morphisms $M_1 \to M_3$ and $M_2 \to M_3$ respectively.

(1) First note $M_3 = g_1(M_1)g_2(M_2)$. Take $a_1 \in M_1$ and $a_2 \in M_2$ and assume $\alpha_3(g_1(a_1)g_2(a_2)) \in \mathcal{O}_X^*$. Then

$$\alpha_1(a_1) = \alpha_3(g_1(a_1)) \in \mathcal{O}_X^* \quad \text{and} \quad \alpha_2(a_2) = \alpha_3(g_2(a_2)) \in \mathcal{O}_X^*,$$

that is, $a_1 \in \alpha_1^{-1}(\mathcal{O}_X^*)$ and $a_2 \in \alpha_2^{-1}(\mathcal{O}_X^*)$. Let a be the unique section of $\alpha_0^{-1}(\mathcal{O}_X^*)$ such that $\alpha_0(a) = \alpha_2(a_2)$. Then, since $f_2(a) = a_2$, we have $g_1(f_1(a)) = g_2(f_2(a)) = g_2(a_2)$. Hence $g_1(a_1)g_2(a_2) = g_1(a_1 f_1(a)) \in g_1(\alpha_1^{-1}(\mathcal{O}_X^*))$. Thus we obtain

$$\alpha_3^{-1}(\mathcal{O}_X^*) = g_1(\alpha_1^{-1}(\mathcal{O}_X^*)),$$

which implies that the morphism $\alpha_3^{-1}(\mathcal{O}_X^*) \to \mathcal{O}_X^*$ induced by α_3 is an isomorphism.

(2) Consider the following two diagrams of sheaves of monoids:

$$\begin{array}{ccccc} M_3/\mathcal{O}_X^* & \longleftarrow & M_3 & \xleftarrow{g_2} & M_2 \\ \uparrow & & \uparrow{\scriptstyle g_1} & & \uparrow{\scriptstyle f_2} \\ M_1/\mathcal{O}_X^* & \longleftarrow & M_1 & \xleftarrow{f_1} & M_0 \end{array} \qquad \begin{array}{ccccc} M_3/\mathcal{O}_X^* & \longleftarrow & M_2/\mathcal{O}_X^* & \longleftarrow & M_2 \\ \uparrow & & \uparrow & & \uparrow{\scriptstyle f_2} \\ M_1/\mathcal{O}_X^* & \longleftarrow & M_0/\mathcal{O}_X^* & \longleftarrow & M_0 \end{array}$$

The two squares of the first diagram are cocartesian. Hence the outer square of the second diagram is cocartesian. Since the left square of the second diagram is cocartesian, the right one is also cocartesian. □

Proposition II.1.2. *Consider a cartesian diagram in the category of log schemes*:

$$\begin{array}{ccc} (Z, M_Z) & \xrightarrow{h} & (Y, M_Y) \\ {\scriptstyle k}\downarrow & & \downarrow{\scriptstyle g} \\ (X, M_X) & \xrightarrow{f} & (S, M_S) \end{array}$$

Take $z \in Z$ and let x, y and s be the images of z in X, Y and S respectively. Then, *the diagram of monoids*

$$\begin{array}{ccc} (M_Z/\mathcal{O}_Z^*)_{\bar{z}} & \longleftarrow & (M_Y/\mathcal{O}_Y^*)_{\bar{y}} \\ \uparrow & & \uparrow \\ (M_X/\mathcal{O}_X^*)_{\bar{x}} & \longleftarrow & (M_S/\mathcal{O}_S^*)_{\bar{s}} \end{array}$$

induced by the above diagram of log schemes is cocartesian in the category of monoids.

Proof. Let M be the pushout of the diagram

$$k^*(M_X) \leftarrow (f \circ k)^*(M_S) = (g \circ h)^*(M_S) \rightarrow h^*(M_Y)$$

as sheaves of monoids. Then M endowed with the morphism $M \rightarrow \mathcal{O}_Z$ induced by the structure morphisms $k^*(M_X) \rightarrow \mathcal{O}_Z$ and $h^*(M_Y) \rightarrow \mathcal{O}_Z$ is a log structure by Lemma II.1.1 (1). One can verify that (Z, M) satisfies the universal property of fiber products. Hence $M_Z \cong M$. Now the claim follows from Lemma II.1.1 (2) and [Kato 1989, (1.4.1)]. □

Proposition II.1.3 [Kato 1989, Example (2.5)(2)]. *Let k be an algebraically closed field. Let M be an integral log structure on $s = \mathrm{Spec}(k)$ and set $P = \Gamma(s, M/\mathcal{O}_s^*)$. Then*, *there exists a section α of the projection $\Gamma(s, M) \rightarrow P$. Furthermore*, *such a section induces an isomorphism of log structures $(P_s)^a \xrightarrow{\sim} M$.*

Proof. Since $\Gamma(s, M^{\mathrm{gp}})/k^* \cong P^{\mathrm{gp}}$ and k^* is divisible and hence injective as a $\mathbb{Z}$-module, the projection $\Gamma(s, M^{\mathrm{gp}}) \rightarrow P^{\mathrm{gp}}$ has a section α. One sees easily $\alpha(P) \subset \Gamma(s, M)$. One can also verify that the morphism $(1, \alpha) : k^* \oplus P \rightarrow \Gamma(s, M)$ is an isomorphism and the image of $\alpha(P\backslash\{1\})$ under $\Gamma(s, M) \to k$ is 0. These imply that α induces an isomorphism $(P_s)^a \xrightarrow{\sim} M$. □

Proposition II.1.4. *Let (X, M_X) be a fine log scheme and let $\alpha : P_X \to M_X$ be a chart of M_X. Let $x \in X$ and let $\mathfrak{p}$ be the inverse image of the maximal ideal of $\mathcal{O}_{X,\bar{x}}$ under the morphism $P \xrightarrow{\alpha_{\bar{x}}} (M_X)_{\bar{x}} \to \mathcal{O}_{X,\bar{x}}$, which is a prime ideal of P. Then:*

(1) *The morphism α induces an isomorphism $P_{\mathfrak{p}}/P_{\mathfrak{p}}^* \xrightarrow{\sim} (M_X/\mathcal{O}_X^*)_{\bar{x}}$.*

(2) *Let U be the maximal open subscheme of X on which the image of every element of $P\backslash\mathfrak{p}$ under $P \to \Gamma(X, M_X) \to \Gamma(X, \mathcal{O}_X)$ becomes invertible. (Note that $P\backslash\mathfrak{p}$ is finitely generated.) Then, the chart α induces a chart $(P_{\mathfrak{p}})_U \to M_U$ of the restriction M_U of M_X on U.*

Proof. (1) By the definition of associated log structures, the diagram of monoids

$$\begin{array}{ccc} P\backslash\mathfrak{p} & \longrightarrow & P \\ {\scriptstyle\alpha_{\bar{x}}}\downarrow & & {\scriptstyle\alpha_{\bar{x}}}\downarrow \\ \mathcal{O}_{X,\bar{x}}^* & \longrightarrow & M_{X,\bar{x}} \end{array}$$

is cocartesian. Hence $\alpha_{\bar{x}}$ induces an isomorphism $P/(P\backslash\mathfrak{p}) \xrightarrow{\sim} (M_X/\mathcal{O}_X^*)_{\bar{x}}$. Since the image of $P\backslash\mathfrak{p}$ in $M_{X,\bar{x}}$ is contained in $\mathcal{O}_{X,\bar{x}}^*$, this isomorphism factors as

$$P/(P\backslash\mathfrak{p}) \to P_{\mathfrak{p}}/P_{\mathfrak{p}}^* \to (M_X/\mathcal{O}_X^*)_{\bar{x}}.$$

One sees easily that the first morphism is an isomorphism and hence the second one is also an isomorphism.

(2) Since the image of $P\backslash\mathfrak{p}$ in $\Gamma(U, M_U)$ is contained in $\Gamma(U, \mathcal{O}_U^*)$, the morphism α induces a morphism $\beta : (P_{\mathfrak{p}})_U \to M_U$. Let $x \in U$ and let $\mathfrak{q}$ be the inverse image of the maximal ideal of $\mathcal{O}_{U,\bar{x}}$ in $P_{\mathfrak{p}}$ and set $\mathfrak{r} = P \cap \mathfrak{q}$. By (1) and the fact that M_X is integral, it suffices to prove that the morphism $(P_{\mathfrak{p}})_{\mathfrak{q}}/(P_{\mathfrak{p}})_{\mathfrak{q}}^* \to (M_U/\mathcal{O}_U^*)_{\bar{x}}$ induced by β is an isomorphism. This follows from $P_{\mathfrak{r}} = (P_{\mathfrak{p}})_{\mathfrak{q}}$ and the fact that α induces an isomorphism $P_{\mathfrak{r}}/P_{\mathfrak{r}}^* \cong (M_X/\mathcal{O}_X^*)_{\bar{x}}$ by (1). □

II.2. *p-saturated log schemes and p-saturated morphisms.*

Definition II.2.1. Let p be a prime. Let M_X be a log structure on a scheme X. We say the log structure M_X is *p-saturated* (resp. *saturated*) if $\Gamma(U, M_X)$ is p-saturated (resp. saturated) for every étale X-scheme U. We call a scheme with a p-saturated (resp. saturated) log structure a *p-saturated* (resp. *saturated*) *log scheme*.

Note that p-saturated (resp. saturated) log structures are integral. We see easily that a log scheme (X, M_X) is p-saturated (resp. saturated) if and only if $M_{X,\bar{x}}$ is p-saturated (resp. saturated) for every point $x \in X$ and that an integral log scheme (X, M_X) is p-saturated (resp. saturated) if and only if $(M_X/\mathcal{O}_X^*)_{\bar{x}} \cong M_{X,\bar{x}}/\mathcal{O}_{X,\bar{x}}^*$ is p-saturated (resp. saturated) for every point $x \in X$.

Definition II.2.2. Let p be a prime and let P be an integral monoid. We define $P^{p\text{-sat}}$, the *p-saturated monoid associated to P*, and P^{sat}, the *saturated monoid associated to P*, by

$$P^{p\text{-sat}} = \{a \in P^{\text{gp}} \mid \text{there exists an integer } m \geq 0 \text{ such that } a^{p^m} \in P\},$$
$$P^{\text{sat}} = \{a \in P^{\text{gp}} \mid \text{there exists an integer } n \geq 1 \text{ such that } a^n \in P\}.$$

Proposition II.2.3. *Let p be a prime. The functor from the category of integral monoids to the category of p-saturated monoids (resp. saturated monoids) associating $P^{p\text{-sat}}$ (resp. P^{sat}) to P is a left adjoint of the forgetful functor.*

Proof. Straightforward. □

Proposition II.2.4. *Let p be a prime and let P be a finitely generated integral monoid. Then $P^{p\text{-sat}}$ (resp. P^{sat}) is finitely generated.*

Proof. It suffices to prove that $\mathbb{Q}[P^{p\text{-sat}}]$ and $\mathbb{Q}[P^{\text{sat}}]$ are finitely generated $\mathbb{Q}[P]$-modules. Let $\bar{P}$ and $\bar{P}'$ be the image of P and P^{sat} in $P^{\text{gp}}/(P^{\text{gp}})_{\text{tor}}$, where $(P^{\text{gp}})_{\text{tor}}$ denotes the torsion part of P^{gp}. Then, $\mathbb{Q}[\bar{P}]$ is a noetherian integral domain and $\mathbb{Q}[\bar{P}']$ is contained in the integral closure of $\mathbb{Q}[\bar{P}]$, which is finite over $\mathbb{Q}[\bar{P}]$. Hence $\mathbb{Q}[\bar{P}']$ is a finitely generated $\mathbb{Q}[\bar{P}]$-module. Since $P^{\text{sat}} \supset (P^{\text{gp}})_{\text{tor}}$, this implies that $\mathbb{Q}[P^{\text{sat}}]$ is finitely generated over $\mathbb{Q}[P]$ and its submodule $\mathbb{Q}[P^{p\text{-sat}}]$ is also finitely generated. □

Proposition II.2.5. *Let p be a prime. Let Q be the pushout of a diagram of monoids $P \leftarrow S \rightarrow G$. Suppose P is integral (resp. p-saturated, resp. saturated) and G is a group. Then, Q is integral (resp. p-saturated, resp. saturated). In particular, if S is integral (resp. p-saturated, resp. saturated), then Q is also the pushout in the category of integral (resp. p-saturated, resp. saturated) monoids.*

Proof. Straightforward, using [Kato 1989, (1.3) Remark]. □

Corollary II.2.6. *Let p be a prime. Let $f : X \to Y$ be a morphism of schemes and let M_Y be a log structure on Y. If M_Y is p-saturated (resp. saturated), then $f^*(M_X)$ is p-saturated (resp. saturated).*

Proposition II.2.7. *Let p be a prime and let (X, M_X) be a fine p-saturated (resp. fine saturated) log scheme. Let $\alpha : P_X \to M_X$ be a chart of M_X. Then the morphism $\beta : P_X^{p\text{-sat}} \to M_X$ (resp. $\beta : P_X^{\text{sat}} \to M_X$) induced by α is also a chart of M_X.*

Proof. Let P' be $P^{p\text{-sat}}$ (resp. P^{sat}). Let α^a and β^a be the morphisms of log structures $(P_X)^a \to M_X$ and $(P'_X)^a \to M_X$ induced by α and β, respectively. The morphism α^a is an isomorphism by assumption, and we want to prove that β^a is an isomorphism. Let γ be the composition of $(\alpha^a)^{-1} : M_X \xrightarrow{\sim} (P_X)^a$ and the morphism of log structures $(P_X)^a \to (P'_X)^a$ induced by the canonical morphism $P \to P'$. Let δ be the composition $P_X \to P'_X \to (P'_X)^a$. Then we have $\gamma \circ \beta^a \circ \delta = \delta$

and $\beta^a \circ \gamma \circ \alpha = \alpha$. By using the universality of associated log structures and Proposition II.2.3, we see that $\gamma \circ \beta^a$ and $\beta^a \circ \gamma$ are the identity maps. □

Corollary II.2.8. *Let p be a prime and let (X, M_X) be a fine log scheme. Then M_X is p-saturated (resp. saturated) if and only if, étale locally on X, there exists a chart $P_X \to M_X$ such that P is p-saturated (resp. saturated).*

Proof. The necessity follows from Proposition II.2.7. The sufficiency follows from the definition of associated log structures and Proposition II.2.5. □

Proposition II.2.9. *Let (X, M_X) be a fine saturated log scheme. Then, for any $x \in X$, there exists a chart $P_U \to M_X|_U$ for an étale neighborhood U of x which induces an isomorphism $P \cong (M_X/\mathcal{O}_X^*)_{\bar{x}}$.*

Proof. Set $P = (M_X/\mathcal{O}_X^*)_{\bar{x}} \cong M_{X,\bar{x}}/\mathcal{O}_{X,\bar{x}}^*$. Since P is a finitely generated saturated monoid such that $P^* = \{1\}$, P^{gp} is a finitely generated free abelian group. Hence there exists a section $s : P \to M_{X,\bar{x}}$ of the projection $M_{X,\bar{x}} \to P$. We see easily that the inverse image of $M_{X,\bar{x}}$ under the morphism $s^{\mathrm{gp}} : P^{\mathrm{gp}} \to M_{X,\bar{x}}^{\mathrm{gp}}$ is P. Hence, by [Kato 1989, Lemma (2.10)], the section s is extended to a chart $P_U \to M_X|_U$ for an étale neighborhood U of x. □

Definition II.2.10. Let p be a prime. We say a morphism of integral log schemes $f : (X, M_X) \to (Y, M_Y)$ is *p-saturated* (resp. *saturated*) if, for every $x \in X$ and $y = f(x) \in Y$, the morphism $(M_Y/\mathcal{O}_Y^*)_{\bar{y}} \to (M_X/\mathcal{O}_X^*)_{\bar{x}}$ induced by f is p-saturated (resp. saturated).

Note that p-saturated morphisms and saturated morphisms are integral and that a morphism of integral log schemes is saturated if and only if it is p-saturated for every prime p.

Proposition II.2.11. *Let p be a prime.*

(1) *Let $f : (X, M_X) \to (Y, M_Y)$ and $g : (Y, M_Y) \to (Z, M_Z)$ be morphisms of integral log schemes. If f and g are p-saturated (resp. saturated), then $g \circ f$ is also p-saturated (resp. saturated).*

(2) *Let $f : (X, M_X) \to (Y, M_Y)$ and $g : (Y', M_{Y'}) \to (Y, M_Y)$ be morphisms of integral log schemes. If f is p-saturated (resp. saturated), then the base change $f' : (X', M_{X'}) \to (Y', M_{Y'})$ of f by g in the category of log schemes, is also p-saturated (resp. saturated).*

Proof. The claim (1) follows from Propositions I.2.3 (1) and I.3.6 (1), and (2) follows from Propositions II.1.2, I.2.3 (2) and I.3.6 (2). □

Proposition II.2.12. *Let p be a prime. Let $f : (X, M_X) \to (Y, M_Y)$ be a morphism of integral log schemes. If f is p-saturated (resp. saturated) and M_Y is p-saturated (resp. saturated), then M_X is p-saturated (resp. saturated).*

Proof. Take $x \in X$ and $y = f(x) \in Y$. If M_Y is p-saturated (resp. saturated), then $(M_Y/\mathcal{O}_Y^*)_{\bar{y}}$ is p-saturated (resp. saturated). Hence, by Proposition I.3.9, if f is p-saturated (resp. saturated), then $(M_X/\mathcal{O}_X^*)_{\bar{x}}$ is p-saturated (resp. saturated). Since M_X is integral, this implies that $(M_X)_{\bar{x}}$ is p-saturated (resp. saturated). □

Proposition II.2.13. *Let p be a prime.*

(1) *Let $f : (X, M_X) \to (Y, M_Y)$ be an integral morphism of p-saturated* (*resp. saturated*) *log schemes. Then f is p-saturated* (*resp. saturated*) *if and only if, for any p-saturated* (*resp. saturated*) *log scheme $(Y', M_{Y'})$ and any morphism $g : (Y', M_{Y'}) \to (Y, M_Y)$, the base change $(X', M_{X'})$ of (X, M_X) by g in the category of log schemes is p-saturated* (*resp. saturated*).

(2) *Let $f : (X, M_X) \to (Y, M_Y)$ be an integral morphism of fine and p-saturated* (*resp. saturated*) *log schemes. Then f is p-saturated* (*resp. saturated*) *if and only if, for any fine and p-saturated* (*resp. saturated*) *log scheme $(Y', M_{Y'})$ and any morphism $g : (Y', M_{Y'}) \to (Y, M_Y)$, the base change $(X', M_{X'})$ of (X, M_X) by g in the category of log schemes is p-saturated* (*resp. saturated*).

Proof. The necessity follows from Propositions II.2.11 (2) and II.2.12. Let us prove the sufficiency. Let $f : (X, M_X) \to (Y, M_Y)$ be an integral morphism of integral log schemes. Take $x \in X$ and $y = f(x) \in Y$. Let k be an algebraic closure of the residue field of Y at y and set $\bar{y} := \mathrm{Spec}(k)$. Let N be the inverse image of M_Y under the canonical morphism $i_{\bar{y}} : \bar{y} \to Y$. Then, by Proposition II.1.3, there exists a section α of the projection $\Gamma(\bar{y}, N) \to \Gamma(\bar{y}, N)/k^* =: P$, which induces an isomorphism $(P_{\bar{y}})^a \cong N$. Let n be a positive integer and define a morphism $g : (\bar{y}, N) \to (\bar{y}, N)$ by the multiplication by n on P and the identity on k. Let $(X', M_{X'})$ be the base change of (X, M_X) by the morphism $i_{\bar{y}} \circ g : (\bar{y}, N) \to (Y, M_Y)$. Let x' be a point on X' whose image in X is x. Then, by Proposition II.1.2, the following diagram of monoids is cocartesian:

$$\begin{array}{ccc} (M_{X'}/\mathcal{O}_{X'}^*)_{\bar{x}'} & \longleftarrow & (M_X/\mathcal{O}_X^*)_{\bar{x}} \\ \uparrow & & \uparrow \\ P = N_{\bar{y}}/k^* & \xleftarrow{\ n\ } & P = N_{\bar{y}}/k^* = (M_Y/\mathcal{O}_Y^*)_{\bar{y}} \end{array}$$

If M_X, M_Y and $M_{X'}$ are p-saturated (resp. saturated), then the log structure N is p-saturated (resp. saturated) and the monoids $(M_X/\mathcal{O}_X^*)_{\bar{x}}$, $(M_Y/\mathcal{O}_Y^*)_{\bar{y}}$, P and $(M_{X'}/\mathcal{O}_{X'}^*)_{\bar{x}'}$ are p-saturated (resp. saturated). Now the claim (1) follows from Propositions I.3.13 and I.3.14. The claim (2) follows from the same propositions and the fact that N is fine if M_Y is fine. □

Proposition II.2.14. *Let p be a prime and let $f : (X, M_X) \to (Y, M_Y)$ be a morphism of integral log schemes over $\mathbb{F}_p$. Then f is p-saturated if and only if f is of Cartier type.*

Proof. This follows from Proposition II.1.2 and the fact that, for $x \in X$ and $y = f(x) \in Y$, the absolute Frobenius of (X, M_X) (resp. (Y, M_Y)) induces the multiplication by p on $(M_X/\mathcal{O}_X^*)_{\bar{x}}$ (resp. $(M_Y/\mathcal{O}_Y^*)_{\bar{y}}$). □

II.3. *Some properties of saturated morphisms.*

Theorem II.3.1. *Let p and q be two different primes. Let $f : (X, M_X) \to (Y, M_Y)$ be a morphism of fine log schemes. If f is p-saturated and M_X is q-saturated, then f is q-saturated.*

Proof. This follows from Corollary I.4.5. □

By Proposition II.2.14, this theorem implies that a morphism of fine saturated log schemes over $\mathbb{F}_p$ is of Cartier type if and only if it is saturated. This is an unpublished result of K. Kato.

Definition II.3.2. We say a morphism of log schemes $f : (X, M_X) \to (Y, M_Y)$ is *vertical* if, for every $x \in X$ and $y = f(x) \in Y$, the morphism $M_{Y,\bar{y}} \to M_{X,\bar{x}}$ induced by f is vertical (Definition I.4.6), or equivalently, the morphism $(M_Y/\mathcal{O}_Y^*)_{\bar{y}} \to (M_X/\mathcal{O}_X^*)_{\bar{x}}$ induced by f is vertical.

Theorem II.3.3. *Let p be a prime and let $f : (X, M_X) \to (Y, M_Y)$ be a morphism of fine log schemes. If f is p-saturated and vertical, then f is saturated.*

Proof. This follows from Corollary I.4.7. □

Theorem II.3.4. *Let $f : (X, M_X) \to (Y, M_Y)$ be an integral morphism of fine saturated log schemes and assume that we are given a chart $\beta : Q_Y \to M_Y$ of M_Y with Q saturated. If X is quasi-compact, then there exists a positive integer n satisfying the following property: Define a fine saturated log scheme $(Y', M_{Y'})$ to be*

$$(Y, M_Y) \times_{(\mathrm{Spec}(\mathbb{Z}[Q]),\text{can. log}),g} (\mathrm{Spec}(\mathbb{Z}[Q]), \text{can. log}),$$

where $g : (\mathrm{Spec}(\mathbb{Z}[Q]), \text{can. log}) \to (\mathrm{Spec}(\mathbb{Z}[Q]), \text{can. log})$ denotes the morphism induced by the multiplication by n on Q. Then, the base change $f' : (X', M_{X'}) \to (Y', M_{Y'})$ of f by the projection $(Y', M_{Y'}) \to (Y, M_Y)$ in the category of fine saturated log schemes is saturated.

Proof. Note first that the question is étale local on Y and on X. So we may assume that there exists a chart $(\alpha : P_X \to M_X, \beta, h : Q \to P)$ of the morphism f. Take $x \in X$ and $y = f(x) \in Y$. Let $\mathfrak{p}$ (resp. $\mathfrak{q}$) be the inverse image of the maximal ideal of $\mathcal{O}_{X,\bar{x}}$ (resp. $\mathcal{O}_{Y,\bar{y}}$) in P (resp. Q), which is a prime ideal. Since $((Q\backslash\mathfrak{q})^n)^{-1}Q \cong Q_{\mathfrak{q}}$, we may replace P, Q by $P_{\mathfrak{p}}$, $Q_{\mathfrak{q}}$ using Proposition II.1.4, and assume that α (resp. β) induces an isomorphism $P/P^* \cong (M_X/\mathcal{O}_X^*)_{\bar{x}}$ (resp. $Q/Q^* \cong (M_Y/\mathcal{O}_Y^*)_{\bar{y}}$). Since M_X is saturated and P is integral, P is saturated by Lemma I.3.15. Furthermore, since the morphism $(M_Y/\mathcal{O}_Y^*)_{\bar{y}} \to (M_X/\mathcal{O}_X^*)_{\bar{x}}$ is integral by assumption, the morphism $h : Q \to P$ is integral by Proposition I.2.5. Now we can apply Corollary I.5.4

to $h : Q \to P$ and find a positive integer n satisfying the following property: If we denote by P' the pushout of the diagram $Q \xleftarrow{n} Q \xrightarrow{h} P$ in the category of monoids, then the canonical morphism $h' : Q \to P' \to (P')^{\mathrm{sat}}$ is saturated. We assert that this n is the desired integer. Let $(X'', M_{X''})$ be the base change of (X, M) by $(Y', M_{Y'}) \to (Y, M_Y)$ in the category of log schemes. Then, since the diagram of log schemes

$$\begin{array}{ccc} (\mathrm{Spec}(\mathbb{Z}[P']), \text{can. log}) & \longrightarrow & (\mathrm{Spec}(\mathbb{Z}[P]), \text{can. log}) \\ \downarrow & & \downarrow \\ (\mathrm{Spec}(\mathbb{Z}[Q]), \text{can. log}) & \xrightarrow{g} & (\mathrm{Spec}(\mathbb{Z}[Q]), \text{can. log}) \end{array}$$

is cartesian, the three strict morphisms

$$(X, M_X) \to (\mathrm{Spec}(\mathbb{Z}[P]), \text{can. log}), \quad (Y, M_Y) \to (\mathrm{Spec}(\mathbb{Z}[Q]), \text{can. log}),$$
$$(Y', M_{Y'}) \to (\mathrm{Spec}(\mathbb{Z}[Q]), \text{can. log})$$

induce a strict morphism $(X'', M_{X''}) \to (\mathrm{Spec}(\mathbb{Z}[P']), \text{can. log})$ and hence a strict morphism $(X', M_{X'}) \to (\mathrm{Spec}(\mathbb{Z}[(P')^{\mathrm{sat}}], \text{can. log}))$. (Recall that we say a morphism of log schemes $\varphi : (S, M_S) \to (T, M_T)$ is strict if the morphism $\varphi^*(M_T) \to M_S$ is an isomorphism.) Thus, we obtain a chart

$$\big(((P')^{\mathrm{sat}})_{X'} \to M_{X'},\ Q_{Y'} \to M_{Y'},\ h' : Q \to (P')^{\mathrm{sat}}\big)$$

of f' such that h' is saturated. Now the claim follows from Lemma II.3.5 below. □

Lemma II.3.5. *Let $f : (X, M_X) \to (Y, M_Y)$ be a morphism of fine saturated log schemes. Suppose that there exists a chart $(\alpha : P_X \to M_X, \beta : Q_Y \to M_Y, h : Q \to P)$ of f such that P and Q are saturated and h is saturated. Then, the morphism f is saturated.*

Proof. Take $x \in X$ and $y = f(x) \in Y$. Let $\mathfrak{p}$ (resp. $\mathfrak{q}$) be the inverse image of the maximal ideal of $\mathcal{O}_{X,\bar{x}}$ (resp. $\mathcal{O}_{Y,\bar{y}}$) in P (resp. Q), which is a prime ideal. Then, by Proposition II.1.4 (1), the morphism α (resp. β) induces an isomorphism $P_{\mathfrak{p}}/P^*_{\mathfrak{p}} \cong (M_X/\mathcal{O}^*_X)_{\bar{x}}$ (resp. $Q_{\mathfrak{q}}/Q^*_{\mathfrak{q}} \cong (M_Y/\mathcal{O}^*_Y)_{\bar{y}}$). Since the morphism $Q_{\mathfrak{q}}/Q^*_{\mathfrak{q}} \to P_{\mathfrak{p}}/P^*_{\mathfrak{p}}$ induced by h is saturated by Propositions I.3.16 and I.3.18, the morphism $(M_Y/\mathcal{O}^*_Y)_{\bar{y}} \to (M_X/\mathcal{O}^*_X)_{\bar{x}}$ induced by f is saturated. □

II.4. *Criteria of saturated morphisms.*

Proposition II.4.1. *Let $f : (X, M_X) \to (Y, M_Y)$ be a smooth integral morphism of fine saturated log schemes. Then, every fiber of the underlying morphism of schemes of f is Cohen–Macaulay.*

Proof. First note that the question is étale local on X and on Y. Take $x \in X$ and $y = f(x) \in Y$. By Proposition II.2.9, we may assume that we have a chart

$\beta : Q_Y \to M_Y$ which induces an isomorphism $Q \cong (M_Y/\mathcal{O}_Y^*)_{\bar{y}}$. By [Kato 1989, Theorem (3.5)], we may assume that, there exists a chart of f,

$$(\alpha : P_X \to M_X,\ \beta : Q_Y \to M_Y,\ h : Q \to P),$$

such that h is injective, the order of the torsion part of the cokernel of $h^{\mathrm{gp}} : Q^{\mathrm{gp}} \to P^{\mathrm{gp}}$ is invertible on X and the morphism $X \to Y \times_{\mathrm{Spec}(\mathbb{Z}[Q])} \mathrm{Spec}(\mathbb{Z}[P])$ induced by the chart is étale. Let $\mathfrak{p}$ be the inverse image of the maximal ideal of $\mathcal{O}_{X,\bar{x}}$ in P. By Proposition II.1.4, we may replace P by $P_{\mathfrak{p}}$ and assume that α induces an isomorphism $P/P^* \cong (M_X/\mathcal{O}_X^*)_{\bar{x}}$. Since P is integral and $P/P^* \cong (M_X/\mathcal{O}_X^*)_{\bar{x}}$ is saturated, P is saturated by Lemma I.3.15. Since the morphism $(M_Y/\mathcal{O}_Y^*)_{\bar{y}} \to (M_X/\mathcal{O}_X^*)_{\bar{x}}$ induced by f is integral by assumption, the morphism h is integral by Proposition I.2.5. Furthermore, we have $h^{-1}(P^*) = Q^* = \{1\}$. Hence, by Corollary I.6.6, the ring $k[P]/h(Q\backslash\{1\})k[P]$ is Cohen–Macaulay for any field k. If we choose the residue field of Y at y as k, then we have an étale morphism $f^{-1}(y) \to \mathrm{Spec}(k[P]/h(Q\backslash\{1\})k[P])$ by the choice of the chart. Hence $f^{-1}(y)$ is Cohen–Macaulay. □

Theorem II.4.2. *Let $f : (X, M_X) \to (Y, M_Y)$ be a smooth integral morphism of fine saturated log schemes. Then the following conditions are equivalent*:

(1) *f is saturated.*

(2) *There exists a prime p such that f is p-saturated.*

(3) *Every fiber of the underlying morphism of schemes of f is reduced.*

(4) *Every fiber of the underlying morphism of schemes of f satisfies (R_0).*

Proof. By Theorem II.3.1, (1) and (2) are equivalent. By Proposition II.4.1, (3) and (4) are equivalent. We will prove that (1) and (3) are equivalent.

Take $x \in X$ and $y = f(x) \in Y$. As in the proof of Proposition II.4.1, we may assume that there exists a chart $(\alpha : P_X \to M_X, \beta : Q_Y \to M_Y, h : Q \to P)$ of the morphism f such that $h^{\mathrm{gp}} : Q^{\mathrm{gp}} \to P^{\mathrm{gp}}$ is injective, the order of the torsion part of the cokernel of h^{gp} is invertible on X, the morphism $X \to Y \times_{\mathrm{Spec}(\mathbb{Z}[Q])} \mathrm{Spec}(\mathbb{Z}[P])$ induced by the chart is étale, and the morphism α (resp. β) induces an isomorphism $P/P^* \cong (M_X/\mathcal{O}_X^*)_{\bar{x}}$ (resp. $Q \cong (M_Y/\mathcal{O}_Y^*)_{\bar{y}}$). Furthermore, as in the proof of Proposition II.4.1, these properties imply that P and Q are saturated, the morphism h is integral, and $h^{-1}(P^*) = Q^* = \{1\}$. We also see that Q^{gp} is torsion-free, and the order of the torsion part of P^{gp} is invertible on X.

(1) $\Rightarrow$ (3): We will prove that $f^{-1}(y)$ is reduced. Since $(M_Y/\mathcal{O}_Y^*)_{\bar{y}} \to (M_X/\mathcal{O}_X^*)_{\bar{x}}$ is saturated, the morphism $h : Q \to P$ is saturated by Proposition I.3.16. Let k be the residue field of Y at y. Then the scheme $\mathrm{Spec}(k[P]/h(Q\backslash\{1\})k[P])$ is reduced, by Theorem I.6.3. Since $f^{-1}(y)$ is étale over the last scheme by the choice of the chart, the scheme $f^{-1}(y)$ is also reduced.

(3) $\Rightarrow$ (1): We will prove that the morphism $(M_Y/\mathcal{O}_Y^*)_{\bar{y}} \to (M_X/\mathcal{O}_X^*)_{\bar{x}}$ induced by f is saturated. Let k be the residue field of Y at y. Then, by the choice of the chart, the morphism $f^{-1}(y) \to \mathrm{Spec}(k[P]/h(Q\backslash\{1\})k[P])$ induced by the chart is étale. Let $\bar{P}$ be the quotient P/P^* and let $\bar{h} : Q \to \bar{P}$ be the morphism induced by $h : Q \to P$. Then, $\bar{P}^* = \{1\}$, $\bar{h}^{-1}(\bar{P}^*) = Q^*(= \{1\})$, and the morphism $\bar{h}$ is integral (Proposition I.2.5). By the choice of the chart of f, we have the following commutative diagram whose horizontal arrows are isomorphisms:

$$\begin{array}{ccc} (M_X/\mathcal{O}_X^*)_{\bar{x}} & \xleftarrow{\sim} & \bar{P} \\ \uparrow{\scriptstyle f_{\bar{x}}^*} & & \uparrow{\scriptstyle \bar{h}} \\ (M_Y/\mathcal{O}_Y^*)_{\bar{y}} & \xleftarrow{\sim} & Q \end{array}$$

Hence, by Theorem I.6.3, it suffices to prove that the scheme

$$\bar{Z} := \mathrm{Spec}(k[\bar{P}]/\bar{h}(Q\backslash\{1\})k[\bar{P}])$$

satisfies (R_0). Choose a section $s : \bar{P} \to P$ of the projection $P \to \bar{P}$. Such a section exists and it induces an isomorphism $(\iota, s) : P^* \oplus \bar{P} \xrightarrow{\sim} P$ by Lemma I.6.7. We have $h(Q\backslash\{1\})k[P] = s \circ \bar{h}(Q\backslash\{1\})k[P]$ because, for any $b \in Q$, there exists $a \in P^*$ such that $h(b) = s \circ \bar{h}(b)a$. On the other hand, we see that the morphism $\mathrm{Spec}(k[P]/s \circ \bar{h}(Q\backslash\{1\})k[P]) \to \bar{Z} = \mathrm{Spec}(k[\bar{P}]/\bar{h}(Q\backslash\{1\})k[\bar{P}])$ induced by s is smooth as follows. Since the order of the torsion part of $P^*(\subset P^{\mathrm{gp}})$ is invertible on k, $\mathrm{Spec}(k[P^*])$ is smooth over k and hence $\mathrm{Spec}(k[P]) \cong \mathrm{Spec}(k[P^*] \otimes_k k[\bar{P}])$ is smooth over $\mathrm{Spec}(k[\bar{P}])$. Now we have smooth morphisms

$$\begin{aligned} f^{-1}(y) \longrightarrow \mathrm{Spec}(k[P]/h(Q\backslash\{1\})k[P]) &= \mathrm{Spec}(k[P]/s \circ \bar{h}(Q\backslash\{1\})k[P]) \\ &\longrightarrow \bar{Z} = \mathrm{Spec}(k[\bar{P}]/\bar{h}(Q\backslash\{1\})k[\bar{P}]). \end{aligned}$$

Since $f^{-1}(y)$ is reduced by assumption, $\bar{Z}$ is reduced on an open neighborhood of the image x_0 of x. In fact, x_0 is the closed point defined by the ideal generated by $\bar{P}\backslash\{1\}$ because we have $s(\bar{P}\backslash\{1\}) \subset P\backslash P^*$ and the image of $P\backslash P^*$ in $\mathcal{O}_{X,\bar{x}}$ under $\alpha_{\bar{x}} : P \to \mathcal{O}_{X,\bar{x}}$ is contained in the maximal ideal. Hence, by Lemma II.4.3 below, the scheme $\bar{Z}$ satisfies (R_0). □

Lemma II.4.3. *Let P be a finitely generated integral monoid such that P^{gp} is torsion-free, and let I be an ideal of P. Let k be a field. Then, for any point z of codimension* 0 *of the scheme* $Z := \mathrm{Spec}(k[P]/Ik[P])$, $\overline{\{z\}}$ *contains the underlying set of the closed subscheme* $\mathrm{Spec}(k[P]/(P\backslash P^*)k[P])$ *of Z.*

Proof. Let $\mathfrak{p}$ be the inverse image of the maximal ideal of $\mathcal{O}_{Z,z}$ in P, which obviously contains I. Then we have $\mathfrak{p} \subset P\backslash P^*$, and z is of codimension 0 in the closed subscheme $\mathrm{Spec}(k[P]/\mathfrak{p}k[P])$ of Z. Hence the claim follows from Sublemma II.4.4 below. □

Sublemma II.4.4. *Let P be a finitely generated integral monoid such that P^{gp} is torsion-free. Then, for any prime ideal $\mathfrak{p}$ of P and any field k, the ring $k[P]/\mathfrak{p}k[P]$ is an integral domain.*

Proof. The morphism of monoids $P\backslash\mathfrak{p} \to P$ induces an isomorphism $k[P\backslash\mathfrak{p}] \xrightarrow{\sim} k[P]/\mathfrak{p}k[P]$. The ring $k[P\backslash\mathfrak{p}]$ is a subring of $k[(P\backslash\mathfrak{p})^{\mathrm{gp}}]$, and $k[(P\backslash\mathfrak{p})^{\mathrm{gp}}]$ is an integral domain because $(P\backslash\mathfrak{p})^{\mathrm{gp}}$ is torsion-free by assumption. □

Definition II.4.5 (cf. [Kato 1994, (2.1) Definition]). Let (X, M_X) be a fine saturated log scheme such that X is locally noetherian. We say (X, M_X) is *regular* at $x \in X$ if $\mathcal{O}_{X,\bar{x}}/I_{\bar{x}}\mathcal{O}_{X,\bar{x}}$ is regular and

$$\dim(\mathcal{O}_{X,\bar{x}}) = \dim(\mathcal{O}_{X,\bar{x}}/I_{\bar{x}}\mathcal{O}_{X,\bar{x}}) + \mathrm{rank}_{\mathbb{Z}}((M_X^{\mathrm{gp}}/\mathcal{O}_X^*)_{\bar{x}}),$$

where $I_{\bar{x}} = M_{X,\bar{x}}\backslash\mathcal{O}^*_{X,\bar{x}}$ and $I_{\bar{x}}\mathcal{O}_{X,\bar{x}}$ denotes the ideal of $\mathcal{O}_{X,\bar{x}}$ generated by the image of $I_{\bar{x}}$. We say (X, M_X) is *regular* if (X, M_X) is regular at every point $x \in X$.

Lemma II.4.6. *Let (X, M_X) be a fine saturated log scheme such that X is locally noetherian, and assume that we are given a chart $P_X \to M_X$ with P saturated. Let M_X^{Zar} be the log structure on the Zariski site [Kato 1994, §1] associated to $P \to \Gamma(X, M_X) \to \Gamma(X, \mathcal{O}_X)$. Then, for any $x \in X$, (X, M_X) is regular at x if and only if (X, M_X^{Zar}) is regular [Kato 1994, (2.1) Definition] at x.*

Proof. Let $\mathfrak{p}$ be the inverse image of the maximal ideal of $\mathcal{O}_{X,\bar{x}}$ in P. Then $\mathfrak{p}$ is also the inverse image of the maximal ideal of $\mathcal{O}_{X,x}$ because the morphism $\mathcal{O}_{X,x} \to \mathcal{O}_{X,\bar{x}}$ is local. Hence, by Proposition II.1.4 and the corresponding fact for log structures in Zariski topology, the canonical morphisms $P_X \to M_X$ on $X_{\text{ét}}$ and $P_X \to M_X^{\mathrm{Zar}}$ on X_{Zar} induce isomorphisms $P_{\mathfrak{p}}/P_{\mathfrak{p}}^* \cong M_{X,\bar{x}}/\mathcal{O}^*_{X,\bar{x}}$ and $P_{\mathfrak{p}}/P_{\mathfrak{p}}^* \cong M^{\mathrm{Zar}}_{X,x}/\mathcal{O}^*_{X,x}$. In particular $\mathrm{rank}_{\mathbb{Z}}((M_X^{\mathrm{gp}}/\mathcal{O}_X^*)_{\bar{x}}) = \mathrm{rank}_{\mathbb{Z}}(((M_X^{\mathrm{Zar}})^{\mathrm{gp}}/\mathcal{O}_X^*)_x)$. On the other hand, if we set $I_{\bar{x}} = M_{X,\bar{x}}\backslash\mathcal{O}^*_{X,\bar{x}}$ and $I_x = (M_X^{\mathrm{Zar}})_x\backslash\mathcal{O}^*_{X,x}$, we have $I_{\bar{x}}\mathcal{O}_{X,\bar{x}} = \mathfrak{p}\mathcal{O}_{X,\bar{x}}$ and $I_x\mathcal{O}_{X,x} = \mathfrak{p}\mathcal{O}_{X,x}$. Hence $\mathcal{O}_{X,\bar{x}}/I_{\bar{x}}\mathcal{O}_{X,\bar{x}}$ is the strict henselization of $\mathcal{O}_{X,x}/I_x\mathcal{O}_{X,x}$. So $\mathcal{O}_{X,\bar{x}}/I_{\bar{x}}\mathcal{O}_{X,\bar{x}}$ is regular if and only if $\mathcal{O}_{X,x}/I_x\mathcal{O}_{X,x}$ is regular. Now the lemma is a direct consequence of the definition. □

Theorem II.4.7 (cf. [Kato 1994, (4.1) Theorem]). *Let (X, M_X) be a fine saturated log scheme. If (X, M_X) is regular, then X is Cohen–Macaulay and normal.*

Proof. Since the question is étale local on X, the proposition follows from [Kato 1994, (4.1) Theorem], Lemma II.4.6 and Corollary II.2.8. □

Proposition II.4.8 (cf. [Kato 1994, (8.2) Theorem]). *Let $f : (X, M_X) \to (Y, M_Y)$ be a smooth morphism of fine saturated log schemes. If (Y, M_Y) is regular, then (X, M_X) is regular.*

Proof. Since the question is étale local on X and on Y, as in the proof of Proposition II.4.1, we may assume that there exists a chart

$$(\alpha : P_X \to M_X,\ \beta : Q_Y \to M_Y,\ h : Q \to P)$$

of the morphism f such that P and Q are saturated, h is injective, the order of the torsion part of the cokernel of $h^{\mathrm{gp}} : Q^{\mathrm{gp}} \to P^{\mathrm{gp}}$ is invertible on X and the morphism $X \to Y \times_{\mathrm{Spec}(\mathbb{Z}[Q])} \mathrm{Spec}(\mathbb{Z}[P])$ induced by the chart is étale. Then the proposition follows from Lemma II.4.6 and [Kato 1994, (8.1) and (8.2) Theorem]. □

Lemma II.4.9 (cf. [Kato 1994, (7.3) Corollary]). *Let (X, M_X) be a regular fine saturated log scheme. Let $x \in X$ and assume that we are given a chart $\alpha : P_X \to M_X$ with P saturated such that the inverse image of the maximal ideal of $\mathcal{O}_{X,\bar{x}}$ under $P \xrightarrow{\alpha_{\bar{x}}} M_{X,\bar{x}} \to \mathcal{O}_{X,\bar{x}}$ is $P\backslash P^*$. Then, for any prime ideal $\mathfrak{p}$ of P, there exists a point $y \in X$ which satisfies the following conditions*:

(1) $x \in \overline{\{y\}}$.

(2) *The inverse image of the maximal ideal of $\mathcal{O}_{X,\bar{y}}$ in P is $\mathfrak{p}$.*

(3) *The image of $\mathfrak{p}$ in $\mathcal{O}_{X,\bar{y}}$ generates the maximal ideal.*

(4) $\dim(\mathcal{O}_{X,y}) = \mathrm{ht}(\mathfrak{p})$.

Proof. Let M_X^{Zar} be the log structure on the Zariski site associated to

$$P \to \Gamma(X, M) \to \Gamma(X, \mathcal{O}_X).$$

By Lemma II.4.6, (X, M_X^{Zar}) is regular. Since the homomorphism $\mathcal{O}_{X,x} \to \mathcal{O}_{X,\bar{x}}$ is local, the inverse image of the maximal ideal of $\mathcal{O}_{X,x}$ in P is also $P\backslash P^*$. Hence the canonical morphism $P/P^* \to M_{X,x}^{\mathrm{Zar}}/\mathcal{O}_{X,x}^*$ is an isomorphism. Thus the map $\mathrm{Spec}(M_{X,x}^{\mathrm{Zar}}) \to \mathrm{Spec}(P)$ induced by $P \to M_{X,x}^{\mathrm{Zar}}$ is bijective. Let $\mathfrak{q}$ be the prime ideal of $M_{X,x}^{\mathrm{Zar}}$ corresponding to $\mathfrak{p}$ under this bijection. Then, $\mathfrak{q}$ is generated by the image of $\mathfrak{p}$ and $\mathrm{ht}(\mathfrak{q}) = \mathrm{ht}(\mathfrak{p})$. Hence, by [Kato 1994, (7.3) Corollary], the ideal $\mathfrak{p}\mathcal{O}_{X,x} (= \mathfrak{q}\mathcal{O}_{X,x})$ is a prime ideal of height $\mathrm{ht}(\mathfrak{p}) (= \mathrm{ht}(\mathfrak{q}))$. Let $y \in \mathrm{Spec}(\mathcal{O}_{X,x}) \subset X$ be the point corresponding to the prime ideal. We assert that y satisfies the required conditions. The conditions (1), (3) and (4) are trivial. For (2), it suffices to prove that the inverse image of the maximal ideal of $\mathcal{O}_{X,y}$ in P is $\mathfrak{p}$. Let $\mathfrak{p}'$ be the inverse image. By the analogue of Proposition II.1.4 (1) for log structures in Zariski topology, we have $P_{\mathfrak{p}'}/P_{\mathfrak{p}'}^* \cong (M_X^{\mathrm{Zar}}/\mathcal{O}_X^*)_y$. Since the image of $\mathfrak{p}$ ($\subset P$) in $\mathcal{O}_{X,y}$ generates the maximal ideal and (X, M_X^{Zar}) is regular, we have $\mathrm{ht}(\mathfrak{p}) = \mathrm{ht}(\mathfrak{p}\mathcal{O}_{X,x}) = \dim(\mathcal{O}_{X,y}) = \mathrm{rank}_{\mathbb{Z}}((M_X^{\mathrm{Zar}}/\mathcal{O}_X^*)_y) = \mathrm{rank}_{\mathbb{Z}}(P_{\mathfrak{p}'}/P_{\mathfrak{p}'}^*) = \mathrm{ht}(\mathfrak{p}')$. (The last equality follows from Proposition I.1.3 (2).) Since $\mathfrak{p} \subset \mathfrak{p}'$, this implies $\mathfrak{p} = \mathfrak{p}'$. □

Lemma II.4.10. *Let (X, M_X) be a regular fine saturated log scheme and assume that we are given a chart $P_X \to M_X$ with P saturated. Let x be a point of X of codimension 1 such that $M_{X,\bar{x}} \neq \mathcal{O}_{X,\bar{x}}^*$ and let $\mathfrak{p}$ denote the inverse image of the* *maximal ideal of* $\mathcal{O}_{X,\bar{x}}$ *in* P. *Then,* $\mathfrak{p}$ *is a prime ideal of height* 1 *and the composite* $P \to \mathcal{O}_{X,\bar{x}} \xrightarrow{v_{\bar{x}}} \mathbb{Z}$ *coincides with the valuation* $v_{\mathfrak{p}}$ *associated to* $\mathfrak{p}$, *where* $v_{\bar{x}}$ *denotes the discrete valuation of* $\mathcal{O}_{X,\bar{x}}$.

Proof. Note first that $\mathcal{O}_{X,\bar{x}}$ is a discrete valuation ring by Theorem II.4.7. By Proposition II.1.4 (1), we have $P_{\mathfrak{p}}/P_{\mathfrak{p}}^* \cong M_{X,\bar{x}}/\mathcal{O}_{X,\bar{x}}^*$. Since (X, M_X) is regular and $M_{X,\bar{x}}/\mathcal{O}_{X,\bar{x}}^* \neq \{1\}$, the group $M_{X,\bar{x}}^{\mathrm{gp}}/\mathcal{O}_{X,\bar{x}}^*$ has rank 1 and the maximal ideal of $\mathcal{O}_{X,\bar{x}}$ is generated by the image of $I_{\bar{x}} := M_{X,\bar{x}} \backslash \mathcal{O}_{X,\bar{x}}^*$. By Proposition I.1.3 (2), $\mathrm{ht}(\mathfrak{p}) = 1$. On the other hand, we see easily that $I_{\bar{x}}$ is generated by the image of $\mathfrak{p}$ and hence the maximal ideal of $\mathcal{O}_{X,\bar{x}}$ is generated by the image of $\mathfrak{p}$. Since the inverse image of $\mathcal{O}_{X,\bar{x}}^*$ under the morphism $P_{\mathfrak{p}} \to \mathcal{O}_{X,\bar{x}}$ is $P_{\mathfrak{p}}^*$, this implies that the composite $P \to \mathcal{O}_{X,\bar{x}} \xrightarrow{v_{\bar{x}}} \mathbb{Z}$ coincides with $v_{\mathfrak{p}}$. □

Theorem II.4.11. *Let* $f : (X, M_X) \to (Y, M_Y)$ *be a smooth integral morphism of fine saturated log schemes and assume that* (Y, M_Y) *is regular. Then* f *is saturated if and only if, for every point* y *of* Y *of codimension* 1 *such that* $M_{Y,\bar{y}} \neq \mathcal{O}_{Y,\bar{y}}^*$, *the fiber of the underlying morphism of schemes of* f *over* y *satisfies* (R_0).

Proof. The necessity follows from Theorem II.4.2. We will prove the sufficiency. By Proposition II.4.8, (X, M_X) is regular. Take $x \in X$ and $y = f(x) \in Y$. We will prove that the morphism $(M_Y/\mathcal{O}_Y^*)_{\bar{y}} \to (M_X/\mathcal{O}_X^*)_{\bar{x}}$ induced by f is saturated. By Proposition II.1.4 (2), we may assume that we have a chart of f,

$$(\alpha : P_X \to M_X,\ \beta : Q_Y \to M_Y,\ h : Q \to P),$$

such that α (resp. β) induces an isomorphism $P/P^* \cong (M_X/\mathcal{O}_X^*)_{\bar{x}}$ (resp. $Q/Q^* \cong (M_Y/\mathcal{O}_Y^*)_{\bar{y}}$). By Lemma I.3.15, P and Q are saturated. By Proposition I.2.5, h is integral. Let $\mathfrak{p}$ be a prime ideal of P of height 1 such that the prime ideal $\mathfrak{q} := h^{-1}(\mathfrak{p})$ of Q is also of height 1. By Theorem I.5.1, it suffices to prove that the ramification index of h at $\mathfrak{p}$ is 1. By Lemma II.4.9, there exists a point $x' \in X$ of codimension 1 such that the inverse image of the maximal ideal of $\mathcal{O}_{X,\bar{x}'}$ in P is $\mathfrak{p}$ and the maximal ideal is generated by the image of $\mathfrak{p}$. Set $y' = f(x')$. Then, since the homomorphism $\mathcal{O}_{Y,\bar{y}'} \to \mathcal{O}_{X,\bar{x}'}$ is local, the inverse image of the maximal ideal of $\mathcal{O}_{Y,\bar{y}'}$ in Q is $\mathfrak{q}$ and hence β induces an isomorphism $Q_{\mathfrak{q}}/Q_{\mathfrak{q}}^* \cong (M_Y/\mathcal{O}_Y^*)_{\bar{y}'}$ by Proposition II.1.4 (1). Since $(Q_{\mathfrak{q}})^{\mathrm{gp}}/Q_{\mathfrak{q}}^*$ is of rank 1 and (Y, M_Y) is regular, we have $\dim(\mathcal{O}_{Y,\bar{y}'}) \geq 1$. On the other hand, the underlying morphism of schemes of f is flat by [Kato 1989, Corollary (4.5)]. Hence

$$\dim(\mathcal{O}_{Y,\bar{y}'}) = \dim(\mathcal{O}_{X,\bar{x}'}) = 1$$

and the codimension of x' in $f^{-1}(y')$ is 0. Since $M_{Y,\bar{y}'} \neq \mathcal{O}_{Y,\bar{y}'}^*$, the maximal ideal of $\mathcal{O}_{X,\bar{x}'}$ is generated by the image of the maximal ideal of $\mathcal{O}_{Y,\bar{y}'}$ by the assumption on f. By Lemma II.4.10, it follows that the ramification index of h at $\mathfrak{p}$ is 1. □

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Quantum mean-field asymptotics and multiscale analysis

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We study, via multiscale analysis, a defect-of-compactness phenomenon which occurs in bosonic and fermionic quantum mean-field problems. The approach relies on a combination of mean-field asymptotics and second microlocalized semiclassical measures. The phase space geometric description is illustrated by various examples.

1. Introduction

Motivations. Over the past three decades, microlocal and semiclassical analysis has provided interesting mathematical techniques for the study of quantum field theory and quantum many-body theory; see for instance [Ammari and Nier 2008; Brunetti and Fredenhagen 2000; Fournais et al. 2015; Fröhlich et al. 2007; Gérard and Wrochna 2014; Ivrii and Sigal 1993; Lieb and Yau 1987; Amour et al. 2001]. In the present article we follow this fruitful stream of ideas and study the mathematical problem of defect of compactness for density matrices in the bosonic or fermionic Fock spaces. Previously, in a series of papers [Ammari and Nier 2008; 2009; 2011; 2015], the authors have introduced Wigner (or semiclassical) measures of density matrices in the bosonic Fock space and showed that it is a very useful

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tool to study the mean-field approximation of Bose gases. Moreover, it was noticed that a certain defect of compactness of density matrices is one of the difficulties that occurs in this context. So towards a better understanding of these concentration and defect-of-compactness phenomena we introduced here a multiscale analysis inspired by second microlocalization. We believe that this approach will be of interest to the study of the mean-field theory of Fermi and Bose gases; see, e.g., [Bach et al. 2016; Benedikter et al. 2014; Fournais et al. 2015]. We indeed provide here some simple applications to the Bose and Fermi free gases and leave more involved applications to further investigations.

Let us briefly describe the main question we consider here. As mentioned before, in the analysis of general bosonic mean-field problems the following defect-of-compactness problem arises. In fact, if ϱ_ε are density matrices in the (fermionic or bosonic) Fock space and $\gamma_\varepsilon^{(p)}$ are its p-particle reduced density matrices, one may have

$$\lim_{\varepsilon\to 0} \mathrm{Tr}[\gamma_\varepsilon^{(p)}\tilde{b}] = \mathrm{Tr}[\gamma_0^{(p)}\tilde{b}] \tag{1}$$

for any p-particle *compact* observable $\tilde{b}$, while it is not true for a general bounded $\tilde{b}$; e.g.,

$$\lim_{\varepsilon\to 0} \mathrm{Tr}[\gamma_\varepsilon^{(p)}] > \mathrm{Tr}[\gamma_0^{(p)}].$$

This reflects the difference between the weak* convergence of trace-class operators and convergence with respect to the trace norm. In the fermionic case, it is even worse, because mean-field asymptotics cannot be described in terms of finitely many quantum states and the right-hand side of (1) is usually 0, while $\lim_{\varepsilon\to 0} \mathrm{Tr}[\gamma_\varepsilon^{(p)}] > 0$ (see Proposition 4.6). From the analysis of finite-dimensional partial differential equations, it is known that such a defect of compactness can be localized geometrically with accurate quantitative information by introducing scales and small parameters within semiclassical techniques; see, e.g., [Gérard 1991; Gérard et al. 1997; Tartar 1990]. We are thus led to introduce two small parameters $\varepsilon > 0$ for the mean-field asymptotics and $h > 0$ for the semiclassical quantization of finite-dimensional p-particle phase space. The small parameter ε stands for $\frac{1}{n}$, where $n \to \infty$ is the typical number of particles, while h is the *rescaled* Planck constant measuring the proximity of quantum mechanics to classical mechanics. Such scaling appears already in the mathematical physics literature with a specific relation between h and ε depending on the considered problem; see, e.g., [Fournais et al. 2015; Narnhofer and Sewell 1981; Lieb and Yau 1987]. The combined analysis of this article is concerned with the general situation when $\varepsilon = \varepsilon(h)$ with $\lim_{h\to 0} \varepsilon(h) = 0$. In order to keep track of the information at the quantum level, especially in the bosonic case, we also introduce finite-dimensional multiscale observables in the spirit of [Bony 1986; Fermanian-Kammerer and Gérard 2002; Fermanian Kammerer 2005; Nier 1996].

Framework. The 1-particle space $\mathscr{Z}$ is a separable complex Hilbert space endowed with the scalar product $\langle\ ,\ \rangle$ (antilinear in the left-hand side). For a Hilbert space $\mathfrak{h}$ the set of bounded operators is denoted by $\mathcal{L}(\mathfrak{h})$, while the Schatten classes are denoted by $\mathcal{L}^p(\mathfrak{h})$, $1 \le p \le \infty$, the case $p = \infty$ corresponding to the space of compact operators. Let $\Gamma_\pm(\mathscr{Z})$ be the bosonic $(+)$ or fermionic $(-)$ Fock space built on the separable Hilbert space $\mathscr{Z}$:

$$\Gamma_\pm(\mathscr{Z}) = \bigoplus_{n\in\mathbb{N}}^{\perp} \mathcal{S}_\pm^n \mathscr{Z}^{\otimes n},$$

where tensor products and direct sums are Hilbert completed. The operator $\mathcal{S}_\pm^n$ is the orthogonal projection given by

$$\mathcal{S}_\pm^n(f_1 \otimes \cdots \otimes f_n) = \frac{1}{n!} \sum_{\sigma\in\mathfrak{S}_n} s_\pm(\sigma) f_{\sigma(1)} \otimes \cdots \otimes f_{\sigma(n)}, \tag{2}$$

where $s_+(\sigma)$ equals 1, while $s_-(\sigma)$ denotes the signature of the permutation σ and $\mathfrak{S}_n$ is the n-symmetric group.

The dense set of many-body state vectors with a finite number of particles is

$$\Gamma_\pm^{\text{fin}}(\mathscr{Z}) = \bigoplus_{n\in\mathbb{N}}^{\perp,\text{alg}} \mathcal{S}_\pm^n \mathscr{Z}^{\otimes n},$$

where the $\perp$, alg superscript stands for the algebraic orthogonal direct sum. We shall also use the notation $[A, B]_+ = [A, B] = \mathrm{ad}_A B = AB - BA$ for the commutator of two operators and the notation $[A, B]_- = AB + BA$ for the anticommutator.

One way to investigate the mean-field asymptotics relies on parameter-dependent *canonical* (*anti-*)*commutation relations* (CCR or CAR). The small parameter $\varepsilon > 0$ has to be thought of as the inverse of the typical number of particles and the CCR (resp. CAR) relations are given by

$$[a_\pm(g), a_\pm(f)]_\pm = [a_\pm^*(g), a_\pm^*(f)]_\pm = 0, \quad [a_\pm(g), a_\pm^*(f)]_\pm = \varepsilon\langle g,\ f\rangle.$$

Let $(\varrho_\varepsilon)_{\varepsilon>0}$ be a family of normal states (i.e., nonnegative and normalized trace-class operators) on the Fock space $\Gamma_\pm(\mathscr{Z})$, depending on $\varepsilon > 0$; we want to investigate the asymptotic behavior of reduced density matrices, defined below, as $\varepsilon \to 0$, by possibly introducing another scale $h > 0$ on the p-particle phase space, with $\varepsilon = \varepsilon(h)$ and $\lim_{h\to 0} \varepsilon(h) = 0$.

Outline. In Section 2, we recall how Wick observables are used to define the reduced density matrices $\gamma_\varepsilon^{(p)}$. Note that it is much more convenient here, in the general grand canonical framework, to work with nonnormalized reduced density matrices. Some symmetrization formulas are also recalled in this section. In

Section 3, we present the geometry of the classical p-particle phase space and introduce the formalism of double scale semiclassical measures, after [Fermanian Kammerer 2005; Fermanian-Kammerer and Gérard 2002]. In Section 4, we combine the mean-field asymptotics with semiclassical analysis, the two parameters ε and h being related through $\varepsilon = \varepsilon(h)$ with $\lim_{h\to 0} \varepsilon(h) = 0$. Instead of studying the collection of nonnormalized reduced density matrices $(\gamma^{(p)}_{\varepsilon(h)})_{p\in\mathbb{N}}$, it is more convenient to associate generating functions

$$z \mapsto \mathrm{Tr}[\varrho_{\varepsilon(h)}\, e^{z\, d\Gamma_{\pm}(a^{Q,h})}],$$

and to use holomorphy arguments presented there. In Section 5, some classical examples with various asymptotics illustrate the general framework: coherent states in the bosonic setting; simple Gibbs states in the fermionic case; more involved Gibbs states in the bosonic case, which make explicit the separation of condensate and noncondensate phases for rather general noninteracting steady Bose gases. The appendices collect or revisit known things about multiscale semiclassical measures, the (PI)-condition of bosonic mean-field problems, Wick composition formulas, and traces of non-self-adjoint second quantized contractions.

2. Wick observables and reduced density matrices

2A. *Wick observables.*

Notation. For $n \in \mathbb{N}$, the operator $\mathcal{S}^n_{\pm}$ given in (2) is an orthogonal projection in $\mathscr{Z}^{\otimes n}$ so that $(\mathcal{S}^n_{\pm})^* = \mathcal{S}^n_{\pm}$. However, we consider $\mathcal{S}^n_{\pm}$ as a bounded operator from $\mathscr{Z}^{\otimes n}$ onto $\mathcal{S}^n_{\pm}\mathscr{Z}^{\otimes n}$, and its adjoint, denoted by $\mathcal{S}^{n,*}_{\pm} : \mathcal{S}^n_{\pm}\mathscr{Z}^{\otimes n} \to \mathscr{Z}^{\otimes n}$, is nothing but the natural embedding.

Let $\tilde{b} \in \mathcal{L}(\mathcal{S}^p_{\pm}\mathscr{Z}^{\otimes p}; \mathcal{S}^q_{\pm}\mathscr{Z}^{\otimes q})$. The Wick quantization of $\tilde{b}$ is the operator on $\Gamma^{\mathrm{fin}}_{\pm}(\mathscr{Z})$ defined by

$$\tilde{b}^{\mathrm{Wick}}|_{\mathcal{S}^{n+p}_{\pm}\mathscr{Z}^{\otimes(n+p)}} = \varepsilon^{\frac{p+q}{2}} \frac{\sqrt{(n+p)!\,(n+q)!}}{n!}\, \mathcal{S}^{n+q}_{\pm}(\tilde{b}\otimes \mathrm{Id}_{\mathscr{Z}^{\otimes n}})\mathcal{S}^{n+p,*}_{\pm}.$$

In the bosonic case, an element $\tilde{b} \in \mathcal{L}(\mathcal{S}^p_{+}\mathscr{Z}^{\otimes p}; \mathcal{S}^q_{+}\mathscr{Z}^{\otimes q})$ is determined by a related "symbol" $\mathscr{Z} \ni z \mapsto b(z) = \langle z^{\otimes q}, \tilde{b} z^{\otimes p}\rangle$ which is a homogeneous polynomial. So b admits Gâteaux differentials

$$\partial^k_{\bar{z}}\partial^{k'}_z b(w)[u_1,\dots,u_k,v_1,\dots,v_{k'}] = \bar{\partial}_{u_1}\cdots\bar{\partial}_{u_k}\partial_{v_1}\cdots\partial_{v_{k'}} b(w),$$

where $\bar{\partial}_u, \partial_v$ are the complex directional derivatives relative to $u, v \in \mathscr{Z}$ at the point $w \in \mathscr{Z}$. In particular, we have the relation

$$\tilde{b} = \frac{1}{q!\,p!}\partial^q_{\bar{z}}\partial^p_z b.$$

Observe that $b(w)$ admits higher Gâteaux derivatives with the natural identification of $\partial_z^{k'} b(w)$ as a continuous form on $\mathcal{S}_+^{k'}\mathscr{Z}^{\otimes k}$ and $\partial_{\bar z}^k b(w)$ as a vector in $\mathcal{S}_+^k\mathscr{Z}^{\otimes k}$. With the above form-vector identification we define, for any symbols b_1, b_2,

$$\partial_z^k b_1(w)\cdot\partial_{\bar z}^k b_2(w) = \partial_z^k b(w)[\partial_{\bar z}^k b(w)] \in \mathbb{C}.$$

We shall also use the notation $b^{\mathrm{Wick}} = \tilde b^{\mathrm{Wick}}$.

Examples.

(a) The annihilation operator $a_\pm(f)$, $f\in\mathscr{Z}$, is the Wick quantization of $\tilde b = \langle f| : \mathscr{Z}^{\otimes 1} = \mathscr{Z} \ni \varphi \mapsto \langle f, \varphi\rangle \in \mathscr{Z}^{\otimes 0} = \mathbb{C}$.

(b) The creation operator $a_\pm^*(f)$, $f\in\mathscr{Z}$, is the Wick quantization of $\tilde b = |f\rangle :$ $\mathscr{Z}^{\otimes 0} = \mathbb{C} \ni \lambda \mapsto \lambda f \in \mathscr{Z}^{\otimes 1} = \mathscr{Z}$.

(c) For $\tilde b \in \mathcal{L}(\mathscr{Z})$ its Wick quantization $\tilde b^{\mathrm{Wick}}$ is nothing but

$$d\Gamma_\pm(\tilde b)|_{\mathcal{S}_\pm^n\mathscr{Z}^{\otimes n}} = \varepsilon[\tilde b\otimes \mathrm{Id}_{\mathscr{Z}}\otimes\cdots\otimes\mathrm{Id}_{\mathscr{Z}} + \cdots + \mathrm{Id}_{\mathscr{Z}}\otimes\cdots\otimes\mathrm{Id}_{\mathscr{Z}}\otimes\tilde b].$$

A particular case is $\tilde b = \mathrm{Id}_{\mathscr{Z}}$ associated with the scaled number operator ($\boldsymbol{N}_{\pm,\varepsilon=1}$ stands for the usual ε-independent number operator):

$$\tilde b^{\mathrm{Wick}} = d\Gamma_\pm(\mathrm{Id}_{\mathscr{Z}}) = \boldsymbol{N}_\pm = \varepsilon\boldsymbol{N}_{\pm,\varepsilon=1}.$$

When $\tilde b$ is self-adjoint one has

$$d\Gamma_\pm(\tilde b) = i\,\partial_t e^{-it\,d\Gamma_\pm(\tilde b)}|_{t=0} = i\,\partial_t\Gamma_\pm(e^{-i\varepsilon t\tilde b})|_{t=0},$$

while for a contraction $C\in\mathcal{L}(\mathscr{Z};\mathscr{Z})$,

$$\Gamma_\pm(C)|_{\mathcal{S}_\pm^n\mathscr{Z}^{\otimes n}} = C\otimes\cdots\otimes C.$$

From the definition of the Wick quantization one easily checks the following properties; see [Ammari 2004].

Proposition 2.1. *For $\tilde b\in\mathcal{L}(\mathcal{S}_\pm^p\mathscr{Z}^{\otimes p};\mathcal{S}_\pm^q\mathscr{Z}^{\otimes q})$:*

- $[\tilde b^{\mathrm{Wick}}]^* = [\tilde b^*]^{\mathrm{Wick}}$.

- *The operator $(1+\boldsymbol{N}_\pm)^{-\frac{m}{2}}\,\tilde b^{\mathrm{Wick}}\,(1+\boldsymbol{N}_\pm)^{-\frac{m'}{2}}$ extends to a bounded operator on $\Gamma_\pm(\mathscr{Z})$ if $m+m'\geq p+q$ with*

$$\left\|(1+\boldsymbol{N}_\pm)^{-\frac{m}{2}}\,\tilde b^{\mathrm{Wick}}\,(1+\boldsymbol{N}_\pm)^{-\frac{m'}{2}}\right\|_{\mathcal{L}(\Gamma_\pm(\mathscr{Z}))} \leq C_{m,m'}\|\tilde b\|_{\mathcal{L}(\mathcal{S}_\pm^p\mathscr{Z};\mathcal{S}_\pm^q\mathscr{Z})}, \tag{3}$$

with $C_{m,m'}$ independent of $\tilde b$ and of $\varepsilon\in(0,\varepsilon_0)$.

- $(\tilde b\geq 0) \Longleftrightarrow (\tilde b^{\mathrm{Wick}}\geq 0)$, *while this makes sense only for $q=p$.*

Wick quantized operators are generally unbounded operators on $\Gamma_\pm(\mathscr{Z})$ (e.g., $\boldsymbol{N}_\pm$) but they are well-defined on the dense set $\Gamma^{\mathrm{fin}}_\pm(\mathscr{Z})$, which is preserved by their action. Hence $\tilde{b}_1^{\mathrm{Wick}} \circ \tilde{b}_2^{\mathrm{Wick}}$ makes sense at least on $\Gamma^{\mathrm{fin}}_\pm(\mathscr{Z})$ and the following composition law holds true.

Proposition 2.2 (composition of Wick operators). *Let* $\tilde{b}_j \in \mathcal{L}(\mathcal{S}^{p_j}_\pm \mathscr{Z}^{\otimes p_j}; \mathcal{S}^{q_j}_\pm \mathscr{Z}^{\otimes q_j})$, $j = 1, 2$. *Then*

$$\tilde{b}_1^{\mathrm{Wick}} \circ \tilde{b}_2^{\mathrm{Wick}} = \sum_{k=0}^{\min\{p_1,q_2\}} (\pm 1)^{(p_1-k)(p_2+q_2)} \frac{\varepsilon^k}{k!} (\tilde{b}_1 \sharp^k \tilde{b}_2)^{\mathrm{Wick}}, \tag{4}$$

where

$$\tilde{b}_1 \sharp^k \tilde{b}_2 := \frac{p_1!}{(p_1-k)!} \frac{q_2!}{(q_2-k)!} \mathcal{S}_\pm^{q_1+q_2-k} (\tilde{b}_1 \otimes \mathrm{Id}^{\otimes q_2-k})(\mathrm{Id}^{\otimes p_1-k} \otimes \tilde{b}_2) \mathcal{S}_\pm^{p_1+p_2-k,*}.$$

For the reader's convenience, the proof of Proposition 2.2 is provided in Appendix C.

In the bosonic case the symbols $b(z) = \langle z^{\otimes q}, \tilde{b} z^{\otimes p}\rangle$ are convenient for writing the composition of Wick quantized operators. If $b_1 \sharp^{\mathrm{Wick}} b_2$ denotes the symbol of $\tilde{b}_1^{\mathrm{Wick}} \circ \tilde{b}_2^{\mathrm{Wick}}$, the composition law is summarized below; see [Ammari and Nier 2008, Proposition 2.7].

Proposition 2.3 (composition of Wick symbols in the bosonic case). *We have*

$$b_1 \sharp^{\mathrm{Wick}} b_2(z) = e^{\varepsilon \partial_{z_1} \cdot \partial_{\bar{z}_2}} b_1(z_1) b_2(z_2)|_{z_1=z_2=z} = \sum_{k=0}^{\min\{p_1,q_2\}} \frac{\varepsilon^k}{k!} \partial_z^k b_1(z) \cdot \partial_{\bar{z}}^k b_2(z).$$

The commutator of Wick operators in the bosonic case is given by

$$[b_1^{\mathrm{Wick}}, b_2^{\mathrm{Wick}}] = \Bigg(\sum_{k=1}^{\max\{\min\{p_1,q_2\},\min\{p_2,q_1\}\}} \frac{\varepsilon^k}{k!} \{b_1, b_2\}^{(k)} \Bigg)^{\mathrm{Wick}},$$

where the k-th order Poisson bracket is given by

$$\{b_1, b_2\}^{(k)}(w) = \partial_z^k b_1(w) \cdot \partial_{\bar{z}}^k b_2(w) - \partial_z^k b_2(w) \cdot \partial_{\bar{z}}^k b_1(w).$$

Proposition 2.4. *Let $p, m, m' \in \mathbb{N}$ such that $m + m' \geq 2p - 2$. Then, there exist coefficients $C_{j_1,\dots,j_k} \geq 0$ such that, for any $\tilde{b} \in \mathcal{L}(\mathcal{Z}; \mathcal{Z})$,*

$$d\Gamma_\pm(\tilde{b})^p - (\tilde{b}^{\otimes p})^{\mathrm{Wick}} = \sum_{k=1}^{p-1} \varepsilon^{p-k} \sum_{\substack{0 \leq j_1 \leq \cdots \leq j_k \\ j_1 + \cdots + j_k = p}} C_{j_1,\dots,j_k} (\mathcal{S}_\pm^k \tilde{b}^{j_1} \otimes \cdots \otimes \tilde{b}^{j_k} \mathcal{S}_\pm^{k,*})^{\mathrm{Wick}} \tag{5}$$

and the estimate

$$\left\| (1 + \boldsymbol{N}_\pm)^{-\frac{m}{2}} (d\Gamma_\pm(\tilde{b})^p - (\tilde{b}^{\otimes p})^{\mathrm{Wick}})(1 + \boldsymbol{N}_\pm)^{-\frac{m'}{2}} \right\|_{\mathcal{L}(\Gamma_\pm(\mathcal{Z}))} \leq \varepsilon\, B_p \, \|\tilde{b}\|^p_{\mathcal{L}(\mathcal{Z})}$$

holds in both the bosonic and fermionic cases, with B_p the p-th Bell number.

Remark 2.5. The p-th Bell number B_p can be defined as the number of partitions of a set with p elements and satisfies $B_p < (0.792p/\ln(p+1))^p$, see [Berend and Tassa 2010], and hence it grows much slower than $p!$.

Proof. We first prove formula (5) by induction on $p \in \mathbb{N}^*$.

For $p = 1$, formula (5) holds because $d\Gamma_\pm(\tilde{b}) = (\tilde{b})^{\mathrm{Wick}}$.

We then set $r_p(\tilde{b}) := d\Gamma_\pm(\tilde{b})^p - (\tilde{b}^{\otimes p})^{\mathrm{Wick}}$. Assuming the result holds for some $p \in \mathbb{N}^*$, one can compute

$$d\Gamma_\pm(\tilde{b})^{p+1} = (\tilde{b}^{\otimes p})^{\mathrm{Wick}}(\tilde{b})^{\mathrm{Wick}} + r_p(\tilde{b})^{\mathrm{Wick}}(\tilde{b})^{\mathrm{Wick}}$$

using the composition formula (4) for

$$(\tilde{b}^{\otimes p})^{\mathrm{Wick}}(\tilde{b})^{\mathrm{Wick}} = (\tilde{b}^{\otimes p+1})^{\mathrm{Wick}} + p\varepsilon\,(\mathcal{S}^p_\pm\; \tilde{b}^{\otimes p-1} \otimes \tilde{b}^2\; \mathcal{S}^{p,*}_\pm)^{\mathrm{Wick}}$$

and for

$$\begin{aligned}
&\varepsilon^{p-k}(\mathcal{S}^k_\pm\, \tilde{b}^{j_1} \otimes \cdots \otimes \tilde{b}^{j_k}\, \mathcal{S}^{k,*}_\pm)^{\mathrm{Wick}}(\tilde{b})^{\mathrm{Wick}} \\
&\quad = \varepsilon^{p+1-(k+1)}(\mathcal{S}^{k+1}_\pm\, \tilde{b} \otimes \tilde{b}^{j_1} \otimes \cdots \otimes \tilde{b}^{j_k}\, \mathcal{S}^{k+1,*}_\pm)^{\mathrm{Wick}} \\
&\qquad + k\varepsilon^{p+1-k}\big(\mathcal{S}^k_\pm(\tilde{b}^{j_1} \otimes \cdots \otimes \tilde{b}^{j_k})\mathcal{S}^{k,*}_\pm\, \mathcal{S}^k_\pm\,(\tilde{b} \otimes \mathrm{Id}_{\mathcal{Z}}^{\otimes j_1+\cdots+j_k-1})\mathcal{S}^{k,*}_\pm\big)^{\mathrm{Wick}},
\end{aligned}$$

which yields the expected form for $r_{p+1}(\tilde{b})$, and achieves the induction.

We then remark that the sum of coefficients of order k,

$$S_2(p,k) = \sum_{\substack{0 \le j_1 \le \cdots \le j_k \\ j_1+\cdots+j_k = p}} C_{j_1,\ldots,j_k},$$

satisfies the recurrence relation $S_2(p,k) = kS_2(p-1,k) + S_2(p-1,k-1)$, with $S_2(p,1) = 1 = S_2(1,k)$ for all $p, k \in \mathbb{N}^*$, where the $S_2(p,k)$ are the Stirling numbers of the second kind. Observe that, for $\frac{M}{2} \ge k$, and for any $\tilde{c} \in \mathcal{L}(\mathcal{S}^k_\pm \mathcal{Z}^{\otimes k})$,

$$\|\tilde{c}^{\mathrm{Wick}}(1+N_\pm)^{-\frac{M}{2}}\|_{\mathcal{L}(\Gamma_\pm(\mathcal{Z}))} \le \|\tilde{c}\|_{\mathcal{L}(\mathcal{S}^k_\pm \mathcal{Z}^{\otimes k};\mathcal{S}^k_\pm \mathcal{Z}^{\otimes k})}.$$

We thus get,

$$\begin{aligned}
&\big\|(1+N_\pm)^{-\frac{m}{2}}(d\Gamma_\pm(\tilde{b})^p - (\tilde{b}^{\otimes p})^{\mathrm{Wick}})(1+N_\pm)^{-\frac{m'}{2}}\big\|_{\mathcal{L}(\Gamma_\pm(\mathcal{Z}))} \\
&\qquad\qquad \le \sum_{k=1}^{p-1} \varepsilon^{p-k} S_2(p,k)\, \|\tilde{b}\|^p_{\mathcal{L}(\mathcal{Z})}
\end{aligned}$$

and the estimate then follows from $\sum_{k=1}^{p-1} \varepsilon^{p-k} S_2(p,k) \le \varepsilon \sum_{k=1}^{p} S_2(p,k) = \varepsilon B_p$, with B_p the p-th Bell number. ☐

2B. ***Reduced density matrices.*** Reduced density matrices emerge naturally in the study of correlation functions of quantum gases [Spohn 1980]. In particular, in quantum mean-field theory they are the main quantities to be analyzed; see, e.g., [Bardos et al. 2000; Knowles and Pickl 2010; Lewin et al. 2016]. However, we shall work with *nonnormalized* reduced density matrices, which are easier to handle. Going back to the more natural reduced density matrices with trace equal to 1 requires attention when normalizing and taking the limits.

Definition 2.6. Let $\varrho_\varepsilon \in \mathcal{L}^1(\Gamma_\pm(\mathscr{Z}))$ ($\varepsilon > 0$ is fixed here) be such that $\varrho_\varepsilon \geq 0$, $\mathrm{Tr}[\varrho_\varepsilon] = 1$ and $\mathrm{Tr}(\varrho_\varepsilon e^{c\mathbf{N}_\pm}) < \infty$ for some $c > 0$. The nonnormalized reduced density matrix of order $p \in \mathbb{N}$, $\gamma_\varepsilon^{(p)} \in \mathcal{L}^1(\mathcal{S}_\pm^p \mathscr{Z}^{\otimes p})$, is defined by duality according to,

$$\text{for all } \tilde{b} \in \mathcal{L}(\mathcal{S}_\pm^p \mathscr{Z}^{\otimes p}; \mathcal{S}_\pm^p \mathscr{Z}^{\otimes p}), \quad \mathrm{Tr}[\gamma_\varepsilon^{(p)} \tilde{b}] = \mathrm{Tr}[\varrho_\varepsilon \tilde{b}^{\mathrm{Wick}}].$$

The definition makes sense owing to the number estimate (3) and to

$$(1 + \mathbf{N}_\pm)^k e^{-c\mathbf{N}_\pm} \in \mathcal{L}(\Gamma_\pm(\mathscr{Z})).$$

When $\mathrm{Tr}[\gamma_\varepsilon^{(p)}] \neq 0$, the normalized density matrix $\bar{\gamma}_\varepsilon^{(p)}$ is defined by $\bar{\gamma}_\varepsilon^{(p)} = \gamma_\varepsilon^{(p)} / \mathrm{Tr}[\gamma_\varepsilon^{(p)}]$; that is, for all $\tilde{b} \in \mathcal{L}(\mathcal{S}_\pm^p \mathscr{Z}^{\otimes p})$,

$$\mathrm{Tr}[\bar{\gamma}_\varepsilon^{(p)} \tilde{b}] = \frac{\mathrm{Tr}[\varrho_\varepsilon \tilde{b}^{\mathrm{Wick}}]}{\mathrm{Tr}[\varrho_\varepsilon (\mathrm{Id}_{\mathcal{S}_\pm^p \mathscr{Z}^{\otimes p}})^{\mathrm{Wick}}]} = \frac{\mathrm{Tr}[\varrho_\varepsilon \tilde{b}^{\mathrm{Wick}}]}{\mathrm{Tr}[\varrho_\varepsilon N_\pm (N_\pm - \varepsilon) \cdots (N_\pm - \varepsilon(p-1))]}.$$

These normalized reduced density matrices $\bar{\gamma}_\varepsilon^{(p)}$ are commonly used, especially when $\varrho_\varepsilon \in \mathcal{L}^1(\mathcal{S}_\pm \mathscr{Z}^{\otimes n})$, with $n\varepsilon \sim 1$, for the following reason: when $\varrho_\varepsilon \in \mathcal{L}^1(\mathcal{S}_\pm^n \mathscr{Z}^{\otimes n})$ lies in the n-particle sector in the mean-field regime $n\varepsilon \to 1$, one has

$$\mathrm{Tr}[\bar{\gamma}_\varepsilon^{(p)} \tilde{b}] = \mathrm{Tr}[\varrho_\varepsilon (\tilde{b} \otimes \mathrm{Id}_{\mathscr{Z}^{\otimes (n-p)}})] \quad \text{and} \quad \lim_{\substack{n\varepsilon \sim 1 \\ \varepsilon \to 0}} \mathrm{Tr}[\bar{\gamma}_\varepsilon^{(p)} \tilde{b}] = \lim_{\substack{n\varepsilon \sim 1 \\ \varepsilon \to 0}} \mathrm{Tr}[\gamma_\varepsilon^{(p)} \tilde{b}], \tag{6}$$

since for $n > p$,

$$\tilde{b}^{\mathrm{Wick}}\big|_{\mathcal{S}_\pm^n \mathscr{Z}^{\otimes n}} = \varepsilon^p \frac{n!}{(n-p)!} \mathcal{S}_\pm^n (\tilde{b} \otimes \mathrm{Id}_{\mathscr{Z}^{\otimes (n-p)}}) \mathcal{S}_\pm^{n,*}$$

and $\varepsilon^p \, n(n-1) \cdots (n-p+1) \to 1$ when $n\varepsilon \to 1$.

Moreover, one often works with kernels of (normalized) reduced density matrices $\bar{\gamma}_\varepsilon^{(p)}$ when $\mathscr{Z} = L^2(M; dv)$ with the following relation deduced from the left-hand side of (6):

$$\bar{\gamma}_\varepsilon^{(p)}(x_1, \ldots, x_p; x_1', \ldots, x_p') = \int_{M^{n-p}} \varrho_\varepsilon(x_1, \ldots, x_p, x; x_1', \ldots, x_p', x) \, dv^{\otimes (n-p)}(x).$$

But, if the states ϱ_ε are not localized on the n-particles then $\gamma_\varepsilon^{(p)}$ and $\bar{\gamma}_\varepsilon^{(p)}$ do not coincide even asymptotically in the mean-field regime (i.e., the right-hand side of (6) may not hold true). As well there is no simple relation between the nonnormalized density matrices $\gamma_\varepsilon^{(p+1)}$ and $\gamma_\varepsilon^{(p)}$. Actually, we have

$$\begin{aligned}(\mathcal{S}_\pm^{p+1}(\tilde{b}\otimes \mathrm{Id}_{\mathscr{Z}})\mathcal{S}_\pm^{p+1,*})^{\mathrm{Wick}}\big|_{\mathcal{S}_\pm^{n+p+1}\mathscr{Z}^{\otimes(n+p+1)}} \\ &= \varepsilon^{p+1}\frac{(n+p+1)!}{n!}\mathcal{S}_\pm^{n+p+1}(\tilde{b}\otimes \mathrm{Id}_{\mathscr{Z}^{\otimes n+1}})\mathcal{S}_\pm^{n+p+1,*} \\ &= \varepsilon(n+1)\tilde{b}^{\mathrm{Wick}}\big|_{\mathcal{S}_\pm^{n+p+1}\mathscr{Z}^{\otimes(n+p+1)}},\end{aligned}$$

from which we deduce

$$\mathrm{Tr}[\gamma_\varepsilon^{(p+1)}(\tilde{b}\otimes \mathrm{Id}_{\mathscr{Z}})] = \mathrm{Tr}[\varrho_\varepsilon(\boldsymbol{N}_\pm - \varepsilon p)\tilde{b}^{\mathrm{Wick}}],$$

while

$$\mathrm{Tr}[\gamma_\varepsilon^{(p)}\tilde{b}] = \mathrm{Tr}[\varrho_\varepsilon\tilde{b}^{\mathrm{Wick}}],$$

where we have again identified $\gamma_\varepsilon^{(p+1)}$ as an element of $\mathcal{L}^1(\mathscr{Z}^{\otimes(p+1)})$. We thus conclude with the following important remark.

Remark 2.7. Assume $\varrho_\varepsilon = \varrho_\varepsilon 1_{[\nu-\delta(\varepsilon),\nu+\delta(\varepsilon)]}(\boldsymbol{N}_\pm)$ with $\nu > 0$ and $\lim_{\varepsilon\to 0}\delta(\varepsilon) = 0$. Then the following simple asymptotic relations between $\gamma_\varepsilon^{(p)}$ and $\gamma_\varepsilon^{(p')}$ (or the normalized versions $\bar{\gamma}_\varepsilon^{(p)}$ and $\bar{\gamma}_\varepsilon^{(p')}$) hold true for any $p' > p$ and any $\tilde{b} \in \mathcal{L}(\mathcal{S}_\pm^p\mathscr{Z}^{\otimes p};\mathcal{S}_\pm^p\mathscr{Z}^{\otimes p})$,

$$\lim_{\varepsilon\to 0}\mathrm{Tr}[\gamma_\varepsilon^{(p')}(\tilde{b}\otimes \mathrm{Id}_{\mathscr{Z}^{\otimes(p'-p)}})] = \nu^{p'-p}\lim_{\varepsilon\to 0}\mathrm{Tr}[\gamma_\varepsilon^{(p)}\tilde{b}],$$
$$\lim_{\varepsilon\to 0}\mathrm{Tr}[\bar{\gamma}_\varepsilon^{(p')}(\tilde{b}\otimes \mathrm{Id}_{\mathscr{Z}^{\otimes(p'-p)}})] = \lim_{\varepsilon\to 0}\mathrm{Tr}[\bar{\gamma}_\varepsilon^{(p)}\tilde{b}].$$

We shall use recurrently with variations the following lemma, with the notation

$$\tilde{b}_1\odot\cdots\odot\tilde{b}_p = \frac{1}{p!}\sum_{\sigma\in\mathfrak{S}_p}\tilde{b}_{\sigma(1)}\otimes\cdots\otimes\tilde{b}_{\sigma(p)}$$

for $\tilde{b}_1,\ldots,\tilde{b}_p \in \mathcal{L}(\mathscr{Z})$.

We also abbreviate $(\mathcal{S}_\pm^p(\tilde{b}_1\odot\cdots\odot\tilde{b}_p)\mathcal{S}_\pm^{p,*})^{\mathrm{Wick}}$ by $(\tilde{b}_1\odot\cdots\odot\tilde{b}_p)^{\mathrm{Wick}}$ and $(\mathcal{S}_\pm^p(\tilde{b}^{\otimes p})\mathcal{S}_\pm^{p,*})^{\mathrm{Wick}}$ by $(\tilde{b}^{\otimes p})^{\mathrm{Wick}}$.

Lemma 2.8 (quantum symmetrization lemma). *In the bosonic and fermionic cases for any $p \in \mathbb{N}$, the equality*

$$\mathcal{S}_\pm^p(\tilde{b}_1\otimes\cdots\otimes\tilde{b}_p)\mathcal{S}_\pm^{p,*} = \mathcal{S}_\pm^p(\tilde{b}_1\odot\cdots\odot\tilde{b}_{\sigma(p)})\mathcal{S}_\pm^{p,*} \tag{7}$$

holds in $\mathcal{L}(\mathcal{S}_\pm^p\mathscr{Z}^{\otimes p};\mathcal{S}_\pm^p\mathscr{Z}^{\otimes p})$ for all $\tilde{b}_1,\ldots,\tilde{b}_p \in \mathcal{L}(\mathscr{Z};\mathscr{Z})$.

As a consequence, under the assumptions of Definition 2.6, the nonnormalized (resp. normalized if possible) reduced density matrix $\gamma_\varepsilon^{(p)}$ (resp. $\bar{\gamma}_\varepsilon^{(p)}$), $p \in \mathbb{N}$, is completely determined by the set of quantities $\{\mathrm{Tr}[\varrho_\varepsilon(\tilde{b}^{\otimes p})^{\mathrm{Wick}}], \tilde{b} \in \mathcal{B}\}$ when $\mathcal{B}$ is any dense subset of $\mathcal{L}^\infty(\mathscr{Z};\mathscr{Z})$.

Remark 2.9. While computing $\mathrm{Tr}[\gamma_\varepsilon^{(p)}]$ or studying $\bar{\gamma}_\varepsilon^{(p)}$ one can simply add to $\mathcal{B}$ the element $\mathrm{Id}_{\mathscr{Z}}$ owing to $\mathcal{S}_\pm^p \mathrm{Id}_{\mathscr{Z}}^{\otimes p} \mathcal{S}_\pm^{p,*} = \mathrm{Id}_{\mathcal{S}_\pm^p \mathscr{Z}^{\otimes p}}$. For $\varepsilon > 0$ fixed it is not necessary because compact observables are sufficient to determine the total trace owing to

$$\mathrm{Tr}[\gamma_\varepsilon^{(p)}] = \sup_{\substack{B \in \mathcal{L}^\infty(\mathcal{S}_\pm^p \mathscr{Z}^{\otimes p}) \\ 0 \le B \le \mathrm{Id}}} \mathrm{Tr}[\gamma_\varepsilon^{(p)} B].$$

However, while considering weak*-limits as $\varepsilon \to 0$, adding the identity operator $\mathrm{Id}_{\mathcal{S}_\pm^p \mathscr{Z}^{\otimes p}}$ to the set of compact observables, or possibly replacing $\mathcal{B}$ by the Calkin algebra $\mathbb{C}\mathrm{Id}(\mathscr{Z}) \oplus \mathcal{L}^\infty(\mathscr{Z})$, is useful in order to control the asymptotic total mass.

Proof. For $\tilde{b}_1, \dots, \tilde{b}_p \in \mathcal{L}(\mathscr{Z})$, we decompose

$$\mathcal{S}_\pm^p (\tilde{b}_1 \otimes \cdots \otimes \tilde{b}_p) \mathcal{S}_\pm^{p,*} \mathcal{S}_\pm^p (\psi_1 \otimes \cdots \otimes \psi_p)$$

as

$$\begin{aligned} &\mathcal{S}_\pm^p \bigg[\frac{1}{p!} \sum_{\sigma' \in \mathfrak{S}_p} s_\pm(\sigma') (\tilde{b}_1 \psi_{\sigma'(1)}) \otimes \cdots \otimes (\tilde{b}_p \psi_{\sigma'(p)}) \bigg] \\ &\qquad = \frac{1}{p!\,p!} \bigg[\sum_{\sigma \in \mathfrak{S}_p} \sum_{\sigma' \in \mathfrak{S}_p} s_\pm(\sigma) s_\pm(\sigma') (\tilde{b}_{\sigma(1)} \psi_{\sigma\circ\sigma'(1)}) \otimes \cdots \otimes (\tilde{b}_{\sigma(p)} \psi_{\sigma\circ\sigma'(p)}) \bigg]. \end{aligned}$$

Setting $\sigma'' = \sigma \circ \sigma'$, with $s_\pm(\sigma'') = s_\pm(\sigma) s_\pm(\sigma')$ yields (7), after noting that $\tilde{b}_1 \odot \cdots \odot \tilde{b}_p = \frac{1}{p!} \sum_{\sigma \in \mathfrak{S}_p} \tilde{b}_{\sigma(1)} \otimes \cdots \otimes \tilde{b}_{\sigma(p)}$ commutes with $\mathcal{S}_\pm^p$ in both the bosonic and fermionic cases.

Now the nonnormalized reduced density matrix is determined by

$$\mathrm{Tr}[\gamma_\varepsilon^{(p)} \widetilde{B}] = \mathrm{Tr}[\varrho_\varepsilon \widetilde{B}^{\mathrm{Wick}}]$$

for $\widetilde{B} \in \mathcal{L}^\infty(\mathcal{S}_\pm^p \mathscr{Z}^{\otimes p})$ as $\mathcal{L}^1(\mathcal{S}_\pm^p \mathscr{Z}^{\otimes p})$ is the dual of $\mathcal{L}^\infty(\mathcal{S}_\pm^p \mathscr{Z}^{\otimes p})$. But $\widetilde{B} \in \mathcal{L}^\infty(\mathcal{S}_\pm^p \mathscr{Z}^{\otimes p})$ means $\widetilde{B} = \mathcal{S}_\pm^p \widetilde{B}' \mathcal{S}_\pm^{p,*}$ with $\widetilde{B}' \in \mathcal{L}^\infty(\mathscr{Z}^{\otimes p})$, while the algebraic tensor product $\mathcal{L}^\infty(\mathscr{Z})^{\otimes^{\mathrm{alg}} p}$ is dense in $\mathcal{L}^\infty(\mathscr{Z}^{\otimes p})$.

With the estimate

$$\begin{aligned} \big| \mathrm{Tr}[\varrho_\varepsilon \widetilde{B}^{\mathrm{Wick}}] \big| &= \big| \mathrm{Tr}[e^{\frac{c}{2}\boldsymbol{N}} \varrho_\varepsilon e^{\frac{c}{2}\boldsymbol{N}} e^{-\frac{c}{2}\boldsymbol{N}} \widetilde{B}^{\mathrm{Wick}} e^{-\frac{c}{2}\boldsymbol{N}}] \big| \\ &\le C\, \mathrm{Tr}[\varrho_\varepsilon e^{c\boldsymbol{N}}] \| \widetilde{B} \|_{\mathcal{L}(\mathcal{S}_\pm^p \mathscr{Z}^{\otimes p}; \mathcal{S}_\pm^p \mathscr{Z}^{\otimes p})}, \end{aligned}$$

it suffices to consider $\widetilde{B} = \mathcal{S}_\pm^p \widetilde{B}' \mathcal{S}_\pm^{p,*}$ with $\widetilde{B}' \in \mathcal{L}^\infty(\mathscr{Z})^{\otimes^{\mathrm{alg}} p}$. By linearity and density, $\gamma_\varepsilon^{(p)}$ is determined by the quantities $\mathrm{Tr}[\varrho_\varepsilon \widetilde{B}^{\mathrm{Wick}}]$ with $\widetilde{B}' = \tilde{b}_1 \otimes \cdots \otimes \tilde{b}_p$, $\tilde{b}_i \in \mathcal{B}$. We conclude with

$$\mathcal{S}_\pm^p (\tilde{b}_1 \otimes \cdots \otimes \tilde{b}_p) \mathcal{S}_\pm^{p,*} = \mathcal{S}_\pm^p (\tilde{b}_1 \odot \cdots \odot \tilde{b}_p) \mathcal{S}_\pm^{p,*},$$

and the polarization identity

$$\tilde{b}_1 \odot \cdots \odot \tilde{b}_p = \frac{1}{2^p p!} \sum_{\varepsilon_i = \pm 1} \varepsilon_1 \cdots \varepsilon_p \Big(\sum_{i=1}^{p} \varepsilon_i \tilde{b}_i \Big)^{\otimes p}. \qquad \square$$

Remark 2.10. In the bosonic case, the nonnormalized reduced density matrices $\gamma_\varepsilon^{(p)}$ are also characterized by the values of $\mathrm{Tr}[\gamma_\varepsilon^{(p)} B]$ for B in

$$\mathcal{B} = \big\{ |\psi^{\otimes p}\rangle\langle\psi^{\otimes p}| : \psi \in \mathscr{Z} \big\} \cup \{\mathrm{Id}_{\mathscr{Z}}^{\otimes p}\}.$$

This does not hold in the fermionic case.

The rest of the article is devoted to the asymptotic analysis of $\gamma_\varepsilon^{(p)}$ as $\varepsilon \to 0$. In particular we shall study their concentration at the quantum level while testing with fixed observable $\tilde{b}$ (with $\tilde{b}$ compact) and their semiclassical behavior after taking semiclassically quantized observables, e.g., $a(x, hD_x)$ with some relation $\varepsilon = \varepsilon(h)$ between ε and h.

3. Classical phase-space and h-quantizations

When $\mathscr{Z} = L^2(M^1, dx)$, with $M^1 = M$ a smooth manifold with volume measure dx, the classical 1-particle phase space is $\mathcal{X}^1 = \mathcal{X} = T^*M^1$ and we will focus on the h-dependent quantization which associates with a symbol $a(x,\xi) = a(X)$, $X \in \mathcal{X}^1$ an operator $a^{Q,h} = a(x, hD_x)$ with the standard semiclassical quantization or when $M^1 = \mathbb{R}^d$, $a^{Q,h} = a^{W,h} = a^W(h^t x, h^{1-t} D_x)$, by using the Weyl quantization, $t \in \mathbb{R}$ being fixed.

Note that in later sections the parameters ε and h will be linked through $\varepsilon = \varepsilon(h)$ with $\lim_{h\to 0} \varepsilon(h) = 0$. In relation with the symmetrization result, Lemma 2.8, we introduce the adapted p-particle phase space which was also considered in [Dereziński 1998], and the corresponding semiclassical observables.

3A. ***Classical p-particle phase space.*** A fundamental principle of quantum mechanics is that identical particles are indistinguishable. The classical description is thus concerned with indistinguishable classical particles. If one classical particle is characterized by its position-momentum $(x, \xi) \in \mathcal{X}^1 = T^*M^1$, $x \in M$ being the position coordinate and ξ the momentum coordinates, p indistinguishable particles will be described by their position-momentum coordinates $(X_1, \dots, X_p) = (x_1, \xi_1, \dots, x_p, \xi_p) \in \mathcal{X}^p/\mathfrak{S}_p = (T^*M)^p/\mathfrak{S}_p = T^*(M^p)/\mathfrak{S}_p$, where the quotient by $\mathfrak{S}_p$ simply implements the identification,

$$\text{for all } \sigma \in \mathfrak{S}_p, \quad (X_{\sigma(1)}, \dots, X_{\sigma(p)}) \equiv (X_1, \dots, X_p).$$

The grand canonical description of a classical particles system then takes place in the disjoint union

$$\bigsqcup_{p\in\mathbb{N}} \mathcal{X}^p/\mathfrak{S}_p = \bigsqcup_{p\in\mathbb{N}} (T^*M)^p/\mathfrak{S}_p.$$

A p-particle classical observable will be a function on $\mathcal{X}^p/\mathfrak{S}_p$ and, when the number of particles is not fixed, a collection of functions $(a^{(p)})_{p\in\mathbb{N}}$, each $a^{(p)}$ being a function on $\mathcal{X}^p/\mathfrak{S}_p$. The situation is presented in this way in [Dereziński 1998]. A p-particle observable is a function $a^{(p)}$ on $\mathcal{X}^p/\mathfrak{S}_p$ and a p-particle classical state is a probability measure (and when the normalization is forgotten, a nonnegative measure) on $\mathcal{X}^p/\mathfrak{S}_p$.

However while quantizing a classical observable, it is better to work in $\mathcal{X}^p$, which equals $T^*(M^p)$, a function $a^{(p)}$ on $\mathcal{X}^p/\mathfrak{S}_p$ being nothing but a function on $\mathcal{X}^p$ which satisfies,

$$\text{for all } \sigma \in \mathfrak{S}_p, \quad \sigma^* a^{(p)} = a^{(p)},$$

where,

$$\text{for all } (X_1,\dots,X_p) \in \mathcal{X}^p, \quad \sigma^* a^{(p)}(X_1,\dots,X_p) = a^{(p)}(X_{\sigma(1)},\dots,X_{\sigma(p)}),$$

and

$$a^{(p)} = \frac{1}{p!}\sum_{\sigma\in\mathfrak{S}_p} \sigma^* a^{(p)}.$$

In the same way, we define for a Borel measure ν on $\mathcal{X}^p$ and $\sigma \in \mathfrak{S}_p$, the measure $\sigma_*\nu$ by $\int_{\mathcal{X}^p} \sigma^* a^{(p)}\, d\nu = \int_{\mathcal{X}^p} a^{(p)}\, d(\sigma_*\nu)$ for all $a^{(p)} \in \mathcal{C}_c^0(\mathcal{X}^p)$, or alternatively $\sigma_*\nu(E) = \nu(\sigma^{-1}(E))$ for all Borel subsets E of $\mathcal{X}^p$. A nonnegative measure on $\mathcal{X}^p/\mathfrak{S}_p$ is identified with a nonnegative measure ν on $\mathcal{X}^p$ such that,

$$\text{for all } \sigma \in \mathfrak{S}_p, \quad \sigma_*\nu = \nu = \frac{1}{p!}\sum_{\tilde\sigma\in\mathfrak{S}_p} \tilde\sigma_*\nu. \tag{8}$$

Lemma 3.1 (classical symmetrization lemma). *Any Borel measure $\mu^{(p)}$ on $\mathcal{X}^p/\mathfrak{S}_p$ is characterized by the quantities $\left\{\int_{\mathcal{X}^p} a^{\otimes p}\, d\mu^{(p)} : a \in \mathcal{C}\right\}$ where the tensor power $a^{\otimes p}$ means $a^{\otimes p}(X_1,\dots,X_p) = \prod_{i=1}^p a(X_i)$ and $\mathcal{C}$ is any dense set in $\mathcal{C}_\infty^0(\mathcal{X}^1) = \{f \in \mathcal{C}^0(\mathcal{X}^1) : \lim_{X\to\infty} f(X) = 0\}$.*

Proof. By the Stone–Weierstrass theorem the subalgebra generated by the algebraic tensor product $\mathcal{C}^{\otimes^{\text{alg}} p}$ is dense in $\mathcal{C}_\infty^0(\mathcal{X}^p)$. Hence it suffices to consider

$$a_1 \odot \cdots \odot a_p = \frac{1}{p!}\sum_{\sigma\in\mathfrak{S}_p} a_{\sigma(1)} \otimes \cdots \otimes a_{\sigma(p)}, \quad a_i \in \mathcal{C}.$$

We conclude again with the polarization identity

$$a_1 \odot \cdots \odot a_p = \frac{1}{2^p p!}\sum_{\varepsilon_i=\pm 1} \varepsilon_1 \cdots \varepsilon_p \Big(\sum_{i=1}^p \varepsilon_i a_i\Big)^{\otimes p}. \qquad \square$$

We will work essentially with $M = \mathbb{R}^d$ and $\mathcal{X} = T^*\mathbb{R}^d$ and therefore on $\mathcal{X}^p = T^*\mathbb{R}^{dp} \sim \mathbb{R}^{2dp}$ and recall the invariance properties, if possible, by a change of variable in order to extend it to the general case. Remember that on $\mathbb{R}^{dp}$, the standard and Weyl semiclassical quantization are asymptotically equivalent: $a(x,hD_x)-a^W(x,hD_x)=O(h)$ when $a\in S(1,dX^2)$ ($\sup_{X\in T^*\mathbb{R}^{dp}}|\partial_X^\alpha a(X)|<\infty$ for all $\alpha\in\mathbb{N}^{2d}$). Moreover on $\mathbb{R}^{dp}$, $a^W(x,hD_x)$ is unitary equivalent to $a^W(h^t x,h^{1-t}D_x)$ for any fixed $t\in\mathbb{R}$ so that result can be adapted to different scalings.

3B. ***Semiclassical and multiscale measures.*** We recall the notions of semiclassical (or Wigner) measures and multiscale measures in the finite-dimensional case. We start with the results on $M=\mathbb{R}^D$ (think of $D=dp$) and review the invariance properties for applications to some more general manifolds M.

3B1. *In the Euclidean space.* On $\mathbb{R}^D$ the semiclassical Weyl quantization of a symbol $a\in\mathcal{S}'(\mathbb{R}^{2D})$ will be written $a^{W,h}=a^W(h^t x,h^{1-t}D_x)$, with $t>0$ fixed, while $c^W(x,D_x)$ is given by its kernel:

$$[c^W(x,D_x)](x,y)=\int_{\mathbb{R}^d}e^{i\xi\cdot(x-y)}c\left(\frac{x+y}{2},\xi\right)\frac{d\xi}{(2\pi)^d}.$$

Definition 3.2. Let $(\gamma_h)_{h\in\mathcal{E}}$ with $0\in\bar{\mathcal{E}}$, $\mathcal{E}\subset(0,+\infty)$, be a family of trace-class nonnegative operators on $L^2(\mathbb{R}^D)$ such that $\lim_{h\to 0}\operatorname{Tr}[\gamma_h]<+\infty$. The semiclassical quantization $a\mapsto a^{W,h}=a^W(h^t x,h^{1-t}D_x)$ is said to be *adapted* to the family $(\gamma_h)_{h\in\mathcal{E}}$ if

$$\lim_{\delta\to 0^+}\limsup_{\substack{h\in\mathcal{E}\\ h\to 0}}\operatorname{Re}\operatorname{Tr}[(1-\chi(\delta\,\cdot)^{W,h})\gamma_h]=0$$

for some $\chi\in\mathcal{C}_0^\infty(T^*\mathbb{R}^D)$ such that $\chi\equiv 1$ in a neighborhood of 0.

The set of *Wigner measures* $\mathcal{M}(\gamma_h,h\in\mathcal{E})$ is the set of nonnegative measures ν on $T^*\mathbb{R}^D$ such that there exists $\mathcal{E}'\subset\mathcal{E}$, $0\in\bar{\mathcal{E}}'$, such that,

$$\text{for all } a\in\mathcal{C}_0^\infty(T^*\mathbb{R}^D),\quad \lim_{\substack{h\in\mathcal{E}'\\ h\to 0}}\operatorname{Tr}[\gamma_h a^{W,h}]=\int_{T^*\mathbb{R}^D}a(X)\,d\nu(X).$$

The following well-known statement, see [Colin de Verdière 1985; Helffer et al. 1987; Gérard 1991; Gérard et al. 1997; Lions and Paul 1993; Shnirel'man 1974], results from the asymptotic positivity of the semiclassical quantization and it is actually the finite-dimensional version of bosonic mean-field Wigner measures (with the change of parameter $\varepsilon=2h$); see [Ammari and Nier 2008, Section 3.1].

Proposition 3.3. *Let $(\gamma_h)_{h\in\mathcal{E}}$ with $0\in\bar{\mathcal{E}}$, $\mathcal{E}\subset(0,+\infty)$, such that $\gamma_h\geq 0$ and $\lim_{h\to 0}\operatorname{Tr}[\gamma_h]<+\infty$. The set of semiclassical measures $\mathcal{M}(\gamma_h,h\in\mathcal{E})$ is nonempty. The semiclassical quantization $a^{W,h}$ is adapted to the family $(\gamma_h)_{h\in\mathcal{E}}$ if and only if any $\nu\in\mathcal{M}(\gamma_h,h\in\mathcal{E})$ satisfies $\nu(\mathbb{R}^{2D})=\lim_{h\to 0}\operatorname{Tr}[\gamma_h]$.*

Remark 3.4. (1) The manifold version, with $a^{Q,h}=a(x,hD_x)$ instead of $a^{W,h}$ results from the semiclassical Egorov theorem.

(2) By reducing $\mathcal{E}$ to some subset $\mathcal{E}'$ (think of subsequence extraction), one can always assume that there is a unique semiclassical measure.

(3) While considering a time evolution problem, or adding another uncountable parameter, $(\gamma_{t,h})_{h\in\mathcal{E},t\in\mathbb{R}}$, finding simultaneously the subset $\mathcal{E}'$ for all $t \in \mathbb{R}$ requires some compactness argument with respect to the parameter $t \in \mathbb{R}$, usually obtained by equicontinuity properties.

We now review the multiscale measures introduced in [Fermanian-Kammerer and Gérard 2002; Fermanian Kammerer 2005]. For the reader's convenience, details are given in Appendix A, concerning the relationship between Proposition 3.5 below and the more general statement of [Fermanian Kammerer 2005].

The class of symbols $S^{(2)}$ is defined as the set of $a \in \mathcal{C}^\infty(\mathbb{R}^{2D} \times \mathbb{R}^{2D})$ such that

- there exists $C > 0$ such that for all $Y \in \mathbb{R}^{2D}$, $a(\cdot, Y) \in \mathcal{C}_0^\infty(B(0, C))$;
- there exists a function $a_\infty \in \mathcal{C}_0^\infty(\mathbb{R}^{2D} \times \mathbb{S}^{2D-1})$ such that $a(X, R\omega) \to a_\infty(X, \omega)$, as $R \to \infty$, in $\mathcal{C}^\infty(\mathbb{R}^{2D} \times \mathbb{S}^{2D-1})$.

Those symbols are quantized according to

$$a^{(2),h} = a_h^{W,h}, \quad a_h(X) = a\left(X, \frac{X}{h^{\frac{1}{2}}}\right).$$

A geometrical interpretation of those double scale symbols can be given by matching the compactified quantum phase space with the blow-up at $r = 0$ of the macroscopic phase space; see Figure 1.

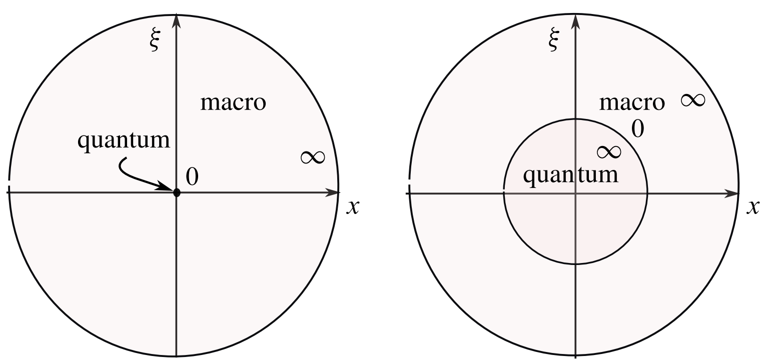

Figure 1. On the left-hand side, the macroscopic phase space with its sphere at infinity. On the right-hand side, the matched quantum and macroscopic phase spaces for which the quantum sphere at infinity and the $r = 0$ macroscopic sphere coincide.

Proposition 3.5. *Let $(\gamma_h)_{h\in\mathcal{E}}$ be a bounded family of nonnegative trace-class operators on $L^2(\mathbb{R}^D)$ with $\lim_{h\to 0}\mathrm{Tr}[\gamma_h] < +\infty$. There exist $\mathcal{E}'\subset\mathcal{E}$, $0\in\bar{\mathcal{E}}'$, nonnegative measures ν and $\nu_{(I)}$ on $\mathbb{R}^{2D}$ and $\mathbb{S}^{2D-1}$, and a $\gamma_0\in\mathcal{L}^1(L^2(\mathbb{R}^D))$ such that $\mathcal{M}(\gamma_h, h\in\mathcal{E}')=\{\nu\}$ and, for all $a\in S^{(2)}$,*

$$\lim_{\substack{h\in\mathcal{E}'\\ h\to 0}} \mathrm{Tr}[\gamma_h a^{(2),h}] = \int_{\mathbb{R}^{2D}\setminus\{0\}} a_\infty\left(X, \frac{X}{|X|}\right) d\nu(X) + \int_{\mathbb{S}^{2D-1}} a_\infty(0,\omega)\, d\nu_{(I)}(\omega) + \mathrm{Tr}[a(0,x,D_x)\gamma_0].$$

Definition 3.6. $\mathcal{M}^{(2)}(\gamma_h, h\in\mathcal{E})$ denotes the set of all triples $(\nu,\nu_{(I)},\gamma_0)$ which can be obtained in Proposition 3.5 for suitable choices of $\mathcal{E}'\subset\mathcal{E}$, $0\in\bar{\mathcal{E}}'$.

Remark 3.7. Actually when $a^{W,h}=a^W(\sqrt{h}x,\sqrt{h}D_x)$, this trace class operator γ_0 is nothing but the weak*-limit of γ_h. Take simply $\tilde{a}(X,Y)=\chi(X)\alpha(Y)$ with $\chi,\alpha\in\mathcal{C}_0^\infty(\mathbb{R}^{2D})$, $\chi\equiv 1$ in a neighborhood of 0 for which

$$\lim_{h\to 0}\|\tilde{a}^{(2),h}-\alpha^W(x,D_x)\|_{\mathcal{L}(L^2)}=0.$$

The above results says $\lim_{h\to 0}\mathrm{Tr}[\gamma_h\alpha^W(x,D_x)]=\mathrm{Tr}[\gamma_0\alpha^W(x,D_x)]$ for all $\alpha\in\mathcal{C}_0^\infty(\mathbb{R}^{2D})\subset L^2(\mathbb{R}^{2D},dX)$, and by the density of the embeddings $\mathcal{C}_0^\infty(\mathbb{R}^{2D})\subset L^2(\mathbb{R}^{2D},dx)\sim\mathcal{L}^2(L^2(\mathbb{R}^D))\subset\mathcal{L}^\infty(L^2(\mathbb{R}^D))$, the test observable $\alpha^W(x,D_x)$ can be replaced by any compact operator $K\in\mathcal{L}^\infty(L^2(\mathbb{R}^D,dx))$. Moreover the relationship between ν and the triple $(1_{(0,+\infty)}(|X|)\nu,\nu_{(I)},\gamma_0)$ can be completed in this case by

$$\nu(\{0\})=\int_{\mathbb{S}^{2D-1}} d\nu_{(I)}(\omega)+\mathrm{Tr}[\gamma_0], \tag{9}$$

and $\nu_{(I)}\equiv 0$ is equivalent to $\nu(\{0\})=\mathrm{Tr}[\gamma_0]$.

Because products of spheres are not spheres, handling the part $\nu_{(I)}$ in the p-particle space, $D=dp$, is not straightforward within a tensorization procedure; see Figure 2.

Actually we expect in the applications that a well chosen quantization will lead to $\nu_{(I)}=0$. This leads to the following definition.

Definition 3.8. Assume that the quantization $a^{W,h}=a^W(\sqrt{h}x,\sqrt{h}D_x)$ is adapted to the family $(\gamma_h)_{h\in\mathcal{E}}$, $\gamma_h\geq 0$, $\mathrm{Tr}[\gamma_h]=1$. We say that the quantization $a^{W,h}=a^W(\sqrt{h}x,\sqrt{h}D_x)$ is *separating* for the family $(\gamma_h)_{h\in\mathcal{E}}$ if one of the three following (equivalent) conditions is satisfied:

(1) For any triple $(\nu,\nu_{(I)},\gamma_0)\in\mathcal{M}^{(2)}(\gamma_h,h\in\mathcal{E})$, we have $\nu_{(I)}=0$.

(2) $$\left.\begin{array}{r}\mathcal{M}(\gamma_h,h\in\mathcal{E}')=\{\nu\},\\ \underset{h\in\mathcal{E}',h\to 0}{\text{w}^*\text{-lim}}\ \gamma_h=\gamma_0 \quad \text{in } \mathcal{L}^1(L^2(\mathbb{R}^D))\end{array}\right\} \implies \nu(\{0\})=\mathrm{Tr}[\gamma_0].$$

(3) For any triple $(\nu,\nu_{(I)},\gamma_0)\in\mathcal{M}^{(2)}(\gamma_h,h\in\mathcal{E})$, we have $\nu(\{0\})=\mathrm{Tr}[\gamma_0]$.

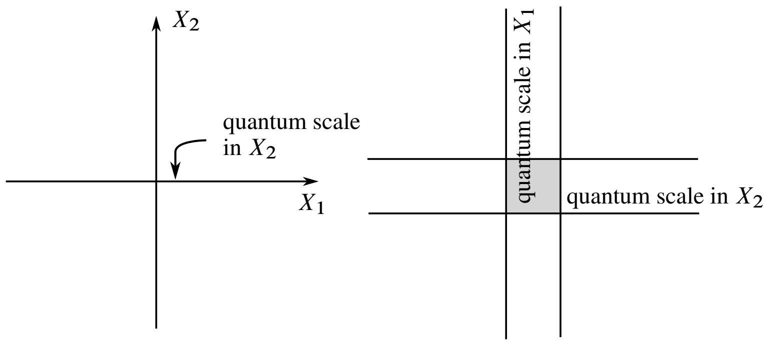

Figure 2. Tensor product of two blow-ups. The product of the two matching spheres is not a sphere: the corners of the gray square correspond to the case when the quantum variables $|X_1|$ and $|X_2|$ go to infinity without any proportionality rule.

Remark 3.9. This terminology expresses the fact that the mass localized at any intermediate scale vanishes asymptotically when $\nu_{(I)} \equiv 0$. Accordingly, the microscopic quantum scale and the macroscopic scale are well-identified and separated.

Hence we can get all the information by computing the weak*-limit of γ_h and the semiclassical measure ν and then by checking a posteriori the equality $\nu(\{0\}) = \mathrm{Tr}[\gamma_0]$.

This will suffice when the quantum part corresponds, within a macroscopic scale, to a point in the phase space. When $M = \mathbb{R}^d$, we have enough flexibility by choosing the small parameter $h > 0$ and using some dilation in $\mathbb{R}^D$ in order to reduce many problems to such a case. On a manifold M if we can first localize the analysis around a point $x_0 \in M$, the problem can be transferred to $\mathbb{R}^D$ and then analyzed with the suitable scaling.

3B2. *On a compact manifold.* We now consider another interesting case of a smooth compact manifold M with the semiclassical calculus $a^{Q,h} = a(x, hD_x)$. This case is not completely treated in [Fermanian Kammerer 2005] because the geometric invariance properties do not follow only from the microlocal equivariance of semiclassical calculus. We assume $\mathscr{Z} = L^2(M, dx)$ to be defined globally on the compact manifold M (e.g., by introducing a metric, dx being the associated volume measure).

Remark 3.10. When M is a general manifold, replace $a^{W,h}$ in Definition 3.2 by $a^{Q,h} = a(x, hD_x)$, and $\chi(\delta\,\cdot)$ with $\delta \to 0$ by some increasing sequence of compactly supported cut-off functions $(\chi_n)_{n\in\mathbb{N}}$ such that $\bigcup_{n\in\mathbb{N}} \chi_n^{-1}(\{1\}) = T^*M$.

To adapt Proposition 3.5 to the case of a compact manifold, we consider another notion instead of the symbols $S^{(2)}$. For the observables we shall consider the pair

(K, a), where $K \in \mathcal{L}^\infty(L^2(M, dx))$ and $a \in \mathcal{C}_0^\infty(S^*M \sqcup (T^*M \setminus M))$, with $S^*M \sqcup (T^*M \setminus M)$ being described in local coordinates through the identification

$$M \times [0, \infty) \times \mathbb{S}^{D-1} \ni (x, r, \omega) \mapsto \begin{cases} (x, \omega) \in S^*M & \text{if } r = 0, \\ (x, \xi = r\omega) \in T^*M \setminus M & \text{otherwise.} \end{cases}$$

We have identified the 0-section of the cotangent bundle T^*M with M. After introducing an additional parameter $\delta > 0$, $\delta \geq h$, and a $\mathcal{C}^\infty$ partition of unity $(1-\chi) + \chi \equiv 1$ on T^*M with $1 - \chi \in \mathcal{C}_0^\infty(T^*M)$, $1 - \chi \equiv 1$ in a neighborhood of M, we can quantize a as

$$a^{(2)\,Q,\delta,h} = [\chi(x, \xi) a(x, h\delta^{-1}\xi)]^{Q,\delta}.$$

Note that K and the quantization of a are geometrically defined modulo $\mathcal{O}(\delta)$ when $h \leq \delta$ in $\mathcal{L}(L^2(M, dx))$: use local charts for the semiclassical calculus with parameter δ, while $\mathcal{L}^\infty(L^2(M, dx))$ is globally defined like all natural spaces associated with $L^2(M, dx)$. Actually in local coordinates the seminorms of the symbol $\chi(x, \xi) a(x, h\delta^{-1}\xi)$ in $S(1, dx^2 + d\xi^2)$ are uniformly bounded with respect to $h \in (0, \delta]$ by seminorms of a in $\mathcal{C}_0^\infty((T^*M \setminus M) \sqcup S^*M)$. Moreover, when the symbol a is nonnegative one has

$$\left\| (\chi a(\cdot, h\delta^{-1}\cdot))^{Q,\delta} - \mathrm{Re}[(\chi a(\cdot, h\delta^{-1}\cdot))^{Q,\delta}] \right\| \leq C_a \delta, \tag{10}$$

$$\|a\|_{L^\infty} + C_a\delta \geq \mathrm{Re}[(\chi a(\cdot, h\delta^{-1}\cdot))^{Q,\delta}] \geq -C_a\delta, \tag{11}$$

uniformly with respect to $h \in (0, \delta]$.

Proposition 3.11. *Let $(\gamma_h)_{h\in\mathcal{E}}$ be a family of nonnegative trace class operators on $L^2(M, dx)$ such that $\lim_{h\to 0} \mathrm{Tr}[\gamma_h] < +\infty$. Then there exist $\mathcal{E}' \subset \mathcal{E}$, $0 \in \bar{\mathcal{E}}'$, with $\mathcal{M}(\gamma_h, h \in \mathcal{E}') = \{\nu\}$, a nonnegative measure $\nu_{(I)}$ on S^*M and a nonnegative $\gamma_0 \in \mathcal{L}^1(L^2(M, dx))$ such that, for any $K \in \mathcal{L}^\infty(L^2(M, dx))$,*

$$\lim_{\substack{h\in\mathcal{E}' \\ h\to 0}} \mathrm{Tr}[\gamma_h K] = \mathrm{Tr}[\gamma_0 K],$$

and, for any $a \in \mathcal{C}_0^\infty(S^*M \sqcup (T^*M \setminus M))$, and any partition of unity $(1-\chi) + \chi \equiv 1$ with $1 - \chi \in \mathcal{C}_0^\infty(T^*M)$, $1 - \chi \equiv 1$ in a neighborhood of M,

$$\lim_{\delta\to 0} \lim_{\substack{h\in\mathcal{E}' \\ h\to 0}} \mathrm{Tr}[\gamma_h\, a^{(2)\,Q,\delta,h}] = \int_{T^*M\setminus M} a(X)\, d\nu(X) + \int_{S^*M} a(X)\, d\nu_{(I)}(X).$$

Additionally $(\nu_{(I)}, \gamma_0)$ is related to ν by

$$\nu(E) = \nu_{(I)}(\pi^{-1}(E)) + \nu_0(E)$$

for any Borel set $E \subset M$ identified with $E \times \{0\}$, when $\pi : S^*M \to M$ is the natural projection and ν_0 is defined by $\int_M \varphi(x)\, d\nu_0(x) = \mathrm{Tr}[\gamma_0 \varphi]$, where $\varphi \in \mathcal{C}^\infty(M)$ is identified with the multiplication operator by the function φ.

Proof. When γ_h is bounded in $\mathcal{L}^1(L^2(M,dx))$, after extraction of a sequence $h_n \to 0$ from $\mathcal{E}$, we have $\mathcal{M}((\gamma_{h_n})_{n\in\mathbb{N}}) = \{\nu\}$, and the weak*-limit γ_0 of (γ_{h_n}), and the associated measure ν_0 are well-defined objects on the manifold M.

Let us construct a measure $\tilde{\nu}$ on

$$(T^*M \setminus M) \sqcup S^*M = \{(x, r\omega) : x \in M,\ \omega \in S^{d-1},\ r \in [0,\infty)\}$$

and a subset $\mathcal{E}' \subset \mathcal{E},\ 0 \in \bar{\mathcal{E}}'$, such that

$$\lim_{\delta\to 0} \lim_{\substack{h\in\mathcal{E}'\\ h\to 0}} \mathrm{Tr}[\gamma_h(\chi a(\cdot\,, h\delta^{-1}\cdot))^{Q,\delta}] = \int_{(T^*M\setminus M)\sqcup S^*M} a\, d\tilde{\nu} \tag{12}$$

holds for all $a \in \mathcal{C}_0^\infty((T^*M \setminus M) \sqcup S^*M)$.

Fix first the partition of unity $(1-\chi) + \chi \equiv 1,\ 1-\chi \in \mathcal{C}_0^\infty(T^*M),\ 1-\chi \equiv 1$ in a neighborhood of M, and $\delta = \delta_0 > 0$. For a given $a \in \mathcal{C}_0^\infty((T^*M \setminus M) \sqcup S^*M)$, the inequalities (10) and (11) imply that one can find a subsequence $(h_{k,\chi,\delta_0,a})_{k\in\mathbb{N}}$ of $(h_n)_{n\in\mathbb{N}}$ such that

$$\lim_{k\to\infty} \mathrm{Tr}[\gamma_{h_{k,\chi,\delta_0,a}}(\chi a(\cdot\,, h_{k,\chi,\delta_0,a}\delta_0^{-1}\cdot))^{Q,\delta_0}] = \ell_{\chi,\delta_0,a} \in \mathbb{C}. \tag{13}$$

For a different partition of unity $(1-\tilde{\chi}) + \tilde{\chi} \equiv 1$ the symbol $[\chi - \tilde{\chi}]a(x, h\delta_0^{-1}\xi)$ is supported in $C^{-1}_{\chi,\tilde{\chi},\delta_0} \le |\xi| \le C_{\chi,\tilde{\chi},\delta_0}$ and equals

$$[\chi - \tilde{\chi}]a(x, h\delta_0^{-1}\xi) = [\chi - \tilde{\chi}]a_0\left(x, \frac{\xi}{|\xi|}\right) + h r_{\chi,\tilde{\chi},\delta_0,h}(x,\xi),$$

where $a_0 = a|_{S^*M}$ and with $r_{\chi,\tilde{\chi},\delta_0,h}$ uniformly bounded in $S(1, dx^2 + d\xi^2)$. For $\delta_0 > 0$ fixed, the operator $[(\chi - \tilde{\chi})a_0]^{Q,\delta_0}$ is a compact operator and we obtain

$$\lim_{h\to 0} \mathrm{Tr}[\gamma_h(\chi a(\cdot, h\delta_0^{-1}\cdot))^{Q,\delta_0}] - \mathrm{Tr}[\gamma_h(\tilde{\chi} a(\cdot, h\delta_0^{-1}\cdot))^{Q,\delta_0}] = \mathrm{Tr}[\gamma_0((\chi - \tilde{\chi})a_0)^{Q,\delta_0}].$$

Therefore the subsequence extraction, which ensures the convergence (13), can be done independently of the choice of $\tilde{\chi}$ and by taking $\tilde{\chi}(x,\xi) = \chi(x, \delta\delta_0^{-1}\xi)$ independently of $\delta > 0$. For $\mathcal{E}_a = (h_{k,a})_{k\in\mathbb{N}}$ such a sequence of parameters, the limits can be compared by

$$\begin{aligned}\ell_{\tilde{\chi},\delta,a} - \ell_{\chi,\delta_0,a} &= \lim_{\substack{h\in\mathcal{E}_a\\ h\to 0}} \mathrm{Tr}[\gamma_h(\tilde{\chi} a(\cdot\,, h\delta^{-1}\cdot))^{Q,\delta}] - \mathrm{Tr}[\gamma_h(\chi a(\cdot\,, h\delta_0^{-1}\cdot))^{Q,\delta_0}]\\ &= \mathrm{Tr}[((\tilde{\chi}(\delta\delta_0^{-1}) - \chi)a_0)^{Q,\delta_0}\gamma_0]. \end{aligned} \tag{14}$$

By choosing $\tilde{\chi} = \chi$ above, the inequality $0 \le (\chi - \chi(\delta\delta_0^{-1}))a_0 \le \chi a_0$ for $a_0 \ge 0$ and $\delta \le \delta_0$, and the δ_0-Gårding inequality implies

$$\left|\mathrm{Tr}[((\tilde{\chi}(\delta\delta_0^{-1}) - \chi)a_0)^{Q,\delta_0}\gamma_0]\right| \le \mathrm{Tr}[(\chi a_0)^{Q,\delta_0}\gamma_0] + \mathcal{O}(\delta_0)$$

uniformly with respect to $\delta \le \delta_0$. Thus the quantity $\ell_{\chi,\delta,a}$ satisfies the Cauchy criterion as $\delta \to 0$ because $\text{s-lim}_{\delta_0\to 0}\,(\chi a_0)^{Q,\delta_0} = 0$ and γ_0 is fixed in $\mathcal{L}^1(L^2(M,dx))$. Hence the limit

$$\ell_{\chi,a} = \lim_{\delta\to 0} \ell_{\chi,\delta,a} = \lim_{\delta\to 0} \lim_{\substack{h\in\mathcal{E}_a\\ h\to 0}} \mathrm{Tr}[\gamma_h(\chi a(\cdot\,, h\delta^{-1}\,\cdot))^{Q,\delta}]$$

exists for any fixed $a \in \mathcal{C}_0^\infty((T^*M \setminus M) \sqcup S^*M)$. Using (14) with $\delta = \delta_0$, but a general pair $(\chi, \tilde{\chi})$, and taking the limit as $\delta \to 0$ shows $\ell_{\tilde{\chi},a} = \ell_{\chi,a} = \ell_a$. The inequalities (10) and (11) give $0 \le \ell_a \le \|a\|_{L^\infty}$. By the usual diagonal extraction process according to a countable set $\mathcal{N} \subset \mathcal{C}_0^\infty((T^*M \setminus M) \sqcup S^*M)$ dense in the set of continuous functions with limit 0 at infinity, we have found a subset $\mathcal{E}' \subset \mathcal{E}$, $0 \in \bar{\mathcal{E}}'$, and a nonnegative measure $\tilde{\nu}$ such that (12) holds. Note that we have also proved

$$\begin{aligned}\int_{(T^*M\setminus M)\sqcup S^*M} a\, d\tilde{\nu} &= \lim_{\delta\to 0} \lim_{\substack{h\in\mathcal{E}'\\ h\to 0}} \mathrm{Tr}[\gamma_h(\chi a(\cdot\,, h\delta^{-1}\,\cdot))^{Q,\delta}]\\ &= \lim_{\delta\to 0} \lim_{\substack{h\in\mathcal{E}'\\ h\to 0}} \mathrm{Tr}[(\gamma_h - \gamma_0)(\chi a(\cdot\,, h\delta^{-1}\,\cdot))^{Q,\delta}],\end{aligned}$$

where neither limit depends on the partition of unity $(1-\chi) + \chi \equiv 1$ with $1-\chi \in \mathcal{C}_0^\infty(T^*M)$ equal to 1 in a neighborhood of M.

We still have to compare $\tilde{\nu}$ and ν. For this take $a \in \mathcal{C}_0^\infty(T^*M)$ and set $a_0(x,\omega) = \varphi(x) = a(x,0)$. The symbol identity

$$\begin{aligned}a(x, h\delta^{-1}\xi) &= a(x, h\delta^{-1}\xi)(1-\chi) + a(x, h\delta^{-1}\xi)\chi\\ &= \varphi(x)(1-\chi) + a(x, h\delta^{-1}\xi)\chi + h r_{a,\chi,\delta,h},\end{aligned}$$

with $r_{a,\delta,\chi,h}$ uniformly bounded in $S(1, dx^2 + d\xi^2)$ with respect to h, leads after δ-quantization to

$$\begin{aligned}\int_{T^*M} a\, d\nu &= \lim_{\substack{h\in\mathcal{E}'\\ h\to 0}} \mathrm{Tr}[\gamma_h a^{Q,h}]\\ &= \lim_{\substack{h\in\mathcal{E}'\\ h\to 0}} \mathrm{Tr}[\gamma_h(\varphi(x)(1-\chi))^{Q,\delta}] + \lim_{\substack{h\in\mathcal{E}'\\ h\to 0}} \mathrm{Tr}[\gamma_h(\chi a(\cdot\,, h\delta^{-1}\,\cdot))^{Q,\delta}].\end{aligned}$$

For $\delta > 0$ fixed, $(\varphi(x)(1-\chi))^{Q,\delta}$ is a fixed compact operator so that the first limit is

$$\lim_{\substack{h\in\mathcal{E}'\\ h\to 0}} \mathrm{Tr}[\gamma_h(\varphi(x)(1-\chi))^{Q,\delta}] = \mathrm{Tr}[\gamma_0(\varphi(x)(1-\chi))^{Q,\delta}],$$

while the second one is exactly the quantity occurring in the definition of $\tilde{\nu}$. Taking the limit as $\delta \to 0$ with $\text{s-lim}_{\delta\to 0}(\varphi(x)(1-\chi))^{Q,\delta} = \varphi(x)$, yields $\nu|_{T^*M\setminus M} =$

$\tilde{\nu}|_{T^*M\setminus M}$. Finally setting $\nu_{(I)} = \tilde{\nu}|_{S^*M}$ yields, for any $a \in \mathcal{C}_0^\infty(T^*M)$,

$$\int_{T^*M} a\,d\nu = \int_{T^*M\setminus M} a\,d\nu + \int_{S^*M} a_0\,d\nu_{(I)} + \int_M \varphi\,d\nu_0,$$

which implies the relation for the measures. □

Definition 3.12. $\mathcal{M}^{(2)}(\gamma_h, h \in \mathcal{E})$ denotes the set of all triples $(\nu, \nu_{(I)}, \gamma_0)$ which can be obtained in Proposition 3.11 for suitable choices of $\mathcal{E}' \subset \mathcal{E},\ 0 \in \bar{\mathcal{E}}'$.

We note that the equality $\nu(M) = \mathrm{Tr}[\gamma_0]$ implies $\nu_{(I)} \equiv 0$ and this leads, as in the previous case, to the following definition.

Definition 3.13. On a compact manifold M, assume that the quantization $a^{Q,h} = a(x, hD_x)$ is adapted to the family $(\gamma_h)_{h\in\mathcal{E}}$, with $\gamma_h \in \mathcal{L}^1(L^2(M)),\ \gamma_h \geq 0$ and $\lim_{h\to 0} \mathrm{Tr}[\gamma_h] < \infty$. We say that the quantization is *separating* if for any $\mathcal{E}' \subset \mathcal{E}$, $0 \in \bar{\mathcal{E}}'$,

$$\left.\begin{array}{r} \mathcal{M}(\gamma_h, h \in \mathcal{E}') = \{\nu\}, \\ \underset{h\in\mathcal{E}', h\to 0}{\mathrm{w}^*\text{-lim}}\ \gamma_h = \gamma_0 \quad \text{in } \mathcal{L}^1(L^2(M)) \end{array}\right\} \implies \nu(\{\xi = 0\}) = \mathrm{Tr}[\gamma_0].$$

While doing the double scale analysis of the nonnormalized reduced density matrices $\bar{\gamma}_h^{(p)}$, especially with the help of tensorization arguments, we will simply study their weak*-limit in $\mathcal{L}^1$ and their semiclassical measures. The equality of Definition 3.8 or 3.13 will be checked a posteriori in order to ensure $\nu_{(I)} \equiv 0$.

4. Mean-field asymptotics with h-dependent observables

We now combine the mean-field asymptotics with semiclassically quantized observables. This means that the parameter ε appearing in CCR (resp. CAR) relations in Section 2 is bound to the semiclassical parameter h of Section 3 parametrizing observables $a^{W,h}$ (or $a^{Q,h}$):

$$\varepsilon = \varepsilon(h) > 0 \quad \text{with } \lim_{h\to 0} \varepsilon(h) = 0.$$

So, from now on we consider families of density matrices on the fermionic or bosonic Fock space $\Gamma_\pm(\mathscr{Z})$ labeled as $(\varrho_{\varepsilon(h)})_{h\in\mathcal{E}}$ with their reduced density matrices denoted by $(\gamma_{\varepsilon(h)}^{(p)})_{h\in\mathcal{E}}$. Firstly, we give a sufficient condition in terms of semiclassical 1-particle observables and of the family $(\varrho_{\varepsilon(h)})_{h\in\mathcal{E}}$ so that a quantization $a^{W,h}$ defined on the p-particle phase space $\mathcal{X}^p$ is adapted to the nonnormalized reduced density matrix $\gamma_{\varepsilon(h)}^{(p)}$ for all $p \in \mathbb{N}$. After this, the quantum and classical symmetrization results, Lemmas 2.8 and 3.1, then provide simple ways to identify the weak*-limits $\gamma_0^{(p)}$ or the semiclassical measures associated with the family $(\gamma_{\varepsilon(h)}^{(p)})_{h\in\mathcal{E}}$ for all $p \in \mathbb{N}$. According to the discussion in Section 2 about Definitions 3.8 and 3.13, a simple mass argument allows one to check that all the multiscale information has been classified. Recall that if

$$\lim_{h\to 0} \mathrm{Tr}[\gamma^{(p)}_{\varepsilon(h)}] = \lim_{h\to 0} \mathrm{Tr}[\varrho_{\varepsilon(h)} \boldsymbol{N}^p_{\pm}] = T^{(p)}$$

then the semiclassical measures $\nu^{(p)} \in \mathcal{M}(\gamma^{(p)}_{\varepsilon(h)}, h \in \mathcal{E})$ (or multiscale asymptotic triples $(\nu^{(p)}, \nu^{(p)}_{(I)}, \gamma^{(p)}_0))$ have a total mass equal to $T^{(p)}$.

Remember that the nonnormalized reduced density matrices $\gamma^{(p)}_{\varepsilon(h)}$ are defined for $h > 0$ by,

$$\text{for all } \tilde{b} \in \mathcal{L}(\mathcal{S}^p_{\pm}\mathscr{Z}^{\otimes p}), \quad \mathrm{Tr}[\gamma^{(p)}_{\varepsilon(h)}\tilde{b}] = \mathrm{Tr}[\varrho_{\varepsilon(h)}\tilde{b}^{\mathrm{Wick}}].$$

They are well-defined and uniformly bounded trace-class operators with respect to $h \in \mathcal{E}$, as soon as $\mathrm{Tr}[\varrho_{\varepsilon(h)}\boldsymbol{N}^p_{\pm}]$ is bounded uniformly with respect to $h \in \mathcal{E}$ for every $p \in \mathbb{N}$. Actually, it is more convenient in many cases, and not so restrictive, to work with exponential weights in terms of the number operator $\boldsymbol{N}_{\pm}$.

Hypothesis 4.1. *The family* $(\varrho_{\varepsilon(h)})_{h\in\mathcal{E}}$ *in* $\mathcal{L}^1(\Gamma_{\pm}(\mathscr{Z}))$ *satisfies*:

(i) *For all* $h \in \mathcal{E}$, *we have* $\varrho_{\varepsilon(h)} \geq 0$ *and* $\mathrm{Tr}[\varrho_{\varepsilon(h)}] = 1$.

(ii) *There exist* $c, C > 0$ *such that* $\mathrm{Tr}[\varrho_{\varepsilon(h)}e^{c\boldsymbol{N}_{\pm}}] \leq C$ *for all* $h \in \mathcal{E}$.

When the 1-particle phase space is $\mathcal{X}^1 = T^*\mathbb{R}^d$ we use the Weyl quantization on $\mathcal{X}^p = T^*\mathbb{R}^{dp}$, $a^{Q,h} = a^{W,h} = a^W(h^t x, h^{1-t}D_x)$, $x \in \mathbb{R}^{dp}$, and when M^1 is a compact manifold, $\mathcal{X}^p = T^*M^p$, we use $a^{Q,h} = a(x, hD_x)$, $x \in M^p$.

Proposition 4.2. *Assume Hypothesis 4.1. Let* $\chi \in \mathcal{C}^\infty_0(T^*M^1)$ *satisfy* $0 \leq \chi \leq 1$ *and* $\chi \equiv 1$ *in a neighborhood of* 0 (*resp. in a neighborhood of the null section* $\{(x,\xi) \in T^*M : \xi = 0\} = M$) *when* $M = \mathbb{R}^d$ (*resp.* M *is a compact manifold*) *and let* $\chi_\delta(X) = \chi(\delta X)$ (*resp.* $\chi_\delta(x,\xi) = \chi(x, \delta\xi)$). *For* $c' < c$, *where* c *is given by Hypothesis 4.1*(*ii*), *if*

$$s_{c',\chi}(\delta) = \limsup_{h\to 0} \mathrm{Re}\,\mathrm{Tr}[\varrho_{\varepsilon(h)}(e^{c'\boldsymbol{N}_{\pm}} - e^{c'd\Gamma_{\pm}(\chi^{Q,h}_\delta)})] \to 0 \quad \text{as } \delta \to 0, \tag{15}$$

then for all $p \in \mathbb{N}$, *the quantization* $a^{Q,h}$ *is adapted to the family* $\gamma^{(p)}_{\varepsilon(h)}$.

Lemma 4.3. *Let* $A \in \mathcal{L}(\mathscr{Z})$ *and* $\alpha \geq \|A\|$. *For* z *in the open disc* $D(0, \alpha/\|A\|) \subset \mathbb{C}$, *the operator* $e^{z d\Gamma_{\pm}(A)}e^{-\alpha\boldsymbol{N}_{\pm}} = e^{d\Gamma_{\pm}(zA - \alpha\mathrm{Id}_{\mathscr{Z}})}$ *is a contraction in* $\Gamma_{\pm}(\mathscr{Z})$ *and the function* $z \mapsto e^{d\Gamma_{\pm}(zA-\alpha\mathrm{Id}_{\mathscr{Z}})}$ *is holomorphic in* $D(0, \alpha/\|A\|)$ *with*

$$\begin{aligned}\frac{1}{p!}d\Gamma_{\pm}(A)^p e^{-\alpha\boldsymbol{N}_{\pm}} &= e^{-\alpha\boldsymbol{N}_{\pm}}\frac{1}{p!}d\Gamma_{\pm}(A)^p \\ &= \frac{1}{2i\pi}\int_{|z|=r} e^{d\Gamma_{\pm}(zA-\alpha\mathrm{Id}_{\mathscr{Z}})}\frac{dz}{z^{p+1}},\end{aligned} \tag{16}$$

which holds true in $\mathcal{L}(\Gamma_{\pm}(\mathscr{Z}))$ *for all* $p \in \mathbb{N}$ *and all* $r \in (0, \alpha/\|A\|)$.

Assume moreover that $A, B \in \mathcal{L}(\mathscr{Z})$, *and* $\alpha > \alpha_0 = \max\{\|A\|, \|B\|\}$. *Then*:

(1) *For all* $z \in D(0, \alpha/\alpha_0)$,

$$\|(e^{zd\Gamma_\pm(B)} - e^{zd\Gamma_\pm(A)})e^{-\alpha \mathbf{N}_\pm}\|_{\mathcal{L}(\Gamma_\pm(\mathscr{Z}))} \leq \frac{\alpha\|B-A\|_{\mathcal{L}(\mathscr{Z})}}{\alpha_0(\alpha-\alpha_0)e}.$$

(2) *For all* $p \in \mathbb{N}$ *and* $r \in (0, \alpha/\alpha_0)$,

$$\|(d\Gamma_\pm(B)^p - d\Gamma_\pm(A)^p)e^{-\alpha \mathbf{N}_\pm}\|_{\mathcal{L}(\Gamma_\pm(\mathscr{Z}))} \leq \frac{\alpha p!\,\|B-A\|_{\mathcal{L}(\mathscr{Z})}}{\alpha_0(\alpha-\alpha_0)er^p}.$$

Proof of Lemma 4.3. After setting $A' = zA$ with $|z| < \alpha/\|A\|$ so that $\|A'\| < \alpha$, notice that $\|e^{\varepsilon(A'-\alpha)}\| \leq e^{\varepsilon\|A'\|}e^{-\varepsilon\alpha} < 1$. Hence, the operators $\Gamma_\pm(e^{-\varepsilon(A'-\alpha)}) = e^{-\alpha \mathbf{N}_\pm}e^{d\Gamma_\pm(A')} = e^{d\Gamma_\pm(A')}e^{-\alpha \mathbf{N}_\pm}$ are contractions on $\Gamma_\pm(\mathscr{Z})$. The holomorphy and the Cauchy formula are then standard.

For the second statement, set $B' = zB$ and $A' = zA$, $|z| < \alpha/\alpha_0$, and use Duhamel's formula:

$$e^{-d\Gamma_\pm(\alpha-B')} - e^{-d\Gamma_\pm(\alpha-A')} = \int_0^1 e^{-(1-t)d\Gamma_\pm(\alpha_0-A')}\, d\Gamma_\pm(B'-A')e^{-(\alpha-\alpha_0)\mathbf{N}_\pm}e^{-td\Gamma_\pm(\alpha_0-B')}\,dt.$$

Since $e^{-(1-t)d\Gamma_\pm(\alpha_0-A')}$ and $e^{-td\Gamma_\pm(\alpha_0-A')}$ are contractions, the inequality

$$\|d\Gamma_\pm(B'-A')e^{-(\alpha-\alpha_0)\mathbf{N}_\pm}\| \leq \frac{\alpha}{\alpha_0}\|B-A\| \sup_{n\in\mathbb{N}} \varepsilon n e^{-(\alpha-\alpha_0)\varepsilon n} \leq \frac{\alpha\|B-A\|}{\alpha_0(\alpha-\alpha_0)e}$$

yields part (1).

Part (2) follows from (16) and part (1). □

Proof of Proposition 4.2. Fix $p \in \mathbb{N}$. We want to find $\tilde{\chi} \in \mathcal{C}_0^\infty(T^*M^p)$, $0 \leq \tilde{\chi} \leq 1$, and $\tilde{\chi} \equiv 1$ in a neighborhood of $\{X \in \mathbb{R}^{2dp} : X = 0\}$ (resp. $\{(x,\xi) \in T^*M^p : \xi = 0\} = M^p$) when $M^p = \mathbb{R}^{dp}$ (resp. when M is a compact manifold), such that

$$\lim_{\delta\to 0} \limsup_{h\to 0} \mathcal{T}(\delta, h) = 0,$$

with

$$\begin{aligned}\mathcal{T}(\delta,h) :=&\ \mathrm{Re}\,\mathrm{Tr}[\gamma^{(p)}_{\varepsilon(h)}(\mathrm{Id}_{\mathcal{S}^p_\pm\mathscr{Z}^{\otimes p}} - \tilde{\chi}^{Q,h}_\delta)]\\ =&\ \mathrm{Re}\,\mathrm{Tr}[\varrho_{\varepsilon(h)}(\mathrm{Id}_{\mathcal{S}^p_\pm\mathscr{Z}^{\otimes p}} - \tilde{\chi}^{Q,h}_\delta)^{\mathrm{Wick}}].\end{aligned}$$

We know that $\chi^{\otimes p} \in \mathcal{C}_0^\infty(T^*M^p)$, with $0 \leq \chi^{\otimes p} \leq 1$. Take $\tilde{\chi}$ such that $\chi^{\otimes p} \leq \tilde{\chi} \leq 1$. For a constant $\kappa_\delta > 0$ to be fixed, the inequalities of symbols

$$\begin{gathered}0 \leq \chi^{\otimes p}_\delta \leq \tilde{\chi}_\delta \leq 1,\\ 0 \leq \chi_\delta + \kappa_\delta h \leq 1 + \kappa_\delta h\end{gathered}$$

and the semiclassical calculus imply

$$\|(1-\tilde{\chi}_\delta)^{Q,h} - \mathrm{Re}[(1-\tilde{\chi}_\delta)^{Q,h}]\|_{\mathcal{L}(\mathscr{Z}^{\otimes p})} \le C_\delta h,$$

$$\|\chi_\delta^{Q,h} - \mathrm{Re}[\chi_\delta^{Q,h}]\| \le C_\delta h,$$

$$\begin{aligned} 0 &\le \mathrm{Re}[(1-\chi_\delta^{\otimes p})^{Q,h}] + C'_\delta h = 1 - (\mathrm{Re}[\chi_\delta^{Q,h}])^{\otimes p} + C'_\delta h \\ &\le (1+2\kappa_\delta h)^p - (\mathrm{Re}[(\chi_\delta+\kappa_\delta h)^{Q,h}])^{\otimes p} + C''_\delta h \quad \text{in } \mathcal{L}(\mathscr{Z}^{\otimes p}) \end{aligned}$$

for some constants $C_\delta, C'_\delta, C''_\delta > 0$, chosen according to $p\in\mathbb{N}$, $\delta>0$ and $\kappa_\delta>0$. Moreover for $\delta>0$ fixed, the constant κ_δ can be chosen so that

$$0 \le \mathrm{Re}[(\chi_\delta+\kappa_\delta h)^{Q,h}] \le 1+2\kappa_\delta h.$$

With

$$\|(1+\boldsymbol{N}_\pm)^p e^{-\frac{c'}{2}\boldsymbol{N}_\pm}\|_{\mathcal{L}(\Gamma_\pm(\mathscr{Z}))} \le C_{p,c'},$$

the number estimate (3) and the positivity property $(\tilde{b}\ge 0) \Rightarrow (\tilde{b}^{\mathrm{Wick}} \ge 0)$, writing

$$\varrho_{\varepsilon(h)} = e^{-\frac{c}{2}\boldsymbol{N}_\pm} e^{\frac{c}{2}\boldsymbol{N}_\pm} \varrho_{\varepsilon(h)} e^{\frac{c}{2}\boldsymbol{N}_\pm} e^{-\frac{c}{2}\boldsymbol{N}_\pm},$$

leads to

$$\begin{aligned} \mathcal{T}(\delta,h) := &\ \mathrm{Re}\,\mathrm{Tr}[\varrho_{\varepsilon(h)}(\mathrm{Id}_{\mathcal{S}^p_\pm \mathscr{Z}^{\otimes p}} - \tilde{\chi}_\delta^{Q,h})^{\mathrm{Wick}}] \\ = &\ \mathrm{Tr}[\varrho_{\varepsilon(h)}(\mathrm{Id}_{\mathcal{S}^p_\pm \mathscr{Z}^{\otimes p}} - \mathrm{Re}[\tilde{\chi}_\delta^{Q,h}])^{\mathrm{Wick}}] + \mathcal{O}_\delta(h) \\ \le &\ \mathrm{Tr}[\varrho_{\varepsilon(h)}((1+2\kappa_\delta h)^p - (\mathrm{Re}[(\chi_\delta+\kappa_\delta h)^{Q,h}])^{\otimes p})^{\mathrm{Wick}}] + \mathcal{O}_\delta(h). \end{aligned}$$

We now use Proposition 2.4 for

$$\mathcal{T}(\delta,h) \le \mathrm{Tr}\big[\varrho_{\varepsilon(h)}\big(d\Gamma_\pm(1+2\kappa_\delta h)^p - d\Gamma_\pm(\mathrm{Re}[(\chi_\delta+\kappa_\delta h)^{Q,h}])^p\big)\big] + \mathcal{O}_\delta(h+\varepsilon(h)).$$

The two operators $\mathcal{A} = d\Gamma_\pm(1+2\kappa_\delta h)$ and $\mathcal{B} = d\Gamma_\pm(\mathrm{Re}[(\chi_\delta+\kappa_\delta h)^{Q,h}])$ are commuting self-adjoint operators such that $0\le\mathcal{B}\le\mathcal{A}$, so that $0\le \mathcal{A}^p - \mathcal{B}^p \le C_{p,c'}[e^{c'\mathcal{A}} - e^{c'\mathcal{B}}]$. We deduce

$$\begin{aligned} \mathcal{T}(\delta,h) \le C_{p,c'}\,\mathrm{Tr}[\varrho_{\varepsilon(h)} e^{cN_\pm} e^{-cN_\pm}(e^{d\Gamma_\pm(c'(1+2\kappa_\delta h))} - e^{d\Gamma_\pm(c'\mathrm{Re}[(\chi_\delta+\kappa_\delta h)^{Q,h}])})] \\ + \mathcal{O}_\delta(h+\varepsilon(h)). \end{aligned}$$

We apply Lemma 4.3 with $z=1$, $A = c'(1+2\kappa_\delta h)$ and $B=c'$, or $A = c'\,\mathrm{Re}[(\chi_\delta+\kappa_\delta h)^{Q,h}]$ and $B = c'\chi_\delta^{Q,h}$, and finally

$$\alpha = c > \alpha_0 = \frac{c+c'}{2} \ge c' \max\{1+2\kappa_\delta h, \|(\chi_\delta+\kappa_\delta h)^{Q,h}\|, \|\chi_\delta^{Q,h}\|\} \quad \text{for } h \le h_{\delta,c,c'}$$

and we get

$$\mathcal{T}(\delta,h) \le \mathrm{Re}\,\mathrm{Tr}[\varrho_{\varepsilon(h)}(e^{c'\boldsymbol{N}_\pm} - e^{c'd\Gamma_\pm(\chi_\delta^{Q,h})})] + \mathcal{O}_\delta(h+\varepsilon(h)).$$

We thus obtain

$$\limsup_{h\to 0} \mathcal{T}(\delta,h) \le s_{c',\chi}(\delta)$$

and our assumption $\lim_{\delta\to 0} s_{c',\chi}(\delta)=0$ gives the desired conclusion. □

Notation. For any open set $\Omega\subseteq\mathbb{C}$ the Hardy space $H^\infty(\Omega)$ is the space of bounded holomorphic functions on Ω.

Proposition 4.4. *Assume Hypothesis 4.1. Then*:

(i) *The set $\mathcal{E}$ can be reduced to $\mathcal{E}'$ so that $\mathcal{M}(\gamma^{(p)}_{\varepsilon(h)}, h\in\mathcal{E}')=\{\nu^{(p)}\}$ for all $p\in\mathbb{N}$, where $\nu^{(p)}$ is a nonnegative measure on $T^*M^p/\mathfrak{S}_p$, i.e., a measure on $(T^*M)^p$ with the invariance (8).*

(ii) *When (15) is satisfied, this implies*

$$\lim_{\substack{h\in\mathcal{E}'\\ h\to 0}} \mathrm{Tr}[\gamma^{(p)}_{\varepsilon(h)}] = \int_{T^*M^p} d\nu^{(p)}(X) \quad \textit{for all } p\in\mathbb{N}.$$

(iii) *For any $a\in\mathcal{C}_0^\infty(\mathbb{R}^{2d})$ there exists $r_a>0$ such that the function $\Phi_{a,h}: s\mapsto \mathrm{Tr}[\varrho_{\varepsilon(h)}e^{s\,d\Gamma_\pm(a^{W,h})}]$ is uniformly bounded in $H^\infty(D(0,r_a))$ and, locally uniformly in s,*

$$\lim_{\substack{h\in\mathcal{E}'\\ h\to 0}} \Phi_{a,h}(s) = \Phi_{a,0}(s) := \sum_{p=0}^{\infty}\frac{s^p}{p!}\int_{T^*M^p} a^{\otimes p}(X)\,d\nu^{(p)}(X). \tag{17}$$

Conversely, if we know that $\Phi_{a,h}$ converges, pointwise on the interval $(-r_a,r_a)$ or in $\mathcal{D}'((-r_a,r_a))$, to some function $\Phi_{a,0}$ as $h\to 0$, $h\in\mathcal{E}$, then $\mathcal{M}(\gamma^{(p)}_{\varepsilon(h)}, h\in\mathcal{E})=\{\nu^{(p)}\}$ for all $p\in\mathbb{N}$ and $\Phi_{a,0}$ is equal to (17) with $\mathcal{E}'=\mathcal{E}$.

Proof. The uniform bound

$$\mathrm{Tr}[\gamma^{(p)}_{\varepsilon(h)}] \le \mathrm{Tr}[\varrho_{\varepsilon(h)}\langle \boldsymbol{N}_\pm\rangle^p] \le C_{p,c}\,\mathrm{Tr}[\varrho_{\varepsilon(h)}e^{c\boldsymbol{N}_\pm}]$$

and Hypothesis 4.1 ensure for each $p\in\mathbb{N}$ the existence of $\mathcal{E}^{(p)}\subseteq\mathcal{E}^{(p-1)}\subseteq\mathcal{E}$, $0\in\bar{\mathcal{E}}^{(p)}$, such that $\mathcal{M}(\gamma^{(p)}_{\varepsilon(h)}, h\in\mathcal{E}^{(p)})=\{\nu^{(p)}\}$ (see Proposition 3.3 and Remark 3.4). A diagonal extraction with respect to p determines $\mathcal{E}'\subset\mathcal{E}$, $0\in\bar{\mathcal{E}}'$, such that $\mathcal{M}(\gamma^{(p)}_{\varepsilon(h)}, h\in\mathcal{E}')=\{\nu^{(p)}\}$ for all $p\in\mathbb{N}$.

The second statement (ii) is a straightforward application of Proposition 4.2 and Proposition 3.3.

In the statement (iii), the holomorphy of the function $\Phi_{a,h}$ on the domain $D(0,c/\|a^{W,h}\|)$ follows by Lemma 4.3. Hypothesis 4.1 now combined with

$$\|e^{-c\boldsymbol{N}_\pm}e^{z\,d\Gamma_\pm(\alpha^{W,h})}\| = \|\Gamma(e^{\varepsilon(z\alpha^{W,h}-c)})\| \le 1 \quad\text{and}\quad \|a^{W,h}\|\le C_a$$

provides the uniform boundedness with respect to $h \in \mathcal{E}$ of $\Phi_{a,h}$ in $H^\infty(D(0,r_a))$ with $r_a = c/C_a$. Moreover, Lemma 4.3(2) shows that $\Phi_{a,h}$ is given by the entire function

$$\Phi_{a,h}(s) = \sum_{p=0}^{\infty} \frac{s^p}{p!} \operatorname{Tr}[\varrho_{\varepsilon(h)} d\Gamma_\pm(a^{W,h})^p],$$

which is absolutely convergent on $s \in D(0,r_a)$ uniformly in $h \in \mathcal{E}$ since the estimate

$$\|d\Gamma_\pm(a^{W,h})^p e^{-c\boldsymbol{N}_\pm}\|_{\mathcal{L}(\Gamma_\pm(\mathscr{Z}))} \lesssim \frac{p!}{r_a^p} \tag{18}$$

holds true uniformly for all $p \in \mathbb{N}$ and $h \in \mathcal{E}$. According to (i) and Proposition 2.4,

$$\begin{aligned}\lim_{\substack{h\in\mathcal{E}'\\ h\to 0}} \operatorname{Tr}[\varrho_{\varepsilon(h)} d\Gamma_\pm(a^{W,h})^p] &= \lim_{\substack{h\in\mathcal{E}'\\ h\to 0}} \operatorname{Tr}[\varrho_{\varepsilon(h)}((a^{W,h})^{\otimes p})^{\mathrm{Wick}}] \\ &= \lim_{\substack{h\in\mathcal{E}'\\ h\to 0}} \operatorname{Tr}[\gamma_{\varepsilon(h)}^{(p)}(a^{W,h})^{\otimes p}] = \int_{T^*M^p} a^{\otimes p}\, d\nu^{(p)}.\end{aligned}$$

Hence, by dominated convergence, $\Phi_{a,h}$ converges locally uniformly in $D(0,r_a)$ to $\Phi_{a,0}$ given by (17) and consequently $\Phi_{a,0}$ belongs to $H^\infty(D(0,r_a))$ as well.

Moreover, assume for any $a \in \mathcal{C}_0^\infty(\mathbb{R}^{2d})$ the convergence of $\Phi_{a,h}$ to $\Phi_{a,0}$ in a weak topology on the interval $(-r_a,r_a)$ as $h \in \mathcal{E}$, $h \to 0$. Let $\nu_1^{(p)}, \nu_2^{(p)} \in \mathcal{M}(\gamma_h^{(p)}, h \in \mathcal{E})$, for $p \in \mathbb{N}$. Then according to (i) and the first part of (iii), one has, for any $s \in (-r_a, r_a)$,

$$\Phi_{a,0}(s) = \sum_{p=0}^{\infty} \frac{s^p}{p!} \int_{T^*M^p} a^{\otimes p}(X)\, d\nu_1^{(p)}(X) = \sum_{p=0}^{\infty} \frac{s^p}{p!} \int_{T^*M^p} a^{\otimes p}(X)\, d\nu_2^{(p)}(X).$$

The uniform estimate (18) shows that $\Phi_{a,0}$ admits a holomorphic extension on $D(0,r_a)$ and consequently

$$\int_{T^*M^p} a^{\otimes p}(X)\, d\nu_1^{(p)}(X) = \int_{T^*M^p} a^{\otimes p}(X)\, d\nu_2^{(p)}(X)$$

for all $p \in \mathbb{N}$. Thanks to Lemma 3.1, the measures $\nu_1^{(p)}$ and $\nu_2^{(p)}$ are determined by integrating with all the test functions $a^{\otimes p}$, $a \in \mathcal{C}_0^\infty(T^*M)$. So $\nu_1^{(p)} = \nu_2^{(p)}$, which ends the proof. □

Replacing the semiclassical symmetrization Lemma 3.1 by the quantum ones, Lemma 2.8 in the above proof leads to the following similar result for the quantum part.

Proposition 4.5. *Assume Hypothesis 4.1. For all $K \in \mathcal{L}^\infty(\mathscr{Z})$ there exists $r_K > 0$ such that the set $\{\Psi_{K,h}, h \in \mathcal{E}\}$ of functions $\Psi_{K,h}(s) := \operatorname{Tr}[\varrho_{\varepsilon(h)} e^{s\, d\Gamma_\pm(K)}]$ is bounded in $H^\infty(D(0,r_K))$.*

The pointwise or $\mathcal{D}'((-r_K, r_K))$*-convergence* $\lim_{h\in\mathcal{E},\, h\to 0}\Psi_{K,h}=\Psi_{K,0}$ *is equivalent to* $\mathrm{w}^*\text{-}\lim_{h\in\mathcal{E},\, h\to 0}\gamma_h^{(p)}=\gamma_0^{(p)}$ *(remember* $\mathcal{L}^1=(\mathcal{L}^\infty)^*$*) with*

$$\Psi_{K,0}(s)=\sum_{p=0}^{\infty}\mathrm{Tr}[\gamma_0^{(p)}K^{\otimes p}]\frac{s^p}{p!}.$$

Let us consider a specific feature of the fermionic case:

Proposition 4.6. *Let* $(\varrho_\varepsilon)_{\varepsilon\in\mathcal{E}}$ be a family of nonnegative, trace-1 operators in $\mathcal{L}^1(\Gamma_-(\mathcal{Z}))$. Let $\gamma_\varepsilon^{(p)}$ *denote the corresponding nonnormalized reduced density matrices of order* p. If $\gamma_0^{(p)}\in\mathcal{L}^1(\mathcal{S}_-^p\mathcal{Z}^{\otimes p})$ is such that,

$$\text{for all } K\in\mathcal{L}^\infty(\mathcal{S}_-^p\mathcal{Z}^{\otimes p}),\qquad \lim_{\substack{\varepsilon\in\mathcal{E}\\ \varepsilon\to 0}}\mathrm{Tr}[\gamma_\varepsilon^{(p)}K]=\mathrm{Tr}[\gamma_0^{(p)}K],$$

then $\gamma_0^{(p)}=0$.

As a consequence, the weak**-limits* $\gamma_0^{(p)}$ *always vanish in the fermionic case.*

Proof. First consider K a nonnegative finite-rank operator. Then

$$\lim_{\substack{\varepsilon\in\mathcal{E}\\ \varepsilon\to 0}}\mathrm{Tr}[\varrho_\varepsilon K^{\mathrm{Wick}}]=\mathrm{Tr}[\gamma_0^{(p)}K].$$

For fermions, $K^{\mathrm{Wick}}\le\varepsilon^p\,\mathrm{Tr}[K]$, and hence $\mathrm{Tr}[\varrho_\varepsilon K^{\mathrm{Wick}}]\le\varepsilon(h)^p\to 0$ as $\varepsilon\to 0$. Since any finite-rank operator is of the form $K=K_1-K_2+i(K_3-K_4)$ for some nonnegative finite-rank operators $K_j,\ j\in\{1,2,3,4\}$, the limit $\mathrm{Tr}[\varrho_\varepsilon K^{\mathrm{Wick}}]\to 0=\mathrm{Tr}[\gamma_0^{(p)}K]$ holds for any finite-rank operator K. Hence, by density of the finite-rank operators in the compact operators for the operator norm, $\mathrm{Tr}[\gamma_0^{(p)}K]=0$ for any $K\in\mathcal{L}^\infty(\mathcal{S}_-^p\mathcal{Z}^{\otimes p})$, i.e., $\gamma_0^{(p)}=0$. ☐

5. Examples

5A. ***h-dependent coherent states in the bosonic case.*** We first recall our normalization for a coherent state. If we use the identification $\mathcal{S}_\pm^0\mathcal{Z}\equiv\mathbb{C}$, then the vacuum-state vector is defined as $\Omega=(1,0,0,\dots)\in\Gamma_\pm(\mathcal{Z})$. We then introduce the usual field operators $\Phi(f)=(1/\sqrt{2})(a^*(f)+a(f))$, with $f\in\mathcal{Z}$, and the Weyl operators are $W(f)=\exp((i/\sqrt{2})\Phi(f))$. A coherent state is a pure state $E_z=W(\sqrt{2}z/(i\varepsilon))\Omega$, with $z\in\mathscr{Z}$. One then can also speak of a coherent state for the corresponding density matrix $|E_z\rangle\langle E_z|$. One of the useful properties of coherent states is that

$$b(z)=\langle E(z),b^{\mathrm{Wick}}E(z)\rangle. \tag{19}$$

See, e.g., [Ammari and Nier 2008, Proposition 2.10]. The case of coherent states is simple:

Proposition 5.1. *Let $(z_\varepsilon)_{\varepsilon\in(0,1]}$ be a bounded family of $\mathscr{Z}$, choose the semiclassical quantization $a \mapsto a^{W,h} = a^W(\sqrt{h}x, \sqrt{h}D_x)$, and fix a function $\varepsilon = \varepsilon(h) \to 0$ as $h \to 0$. Up to an extraction, $z_{\varepsilon(h)} \rightharpoonup z_0 \in \mathcal{Z}$ weakly, and $\mathcal{M}(|z_{\varepsilon(h)}\rangle\langle z_{\varepsilon(h)}|, h \in \mathcal{E}) = \{\nu\}$. Assume that the semiclassical quantization $a^{W,h} = a^W(\sqrt{h}x, \sqrt{h}D_x)$ is adapted to $(|z_{\varepsilon(h)}\rangle\langle z_{\varepsilon(h)}|)_h$ and separating for $(|z_{\varepsilon(h)}\rangle\langle z_{\varepsilon(h)}|)_h$. Then the family $(\varrho_{\varepsilon(h)} = |E_{z_{\varepsilon(h)}}\rangle\langle E_{z_{\varepsilon(h)}}|)_{h\in\mathcal{E}}$ has*

$$\gamma^{(p)}_{\varepsilon(h)} = |z^{\otimes p}_{\varepsilon(h)}\rangle\langle z^{\otimes p}_{\varepsilon(h)}|$$

as (nonnormalized) reduced density matrices of order p, for which the quantization is adapted and separating, and

$$\mathcal{M}^{(2)}(\gamma^{(p)}_{\varepsilon(h)}, h \in \mathcal{E}) = \{(\nu^{\otimes p}, 0, |z_0^{\otimes p}\rangle\langle z_0^{\otimes p}|)\}.$$

Proof. Formula (19) yields, for $B \in \mathcal{L}(\mathcal{S}^p_+\mathcal{Z}^{\otimes p})$,

$$\langle z^{\otimes p}_{\varepsilon(h)}, B z^{\otimes p}_{\varepsilon(h)}\rangle = \langle E_{z_{\varepsilon(h)}}|B^{\mathrm{Wick}}|E_{z_{\varepsilon(h)}}\rangle = \mathrm{Tr}[\varrho_{\varepsilon(h)} B^{\mathrm{Wick}}] = \mathrm{Tr}[\gamma^{(p)}_{\varepsilon(h)} B],$$

which implies the result. □

The case of coherent states, although simple, can already exhibit interesting behaviors for some families $(z_\varepsilon)_{\varepsilon\in(0,1]}$. Indeed,

Remark 5.2. Let $(z_{j,\varepsilon(h)})_{h\in(0,1]}$, $j \in \{1, 2\}$, be families of $\mathcal{Z}$ such that

- $z_{1,\varepsilon(h)} \to z_{1,0} \in \mathcal{Z}$ as $h \to 0$, and
- $(z_{2,\varepsilon(h)})_{h\in(0,1]}$ converges weakly to 0,

$$\lim_{R\to\infty} \limsup_{h\to 0} \|(1 - \chi(R^{-1}\cdot))^{W,h} z_{2,\varepsilon(h)}\| = 0$$

  for some $\chi \in \mathcal{C}^\infty_0(\mathbb{R}^{2d})$, $\chi \equiv 1$ around 0 (no mass escaping at infinity in the phase space), and $\mathcal{M}(|z_{2,\varepsilon(h)}\rangle\langle z_{2,\varepsilon(h)}|, h \in \mathcal{E}) = \{\nu_2\}$, with $\nu_2(\{0\}) = 0$.

Then $(|z_{1,\varepsilon(h)} + z_{2,\varepsilon(h)}\rangle\langle z_{1,\varepsilon(h)} + z_{2,\varepsilon(h)}|)_{h\in(0,1]}$ satisfies the assumptions of Proposition 5.1, and $z_0 = z_{1,0}$, $\nu = \|z_{1,0}\|^2\delta_0 + \nu_2$.

5B. ***Gibbs states.*** For a given nonnegative self-adjoint hamiltonian H defined in $\mathscr{Z}$ with domain $D(H)$, the Gibbs state at positive temperature $\frac{1}{\beta}$ and with the chemical potential $\mu < 0$ is given by

$$\omega_\varepsilon(A) = \frac{\mathrm{Tr}[\Gamma_\pm(e^{-\beta(H-\mu)})A]}{\mathrm{Tr}[\Gamma_\pm(e^{-\beta(H-\mu)})]} = \mathrm{Tr}[\varrho_\varepsilon A].$$

In general $\varrho_\varepsilon \in \mathcal{L}^1(\Gamma_\pm(\mathscr{Z}))$ as soon as $e^{-\beta(H-\mu)} \in \mathcal{L}^1(\mathscr{Z})$ (in the bosonic case $H \geq 0$ and $\mu < 0$ imply $\|e^{-\beta(H-\mu)}\|_{\mathcal{L}(\mathcal{Z})} < 1$, see Lemma D.1). Moreover the quasi-free state formula, see [Bratteli and Robinson 1981], with ε-dependent quantization gives

$$\operatorname{Tr}[\varrho_\varepsilon \boldsymbol{N}_\pm] = \varepsilon \operatorname{Tr}[e^{-\beta(H-\mu)}(1 \mp e^{-\beta(H-\mu)})^{-1}]$$

and additionally, in the case of bosons,

$$\operatorname{Tr}[\varrho_\varepsilon W(f)] = \exp\big[-\tfrac{1}{4}\varepsilon\langle f, (1+e^{-\beta(H-\mu)})(1-e^{-\beta(H-\mu)})^{-1} f\rangle\big].$$

5B1. *The fermionic case.* This case is simpler than the bosonic case for two reasons: first because the quantum part vanishes (see Proposition 4.6), and second because there is no singularity to handle. To fix the ideas we consider the simple case when H is the harmonic oscillator. Actually one can treat more general pseudodifferential operators, and we do that below in the more interesting case of bosons and Bose–Einstein condensation.

Proposition 5.3. *Let* $\beta > 0$, $H = \frac{1}{2}|X|^{2\,W,h}$, $\mu(\varepsilon)$ *be such that* $\mu(\varepsilon) \geq C\varepsilon$ *for some constant* $C > 0$, *and assume that* $\varepsilon = \varepsilon(h) = h^d$. *Let*

$$\varrho_{\varepsilon(h)} = \frac{\Gamma_-(e^{-\beta(H-\mu(\varepsilon))})}{\operatorname{Tr}[\Gamma_-(e^{-\beta(H-\mu(\varepsilon))})]}$$

and $\gamma^{(p)}_{\varepsilon(h)}$ *be its nonnormalized reduced density matrix of order* $p \geq 1$. *Then*

$$\mathcal{M}^{(2)}(\gamma^{(p)}_{\varepsilon(h)}, h \in (0,1]) = \{(\nu^{(p)}, 0, 0)\},$$

where

$$d\nu^{(p)} = \left(\frac{e^{-\frac{\beta}{2}|X|^2}}{1+e^{-\frac{\beta}{2}|X|^2}}\frac{dX}{(2\pi)^d}\right)^{\otimes p}.$$

Proof. From Remark 3.7 and Proposition 4.6, any

$$(\nu^{(p)}, \nu_I^{(p)}, \gamma_0^{(p)}) \in \mathcal{M}^{(2)}(\gamma^{(p)}_{\varepsilon(h)}, h \in (0,1])$$

satisfies $\gamma_0^{(p)} = 0$.

Since we are considering a Gibbs state, the Wick formula yields

$$\gamma^{(p)}_{\varepsilon(h)} = p!\,\mathcal{S}^p_\pm\,\gamma^{(1)\otimes p}_{\varepsilon(h)}\,\mathcal{S}^{p,*}_\pm.$$

Moreover, in the fermionic case,

$$\gamma^{(1)}_{\varepsilon(h)} = \varepsilon(h)\frac{C}{1+C} \quad \text{for } \varrho_{\varepsilon(h)} = \frac{\Gamma_-(C)}{\operatorname{Tr}[\Gamma_-(C)]};$$

that is to say, with $\varepsilon(h) = h^d$,

$$\gamma^{(1)}_{\varepsilon(h)} = h^d\,\frac{e^{-\beta(H-\mu)}}{1+e^{-\beta(H-\mu)}}$$

in our case. The semiclassical calculus combined with the Helffer–Sjöstrand functional calculus formula yields

$$\frac{e^{-\beta\left(\frac{1}{2}|X|^{2\,W,h}-\mu\right)}}{1+e^{-\beta\left(\frac{1}{2}|X|^{2\,W,h}-\mu\right)}}=\left(\frac{e^{-\frac{\beta}{2}|X|^2}}{1+e^{-\frac{\beta}{2}|X|^2}}\right)^{W,h}+\mathcal{O}(h)\quad\text{in}\quad\mathcal{L}(\mathcal{Z}).$$

For details we refer the reader to, e.g., [Dimassi and Sjöstrand 1999; Helffer and Nier 2005] or to the proof of Proposition 5.6. Again by the semiclassical calculus we know $h^d a^{W,h}$ is uniformly bounded in $\mathcal{L}^1(L^2(\mathbb{R}^d))$ for $a\in\mathcal{C}_0^\infty(\mathbb{R}^{2d})$. This leads to

$$\begin{aligned}\operatorname{Tr}[(a^{W,h})^{\otimes p}\gamma_{\varepsilon(h)}^{(p)}]&=\operatorname{Tr}[a^{W,h}\gamma_{\varepsilon(h)}^{(1)}]^p+\mathcal{O}(h)\\&=\operatorname{Tr}\left[\left(\frac{e^{-\frac{\beta}{2}|X|^2}}{1+e^{-\frac{\beta}{2}|X|^2}}\right)^{W,h}h^d a^{W,h}\right]^p+\mathcal{O}(h).\end{aligned}$$

We finally use

$$h^d\operatorname{Tr}[a^{W,h}b^{W,h}]=\int_{\mathbb{R}^{2d}}a(X)b(X)\frac{dX}{(2\pi)^d},$$

which implies

$$\lim_{h\to 0}\operatorname{Tr}[(a^{W,h})^{\otimes p}\,\gamma_{\varepsilon(h)}^{(p)}]=\left(\int_{\mathbb{R}^{2d}}\frac{e^{-\frac{\beta}{2}|X|^2}}{1+e^{-\frac{\beta}{2}|X|^2}}a(X)\frac{dX}{(2\pi)^d}\right)^p.$$

Hence

$$d\nu^{(p)}(X)=\left(\frac{e^{-\frac{\beta}{2}|X|^2}}{1+e^{-\frac{\beta}{2}|X|^2}}\frac{dX}{(2\pi)^d}\right)^{\otimes p}.$$ □

5B2. *Parameter-dependent Gibbs states and Bose–Einstein condensation in the bosonic case.* The Bose–Einstein condensation phenomenon occurs when H has a ground state $\ker H=\mathbb{C}\psi_0$ and the chemical potential is scaled according to

$$-\beta\mu=\frac{\varepsilon}{\nu_C}\quad\text{for some fixed }\nu_C>0.$$

An especially interesting case is when H is a semiclassically quantized symbol with semiclassical parameter h related to ε, or $\varepsilon=\varepsilon(h)$ according to our previous notations. The quantum and semiclassical parts arise simultaneously when $\varepsilon=h^d$. Two cases will be considered: the first one concerns $\mathscr{Z}=L^2(\mathbb{R}^d)$ with a nondegenerate bottom-well hamiltonian; the second one $\mathscr{Z}=L^2(M)$ with the semiclassical Laplace–Beltrami operator on the compact Riemannian manifold M.

In the first case, let $S(\langle X\rangle^m,dX^2/\langle X\rangle^2)$ denote the Hörmander class of symbols satisfying $|\partial_X^\beta a(X)|\le C_\beta\langle X\rangle^{m-\beta}$, and let $\alpha\in S(\langle X\rangle^2,dX^2/\langle X\rangle^2)$ be elliptic in this class with a unique nondegenerate minimum at $X=0$ (e.g., the symbol of the harmonic oscillator hamiltonian). We can even consider small perturbations of this situation after setting

$$H=\alpha^{W,h}+B^h-\lambda_0(\alpha^{W,h}+B^h),\quad \alpha^{W,h}=\alpha(\sqrt{h}x,\sqrt{h}D_x),\quad \varepsilon=h^d,$$

where

$$B^h=B^{h*}\in\mathcal{L}(L^2(\mathbb{R}^d)),\quad \|B^h\|=o(h),\quad \lambda_0(\alpha^{W,h}+B^h)=\inf\sigma(\alpha^{W,h}+B^h).$$

It is convenient in this case to introduce the linear symplectic transformation $T\in\mathrm{Sp}_{2d}(\mathbb{R})$ such that ${}^tX\,{}^tT^{-1}\,\mathrm{Hess}\,\alpha(0)T^{-1}X=\sum_{j=1}^d\beta_jX_j^2$ and to introduce some unitary quantization U_T of T, i.e., a unitary operator on $L^2(\mathbb{R}^d)$ such that $U_T^*b^WU_T=b(T^{-1}\cdot)^W$.

Proposition 5.4. *Under the above assumptions with dimension $d\geq 2$, for any $p\in\mathbb{N}$, we have $\mathcal{M}^{(2)}(\gamma^{(p)}_{\varepsilon(h)},h\in\mathcal{E})=\{(\nu^{(p)},0,\gamma_0^{(p)})\}$ (see Definition 3.12), where*

$$\gamma_0^{(p)}=p!\,\nu_C^p|\psi_0^{\otimes p}\rangle\langle\psi_0^{\otimes p}|\quad \textit{with}\ \ \psi_0(x)=U_T\frac{e^{-\frac{1}{2}x^2}}{\pi^{\frac{d}{4}}}$$

and

$$\nu^{(p)}=\sum_{\sigma\in\mathfrak{S}_p}\sigma_*\Bigg[\sum_{k=0}^p\frac{1}{(p-k)!}\nu_C^k\delta_0^{\otimes k}\otimes\nu(\beta,\cdot)^{\otimes p-k}\Bigg],$$

with

$$d\nu(\beta,X)=\frac{e^{-\beta\alpha(X)}}{1-e^{-\beta\alpha(X)}}\frac{dX}{(2\pi)^d}.$$

The proof is given in Section 5B4 and needs some preliminaries, which are given in Proposition 5.6 and Lemma 5.7.

Another even simpler case, related to the example $M=\mathbb{T}^d$ presented in [Ammari and Nier 2008], is $\mathscr{Z}=L^2(M,dv_g(x))$ when (M,g) is a compact Riemannian manifold with volume $dv_g(x)$ and

$$H=-h^2\Delta_g+B_h-\lambda_0(-h^2\Delta_g+B_h),$$

where Δ_g is the Laplace Beltrami operator on (M,g) and $B_h=B_h^*\in\mathcal{L}(L^2(M))$, $\|B_h\|=\underline{o(h^2)}$.

Proposition 5.5. *Under the above assumptions with $d\geq 3$, for any $p\in\mathbb{N}$, we have $\mathcal{M}^{(2)}(\gamma^{(p)}_{\varepsilon(h)},h\in\mathcal{E})=\{(\nu^{(p)},0,\gamma_0^{(p)})\}$, where*

$$\gamma_0^{(p)}=p!\,\nu_C^p|\psi_0^{\otimes p}\rangle\langle\psi_0^{\otimes p}|,\quad \psi_0=\frac{1}{v_g(M)^{\frac{1}{2}}},$$

$$\nu^{(p)}=\sum_{\sigma\in\mathfrak{S}_p}\sigma_*\Bigg[\sum_{k=0}^p\frac{1}{(p-k)!}\nu_C^k\bigg(\frac{1}{v_g(M)}dv_g(x)\otimes\delta_0(\xi)\bigg)^{\otimes k}\otimes\nu(\beta)^{\otimes(p-k)}\Bigg],$$

with

$$d\nu(\beta,X)=\frac{e^{-\beta|\xi|^2_{g(x)}}}{1-e^{-\beta|\xi|^2_{g(x)}}}\frac{dx\,d\xi}{(2\pi)^d},$$

and

$$|\xi|^2_{g(x)}=\sum_{i,j\le d}g^{ij}(x)\xi_i\xi_j\quad\textit{when } g=\sum_{i,j\le d}g_{ij}(x)\,dx^i\,dx^j,\ \ (g_{ij})^{-1}=(g^{ij}).$$

We shall focus on the first case, which requires a more careful analysis, while $\sigma(-h^2\Delta_g)=h^2\sigma(-\Delta_g)$ reduces the problem even more easily to the integrability of $e^{-\beta|\xi|^2_{g(x)}}/(1-e^{-\beta|\xi|^2_{g(x)}})$, valid when $d\ge 3$. The proof of Proposition 5.5 is left as an exercise, which requires the adaptation of the following arguments in the case of Proposition 3.11 with the associated Definitions 3.13 and 3.12.

5B3. *Semiclassical asymptotics with a singularity at $X=0$.* We give here a general semiclassical result in $T^*\mathbb{R}^d$, which involves traces and symbols with a singularity at $X=0$.

Proposition 5.6. *Consider the hamiltonian $H=\alpha^{W,h}+B_h-\lambda_0(\alpha^{W,h}+B^h)$, with $\alpha^{W,h}=\alpha(\sqrt{h}x,\sqrt{h}D_x)$, $\alpha\in S(\langle X\rangle^2,dX^2/\langle X\rangle^2)$ elliptic and real such that $\alpha(0)=0$ is the unique nondegenerate minimum, $B_h=B_h^*\in\mathcal{L}(L^2(\mathbb{R}^d))$, $\|B_h\|=o(h)$, and $\lambda_0(\alpha^{W,h}+B_h)=\inf\sigma(\alpha^{W,h}+B_h)$. Assume that $f\in\mathcal{C}^\infty((0,+\infty);\mathbb{R})$ is decreasing and satisfies*

$$0\le f(u)\le Cu^{-\kappa_\infty},\qquad \lim_{u\to 0^+}u^{\kappa_0}f(u)=f_0\in\mathbb{R},\qquad 0<\kappa_0<d<\kappa_\infty.$$

For $c>0$, the operator $f(H+ch^{\frac{d}{\kappa_0}})$ is trace class with

$$\limsup_{h\to 0^+}h^d\|f(H+ch^{\frac{d}{\kappa_0}})\|_{\mathcal{L}^1(L^2(\mathbb{R}^d))}<+\infty.$$

Moreover the convergence

$$\lim_{h\to 0}h^d\,\mathrm{Tr}[f(H+ch^{\frac{d}{\kappa_0}})a^{W,h}]=\frac{f_0}{c^{\kappa_0}}a(0)+\int_{\mathbb{R}^{2d}}f(\alpha(X))a(X)\frac{dX}{(2\pi)^d}$$

holds for all $a\in S(1,dX^2)$. Finally, all the above estimates and convergences hold uniformly with respect to $c\in(1/A,A)$ for any fixed $A>1$.

The following lemma gives, in a simple way, useful inequalities for our purpose, which are deduced with elementary arguments, and in a robust way with respect to the perturbation B_h, from more accurate and sophisticated results on the spectrum of $\alpha^{W,h}$; see [Charles and Vũ Ngọc 2008; Dimassi and Sjöstrand 1999].

Lemma 5.7. *Let $\alpha\in S(\langle X\rangle^2,dX^2/\langle X\rangle^2)$ be real-valued, elliptic, which means $1+\alpha(X)\ge C^{-1}\langle X\rangle^2$, with a unique nondegenerate minimum at $X=0$ and set*

$\alpha_0(X) = \frac{1}{2}|X|^2$. *Let* $B_h = B_h^* \in \mathcal{L}(L^2(\mathbb{R}^d))$ *be such that* $\|B_h\| = o(h)$. *The ordered eigenvalues are denoted by* $\lambda_j(\alpha^{W,h} + B_h)$ *and* $\lambda_j(\alpha_0^{W,h})$ *for* $j \in \mathbb{N}$:

- *For* $j = 0$, *we have* $\lambda_0(\alpha^{W,h} + B_h) = \mathrm{Tr}[\mathrm{Hess}\,\alpha(0)]h + o(h)$ *and the associated spectral projection satisfies*

$$\lim_{h\to 0} 1_{\{\lambda_0(\alpha^{W,h}+B_h)\}}(\alpha^{W,h} + B_h) = (\pi^{-d} e^{-|TX|^2})^W(x, D_x) \quad \text{in } \mathcal{L}^1(L^2(\mathbb{R}^d)),$$

where $T \in \mathrm{Sp}_{2d}(\mathbb{R})$ *is such that* ${}^t X {}^t T^{-1} \mathrm{Hess}\,\alpha(0) T^{-1} X = \sum_{j=1}^d \beta_j X_j^2$.

- *There exist* $h_0 > 0$ *and* $C' \geq 1$ *such that, for all* $j > 0$ *and* $h \in (0, h_0)$,

$$\begin{aligned}\tfrac{1}{2}C'^{-1}hd &\leq C'^{-1}\lambda_j(\alpha_0^{W,h}) \\ &\leq \lambda_j(\alpha^{W,h} + B_h) - \lambda_0(\alpha^{W,h} + B_h) \leq C'\lambda_j(\alpha_0^{W,h}).\end{aligned} \tag{20}$$

Remark 5.8. Of course $\sigma(\alpha_0^{W,h}) = \left\{h\left(\frac{d}{2} + |n|\right) : n \in \mathbb{N}^d\right\}$ and the bounds (20) are actually written in order to use this later. But for an easy use of the min-max principle it is better to write the eigenvalues $\lambda_j(\alpha_0^{W,h})$ in increasing order, with repetition according to their multiplicity.

Proof of Lemma 5.7. We start by noting that $1 + \alpha \in S(\langle X\rangle^2, dX^2/\langle X\rangle^2)$ is fully elliptic in the sense that $(1 + \alpha)^{-1} \in S(\langle X\rangle^{-2}, dX^2/\langle X\rangle^2)$. Therefore

$$(1 + \alpha)\sharp^{W,h}\frac{1}{1+\alpha} = 1 + h^2 R_+(h), \qquad \frac{1}{1+\alpha}\sharp^{W,h}(1 + \alpha) = 1 + h^2 R_-(h)$$

with $R_\pm(h)$ uniformly bounded in $S(\langle X\rangle^{-2}, dX^2/\langle X\rangle^2)$. The semiclassical calculus with the metric $dX^2/\langle X\rangle^2$ then says

$$(1 + \alpha^{W,h})^{-1} = [(1 + \alpha)^{-1}]^{W,h} + \mathcal{O}(h^2) \quad \text{in } S\left(\langle X\rangle^{-2}, \frac{dX^2}{\langle X\rangle^2}\right). \tag{21}$$

The same of course also holds for $\tau\alpha_0(X) = \frac{1}{2}\tau|X|^2$ with $\tau \in (0, +\infty)$ fixed. Therefore $\alpha^{W,h} + B_h$ and $\alpha_0^{W,h}$ are self-adjoint with the same domain $D(\alpha^{W,h}) = D(\alpha_0^{W,h}) = D(\alpha_0^{W,1})$, and they have a compact resolvent. We shall collect all the necessary information by comparing the eigenvalues of $\alpha^{W,h} + B_h$ and $\alpha_0^{W,h}$ in the intervals $(-\infty, 2|\beta|h]$, $[0, 2]$ and $[1, +\infty[$, with $|\beta| = \sum_{j=1}^d \beta_j$. For the first part, we refer to the ready-made simple statement of [Charles and Vũ Ngọc 2008, Theorem 4.5] and complete the other parts with simple pseudodifferential calculus and the min-max principle.

Interval $(-\infty, 2|\beta|h]$: By Theorem 4.5 of [Charles and Vũ Ngọc 2008], there exist a family of real numbers $(\omega_n^h)_{h>0, n\in\mathbb{N}^d}$ and, for any $t > 0$, a constant $C_t > 0$ such that

$$\sigma(\alpha^{W,h}) \cap (-\infty, th] = \{\omega_n^h, n \in \mathbb{N}^d\} \cap \left[\tfrac{1}{2}|\beta|h, th\right]$$

and

$$\left|\omega_n^h - \sum_{j=1}^{d} h\beta_j\left(\tfrac{1}{2}+n_j\right)\right| \le C_t h^{\frac{3}{2}}.$$

As $\|B_h\| = o(h)$, the min-max principle with $\alpha^{W,h}$ and $\alpha^{W,h}+B_h$ then gives,

$$\sigma(\alpha^{W,h}+B_h)\cap(-\infty, th] = \{\omega_n^h + o(h),\ n\in\mathbb{N}\}\cap[0,th].$$

By choosing $t = 2|\beta|$, the operator $\alpha^{W,h}+B_h$ is nonnegative with $\lambda_0(\alpha^{W,h}+B_h) = \frac{1}{2}|\beta|h + o(h)$ and the spectral gap is bounded from below by, for all $j\in\mathbb{N}\setminus\{0\}$,

$$\begin{aligned}\lambda_j(\alpha^{W,h}+B_h)-\lambda_0(\alpha^{W,h}+B_h) &\ge \lambda_1(\alpha^{W,h}+B_h)-\lambda_0(\alpha^{W,h}+B_h)\\ &\ge \beta_m h + o(h) \ge \tfrac{1}{2}\beta_m h,\end{aligned} \tag{22}$$

with $\beta_m = \min\{\beta_1,\dots,\beta_d\}$.

Let $T\in \mathrm{Sp}_{2d}(\mathbb{R}^d)$ be such that ${}^tX\,{}^tT^{-1}\,\mathrm{Hess}\,\alpha(0)T^{-1}X = \sum_{j=1}^d \beta_j X_j^2$, let U_T be a unitary operator such that $U_T^* b^W U_T = b(T^{-1}\cdot)^W$ and set $\varphi_T(x) = (\pi)^{-\frac{d}{4}} U_T e^{-\frac{1}{2}x^2}$. We compute

$$\begin{aligned}\langle\varphi_T,\, (\alpha^{W,h}+B_h)\varphi_T\rangle &= \mathrm{Tr}[U_T^*\alpha^{W,h}U_T|\varphi_{\mathrm{Id}}\rangle\langle\varphi_{\mathrm{Id}}|] + o(h)\\ &= \int_{\mathbb{R}^{2d}} \alpha(\sqrt{h}T^{-1}X)e^{-|X|^2}\frac{dX}{\pi^d} + o(h).\end{aligned}$$

But since $\alpha(T^{-1}X) = \sum_{j=1}^d \frac{1}{2}\beta_j|X_j|^2 + P_3(X) + \mathcal{O}(|X|^4)$, with P_3 a homogeneous polynomial of degree 3, we obtain

$$\langle\varphi_T,\, (\alpha^{W,h}+B_h)\varphi_T\rangle = \tfrac{1}{2}h|\beta| + o(h) = \lambda_0(\alpha^{W,h}+B_h) + o(h).$$

With the spectral gap (22) this implies that the ground state ψ_0^h of $\alpha^{W,h}+B_h$ satisfies $\lim_{h\to 0}\|\psi_0^h - \varphi_T\|_{L^2} = 0$ and

$$\lim_{h\to 0}\|1_{\{\lambda_0(\alpha^{W,h}+B_h)\}}(\alpha^{W,h}+B_h) - \pi^{-d}(e^{-|TX|^2})^{W,1}\|_{\mathcal{L}^1} = 0.$$

<u>Interval $[0,2]$</u>: Our assumptions on α provide a constant $C_2\ge 1$ such that $C_2^{-1}\alpha_0 \le \alpha \le C_2\alpha_0$ and therefore

$$\frac{C_2^{-1}\alpha_0}{1+C_2^{-1}\alpha_0} \le \frac{\alpha}{1+\alpha} \le \frac{C_2\alpha_0}{1+C_2\alpha_0},$$

as $x\mapsto \frac{x}{1+x}$ is increasing on $\mathbb{R}^*$. Since all those symbols belong to $S(1, dX^2)$, the semiclassical Fefferman–Phong inequality for the constant metric dX^2, see [Hörmander 1985, Lemma 18.6.1], says

$$\frac{C_2^{-1}\alpha_0^{W,h}}{1+C_2^{-1}\alpha_0^{W,h}} - \mathcal{O}(h^2) \le \frac{\alpha^{W,h}}{1+\alpha^{W,h}} \le \frac{C_2\alpha_0^{W,h}}{1+C_2\alpha_0^{W,h}} + \mathcal{O}(h^2),$$

after using

$$\left(\frac{\alpha_{.}}{1+\alpha_{.}}\right)^{W,h} = \frac{\alpha_{.}^{W,h}}{1+\alpha_{.}^{W,h}} + \mathcal{O}(h^2).$$

With $\|(1+\alpha^{W,h})^{-1}-(1+\alpha^{W,h}+B_h)^{-1}\| = \mathcal{O}(\|B_h\|) = o(h)$ and $\frac{x}{1+x} = 1-\frac{1}{1+x}$, we deduce

$$\frac{C_2^{-1}\alpha_0^{W,h}}{1+C_2^{-1}\alpha_0^{W,h}} - o(h) \leq \frac{\alpha^{W,h}+B_h}{1+\alpha^{W,h}+B_h} \leq \frac{C_2\alpha_0^{W,h}}{1+C_2\alpha_0^{W,h}} + o(h).$$

For $r = 2(1+C_2)$ and $h_0 > 0$ small enough, the above operators have a discrete spectrum in $\left[0, \frac{r}{1+r}\right]$ with eigenvalues in this interval, while the function $x \mapsto \frac{x}{1+x}$ increases on $[0, +\infty)$. Hence the min-max principle implies that there exists $C_2' \geq 1$ such that

$$\begin{aligned}&\left[\lambda_j(\alpha^{W,h}+B_h) \leq 2\right] \\ &\quad \Longrightarrow \left[C_2'^{-1}\lambda_j(\alpha_0^{W,h}) - o(h) \leq \lambda_j(\alpha^{W,h}+B_h) \leq C_2'\lambda_j(\alpha_0^{W,h}) + o(h)\right] \qquad (23)\end{aligned}$$

holds for all $j \in \mathbb{N}$. With the spectral gap (22) and $\lambda_0(\alpha^{W,h}+B_h) = \frac{1}{2}|\beta|h + o(h)$ we conclude that (20) holds when $\lambda_j(\alpha^{W,h}+B_h) \leq 2$.

Interval $[1, +\infty)$: Our assumptions on α provide a constant $C_1 \geq 1$ such that

$$C_1^{-2} \leq \left(\frac{1+\alpha_0}{1+\alpha}\right)^2 \leq C_1^2.$$

With (21), the semiclassical Gårding inequality then gives for h_0 small enough

$$\max\left\{\|(1+\alpha_0^{W,h})(1+\alpha^{W,h})^{-1}\|, \|(1+\alpha^{W,h})(1+\alpha_0^{W,h})^{-1}\|\right\} \leq 2C_1.$$

Owing to $\|B_h\| = o(h)$, this is also true when $\alpha^{W,h}$ is replaced by $\alpha^{W,h} + B_h$. We obtain for all $\psi \in D(\alpha_0^{W,1})$,

$$(2C_1)^{-2}\langle\psi, (1+\alpha_0^{W,h})^2\psi\rangle \leq \langle\psi, (1+\alpha^{W,h}+B_h)^2\psi\rangle \leq (2C_1)^2\langle\psi, (1+\alpha_0^{W,h})^2\psi\rangle,$$

and the min-max principle gives, for all $j \in \mathbb{N}$,

$$(2C_1)^{-2}\lambda_j((1+\alpha_0^{W,h})^2) \leq \lambda_j((1+\alpha^{W,h}+B_h)^2) \leq (2C_1)^2\lambda_j((1+\alpha_0^{W,h})^2).$$

By taking the square roots, for all $j \in \mathbb{N}$,

$$(2C_1)^{-1}(1+\lambda_j(\alpha_0^{W,h})) \leq 1+\lambda_j(\alpha^{W,h}+B_h) \leq 2C_1(1+\lambda_j(\alpha_0^{W,h})),$$

which yields (20) for $\lambda_j(\alpha^{W,h}+B_h) \geq 1$. □

Proof of Proposition 5.6. With $H = \alpha^{W,h} + B_h - \lambda_0(\alpha^{W,h}+B_h)$, Lemma 5.7 provides a constant $C' > 0$ such that,

$$\text{for all } j \in \mathbb{N}\setminus\{0\}, \quad C'^{-1}\lambda_j(\alpha_0^{W,h}) \leq \lambda_j(H) \leq C'\lambda_j(\alpha_0^{W,h}),$$

while $\lambda_0(H) = 0$ and the ground state of H is the same as the one of $\alpha^{W,h} + B_h$.

When the function f is nonnegative and decaying, we deduce

$$\begin{aligned} Tr[f(H + ch^{\frac{d}{\kappa_0}})] &= f(ch^{\frac{d}{\kappa_0}}) + \sum_{j=1}^{\infty} f(\lambda_j(H) + ch^{\frac{d}{\kappa_0}}) \\ &\leq f(ch^{\frac{d}{\kappa_0}}) + \sum_{j=1}^{\infty} f(\lambda_j(H)) \\ &\leq f(ch^{\frac{d}{\kappa_0}}) + \sum_{\substack{n\in\mathbb{N}^d \\ n\neq 0}} f(C_4^{-1} h|n|), \end{aligned} \tag{24}$$

with $C_4 = C_3(1 + 4|\beta|/\beta_m)$, and for $R > 0$,

$$\begin{aligned} \mathrm{Tr}[f(H + ch^{\frac{d}{\kappa_0}})1_{[R,+\infty)}(H)] &= \sum_{\lambda_j(H)\geq R} f(\lambda_j(H) + ch^{\frac{d}{\kappa_0}}) \\ &\leq \sum_{\substack{n\in\mathbb{N}^d \\ h|n|\geq \frac{R}{2C_3}}} f(C_4^{-1} h|n|). \end{aligned}$$

Apply (24) first, with $f = s^{-\kappa_0}\langle s\rangle^{-\kappa_\infty+\kappa_0}$:

$$h^d\,\mathrm{Tr}[f(H + ch^{\frac{d}{\kappa_0}})] \leq c^{-\kappa_0} + Ch^d \sum_{\substack{n\in\mathbb{N}^d \\ n\neq 0}} (h|n|)^{-\kappa_0}\langle h|n|\rangle^{-\kappa_\infty+\kappa_0}.$$

After splitting the sum into $\sum_{h|n|\leq 1}$ and $\sum_{h|n|\geq 1}$ and with $\#\{n \in \mathbb{N}^d : |n| = m\} = C_{m+d-1}^{d-1} = \mathcal{O}(m^{d-1})$, it becomes

$$\begin{aligned} &h^d\,\mathrm{Tr}[f(H + ch^{\frac{d}{\kappa_0}})] \\ &\quad\leq c^{-\kappa_0} + C'h^d \sum_{m=1}^{\lceil h^{-1}\rceil} h^{-\kappa_0} m^{d-1-\kappa_0} + C'h^d \sum_{m=\lfloor h^{-1}\rfloor}^{\infty} h^{-\kappa_\infty} m^{d-1-\kappa_\infty}. \\ &\quad\leq c^{-\kappa_0} + C''h^{d-\kappa_0}\lceil h^{-1}\rceil^{d-\kappa_0} + C''h^{d-\kappa_\infty}\lfloor h^{-1}\rfloor^{d-\kappa_\infty} \leq c^{-\kappa_0} + C''', \end{aligned}$$

owing to $\kappa_\infty > d$ and $\kappa_0 \in (0, d)$. With a function $f(s) = s^{-\kappa_0}\chi(s/\delta)$ with $0 \leq \chi \leq 1$ compactly supported and decaying on $[0, +\infty)$ we get similarly

$$\lim_{\delta\to 0^+} \limsup_{h\to 0} h^d\,\mathrm{Tr}[f(H + ch^{\frac{d}{\kappa_0}})] - c^{-\kappa_0} = 0,$$

while with $f(s) = \langle s\rangle^{-\kappa_\infty}$, the truncated trace $\mathrm{Tr}[f(H + ch^{\frac{d}{\kappa_0}})1_{[\delta^{-1},+\infty)}(H)]$ satisfies

$$\lim_{\delta\to 0^+} \limsup_{h\to 0} h^d\,\mathrm{Tr}[f(H + ch^{\frac{d}{\kappa_0}})1_{[\delta^{-1},+\infty)}(H)] = 0.$$

The comparison of $\lambda_j(H)$ with $\lambda_j(\alpha_0^{W,h})$, $j \in \mathbb{N}$, stated in Lemma 5.7 does not depend on the parameter c. Neither do the constants C_3, C_4, C, C', C'' and C''' (f is nonnegative and decaying) depend on c. Therefore the previous asymptotic trace estimates are uniform with respect to $c \in \left(\frac{1}{A}, A\right)$ for any fixed $A > 1$.

Thus if $\chi \in \mathcal{C}_0^\infty(\mathbb{R})$ is a cut-off function such that $0 \le \chi \le 1$, $\chi \equiv 1$ in $(-1, 1)$ and if a general $f \in \mathcal{C}^\infty((0, +\infty))$ fulfills all the assumptions of Proposition 5.6, then

$$\lim_{\delta \to 0^+} \limsup_{h \to 0^+} h^d \left\| [f(H + ch^{\frac{d}{\kappa_0}}) 1_{(0,+\infty)}(H)[\chi(\delta^{-1}H) + (1 - \chi(\delta H))] \right\|_{\mathcal{L}^1} = 0. \tag{25}$$

For $g \in \mathcal{C}_0^\infty(\mathbb{R})$, with an almost analytic extension $\tilde{g} \in \mathcal{C}_0^\infty(\mathbb{C})$, the Helffer–Sjöstrand formula

$$g(\alpha^{W,h}) = \frac{1}{2i\pi} \int_{\mathbb{C}} \partial_{\bar{z}} \tilde{g}(z)(z - \alpha^{W,h})\, dz \wedge d\bar{z},$$

combined with the semiclassical Beals criterion [Dimassi and Sjöstrand 1999; Helffer and Nier 2005; Nataf and Nier 1998] with the constant metric dX^2 implies

$$g(\alpha^{W,h}) - g(\alpha)^{W,h} = h\, r(h)^{W,h},$$

with $r(h)$ uniformly bounded (with respect to h) in $S(1, dX^2)$. Since $(1 + \alpha) \in S(\langle X \rangle^2, dX^2/\langle X \rangle^2)$ is an invertible elliptic symbol,

$$(1 + \alpha^{W,h})^{-N} - [(1 + \alpha)^{-N}]^{W,h} = h^2 r'(h)^{W,h},$$

with $r'(h)$ uniformly bounded in $S(\langle X \rangle^{-2N-2}, dX^2/\langle X \rangle^2) \subset S(\langle X \rangle^{-2N}, dX^2)$. For a function $f_\delta \in \mathcal{C}_0^\infty((0, +\infty))$, we take $g(s) = (1 + s)^N f_\delta(s)$ and write

$$f_\delta(\alpha^{W,h}) = g(\alpha^{W,h})(1 + \alpha^{W,h})^{-N},$$

so that

$$\begin{aligned} f_\delta(\alpha^{W,h}) - f_\delta(\alpha)^{W,h} \\ &= [g(\alpha^{W,h}) - g(\alpha)^{W,h}](1 + \alpha^{W,h})^{-N} + g(\alpha)^{W,h}(1 + \alpha^{W,h})^{-N} - f_\delta(\alpha)^{W,h} \\ &= h\, r''(h)^{W,h}, \end{aligned}$$

with $r''(h)$ uniformly bounded in $S(\langle X \rangle^{-2N}, dX^2)$. In particular, $h^d r''(h)^{W,h}$ is uniformly bounded in $\mathcal{L}^1(L^2(\mathbb{R}^d))$ if we choose $N > d$.

Similarly, the Helffer–Sjöstrand formula can be used to prove $g(H + ch^{\frac{d}{\kappa_0}}) - g(\alpha^{W,h}) = o(h)$ in $\mathcal{L}(L^2(\mathbb{R}^d))$. With $h^d[(1 + H + ch^{\frac{d}{\kappa_0}})^{-N} - (1 + \alpha^{W,h})^{-N}] = o(h)$ in $\mathcal{L}^1(L^2(\mathbb{R}^d))$ due to

$$(1 + H + ch^{\frac{d}{\kappa_0}})^{-1} = [1 + (1 + \alpha^{W,h})^{-1}(B_h + ch^{\frac{d}{\kappa_0}})]^{-1}(1 + \alpha^{W,h})^{-1},$$

the same trick as above transforms the $\mathcal{L}(L^2(\mathbb{R}^d))$ estimate into

$$h^d[f_\delta(H+ch^{\frac{d}{\kappa_0}})-f_\delta(\alpha^{W,h})]=o(h) \quad \text{in } \mathcal{L}^1(L^2(\mathbb{R}^d)) \tag{26}$$

Note again that this holds uniformly with respect to $c\in\left(\frac{1}{A},A\right)$ for any fixed $A>1$.

Now take $f_\delta(s)=(1-\chi(\delta^{-2}s))\chi(\delta^2 s)f(s)$ for which we note that the inequality,

$$\text{for all } s\geq 0,\quad 1-(1-\chi(\delta^{-2}s))\chi(\delta^2 s)\leq \chi(\delta^{-1}s)+(1-\chi(\delta s))$$

as soon as $\delta<\delta_\chi$ implies,

$$\text{for all } s\geq 0,\quad 0\leq f(s)-f_\delta(s)\leq f(s)[\chi(\delta^{-1}s)+(1-\chi(\delta s))]. \tag{27}$$

In the expression $h^d\,\mathrm{Tr}[f(H+ch^{\frac{d}{\kappa_0}}a^{W,h}]$, we decompose $f(H+ch^{\frac{d}{\kappa_0}})$ into $(I)+(II)+(III)$, where

$$\begin{aligned}(I)&=f_\delta(H+ch^{\frac{d}{\kappa_0}}),\\ (II)&=(f(H+ch^{\frac{d}{\kappa_0}})-f_\delta(H+ch^{\frac{d}{\kappa_0}}))1_{(0,+\infty)}(H),\\ (III)&=1_{\{0\}}(H)f(ch^{\frac{d}{\kappa_0}}).\end{aligned}$$

We now conclude with the following steps:

- The estimate (26) yields

$$\begin{aligned}\lim_{h\to 0}h^d\,\mathrm{Tr}[f_\delta(H+ch^{\frac{d}{\kappa_0}})a^{W,h}]&=\lim_{h\to 0}h^d\,\mathrm{Tr}[f_\delta(\alpha)^{W,h}a^{W,h}]\\ &=\int_{\mathbb{R}^{2d}}f_\delta(\alpha(X))a(X)\frac{dX}{(2\pi)^d},\end{aligned}$$

which provides the contribution of (I).

- The upper bound (27) combined with (25) leads to

$$\lim_{\delta\to 0+}\limsup_{h\to 0}\left|h^d\,\mathrm{Tr}\left[[f(H+ch^{d/\kappa_0})-f_\delta(H+ch^{\frac{d}{\kappa_0}})]1_{(0,+\infty)}(H)a^{W,h}\right]\right|=0,$$

which says that (II) has a null contribution in the limit $\delta\to 0$.

- The contribution of (III) is simply computed as

$$h^d\,\mathrm{Tr}[f(H+ch^{\frac{d}{\kappa_0}})1_{\{0\}}(H)a^{W,h}]=\frac{f_0}{c^{\kappa_0}}\langle\psi_0^h,a^{W,h}\psi_0^h\rangle,$$

where ψ_0^h is the ground state of $H+ch^{\frac{d}{\kappa_0}}$ with $\|\psi^h-\pi^{-\frac{d}{4}}e^{-\frac{1}{2}x^2}\|\to 0$ as $h\to 0$. This implies $\lim_{h\to 0}\langle\psi^h,a^{W,h}\psi^h\rangle=a(0)$.

- Finally, the assumptions on f ensure $f(\alpha)\in L^1(\mathbb{R}^{2d})$ and

$$\lim_{\delta\to 0}\int_{\mathbb{R}^{2d}}f_\delta(\alpha(X))a(X)\,dX=\int_{\mathbb{R}^{2d}}f(\alpha(X))a(X)\,dX. \qquad \square$$

5B4. *Semiclassical analysis of the reduced density matrices in the bosonic case.*

Proof of Proposition 5.4. This will be made in two parts: we first compute the semiclassical measures $\nu^{(p)}$ and then identify the weak*-limit $\gamma_0^{(p)}$.

For the first part Proposition 4.4 says that it suffices to find the limit $\Phi_{a,0}(s)$ of $\Phi_{a,h}(s)$ for $a \in \mathcal{C}_0^\infty(T^*\mathbb{R}^d)$, real-valued, and $s \in (-r_a, r_a)$. Actually Proposition 5.6 allows to consider more generally $a \in S(1, dX^2)$. For $a \in S(1, dX^2)$, real-valued, take $s \in \mathbb{R}$, $|s| < r_a = 1/(\nu_C C_a)$, $4\|a^{W,h}\| \le C_a$ and set

$$\begin{aligned}DT_{a,h}(s) &= \log \operatorname{Tr}[\varrho_\varepsilon \Gamma(e^{\varepsilon s a})] = -\operatorname{Tr}[\log(1 - CB_s)] + \operatorname{Tr}[\log(1 - C)],\\ \Phi_{a,h}(s) &= \operatorname{Tr}[\varrho_\varepsilon \Gamma(e^{\varepsilon s a^{W,h}})] = \exp DT_{a,h}(s), \quad \varepsilon = h^d,\end{aligned}$$

with $C = e^{-\beta(H + \frac{\varepsilon}{\beta \nu_C})}$ and $B_s = e^{\varepsilon s a^{W,h}}$.

Assume $s \in (-r_a, r_a)$ and compute

$$\begin{aligned}DT_{a,h}(s) &= \int_0^1 \operatorname{Tr}\Big[\frac{C_{ts}\widetilde{B}_{ts}}{1 - C_{ts}\widetilde{B}_{ts}} \varepsilon s a^{W,h}\Big]\,dt\\ &= \int_0^1 \operatorname{Tr}\Big[\varepsilon s f\Big(H + \frac{\varepsilon}{\beta}(\nu_C^{-1} - tsa(0))\Big) a^{W,h}\Big]\,dt\\ &\qquad + \int_0^1 \operatorname{Tr}\big[\varepsilon s[-(1 - C_{ts})^{-1} + (1 - C_{ts}\widetilde{B}_{ts})^{-1}]a^{W,h}\big]\,dt,\end{aligned}$$

with

$$C_{ts} = e^{-\beta(H + \frac{\varepsilon}{\beta}(\nu_C^{-1} - tsa(0)))}, \quad \widetilde{B}_{ts} = e^{\varepsilon ts(a - a(0))^{W,h}}, \quad f(u) = \frac{e^{-\beta u}}{1 - e^{-\beta u}}.$$

Note that for $t \in [0, 1]$ the parameter $\frac{1}{\beta}(\nu_C^{-1} - tsa(0))$ remains in a compact subset of $(0, +\infty)$. Proposition 5.6 implies for all $t \in [0, 1]$

$$\lim_{h\to 0} \operatorname{Tr}\Big[\varepsilon s f\Big(H + \frac{\varepsilon}{\beta}(\nu_C^{-1} - tsa(0))\Big) a^{W,h}\Big] = \frac{\nu_C s a(0)}{1 - t\nu_C s a(0)} + s\int_{\mathbb{R}^{2d}} \frac{e^{-\beta\alpha(X)}}{1 - e^{-\beta\alpha(X)}} a(X) \frac{dX}{(2\pi)^d}.$$

With the uniform control with respect to $\frac{1}{\beta}(\nu_C^{-1} - tsa(0)) = c \in \big[\frac{1}{A}, A\big]$ in Proposition 5.6, we obtain for the first term

$$\lim_{h\to 0} \int_0^1 \operatorname{Tr}\Big[\varepsilon s f\Big(H + \frac{\varepsilon}{\beta}(\nu_C^{-1} - tsa(0))\Big) a^{W,h}\Big]\,dt = -\log(1 - s\nu_C a(0)) + s\int_{\mathbb{R}^{2d}} \frac{e^{-\beta\alpha(X)}}{1 - e^{-\beta\alpha(X)}} a(X) \frac{dX}{(2\pi)^d}.$$

For the remainder term, define $\Pi_0^h=|\psi_0^h\rangle\langle\psi_0^h|$, where $\psi_0^h=U_T(\pi^{-\frac{d}{4}}e^{-\frac{x^2}{2}})+o(h^0)$ is the ground state of H, and write

$$\begin{aligned}
&(1-C_{ts}\widetilde{B}_{ts})\\
&\quad=1-C_{ts}-C_{ts}(\widetilde{B}_{ts}-1)=(1-C_{ts})\left[1+\frac{C_{ts}}{1-C_{ts}}(1-\widetilde{B}_{ts})\right]\\
&\quad=(1-C_{ts})\left[1+\frac{C_{ts}}{1-C_{ts}}\Pi_0^h(1-\widetilde{B}_{ts})+\frac{C_{ts}}{1-C_{ts}}(1-\Pi_0^h)(1-\widetilde{B}_{ts})\right]\\
&\quad=(1-C_{ts})\Bigg[1+\underbrace{f\left(\frac{\varepsilon}{\beta}(\nu_C^{-1}-tsa(0))\right)\Pi_0^h(1-\widetilde{B}_{ts})}_{I}+\underbrace{\frac{C_{ts}}{1-C_{ts}}(1-\Pi_0^h)(1-\widetilde{B}_{ts})}_{II}\Bigg].
\end{aligned}$$

We know

$$\varepsilon\times f\left(\frac{\varepsilon}{\beta}(\nu_C^{-1}-tsa(0))\right)=\frac{1}{\nu_C^{-1}-tsa(0)}+O(\varepsilon)=\frac{1}{\nu_C^{-1}-tsa(0)}+o(h).$$

We write

$$\varepsilon^{-1}(1-\widetilde{B}_{ts})\psi_0^h=-\int_0^1 e^{\varepsilon uts(a-a(0))^{W,h}}ts(a-a(0))^{W,h}\psi_0^h\,du,$$

where $\psi_0^h=\pi^{-\frac{d}{4}}U_Te^{-\frac{x^2}{2}}+o(h^0)$, and $a(X)-a(0)\le C\min\{1,|X|\}$ for some $C>0$ implies $\lim_{h\to 0}\|(a-a(0))^{W,h}\psi_0^h\|_{L^2(\mathbb{R}^d)}=0$. Therefore the term I in the above brackets satisfies

$$I=f\left(\frac{\varepsilon}{\beta}(\nu_C^{-1}-tsa(0))\right)\Pi_0^h(1-\widetilde{B}_{ts})=o(h^0)\quad\text{in }\mathcal{L}^1(L^2(\mathbb{R}^d)).$$

Note that we have also proved

$$(1-\widetilde{B}_{ts})\Pi_0^h-\Pi_0^h(1-\widetilde{B}_{ts})=o(\varepsilon)\quad\text{in }\mathcal{L}(L^2(\mathbb{R}^d)).$$

By using

$$\|1-\widetilde{B}_{ts}\|=\mathcal{O}(\varepsilon),\qquad\left\|\frac{C_{ts}}{1-C_{ts}}(1-\Pi_0^h)\right\|=\mathcal{O}\left(\frac{1}{h}\right),$$

and

$$\begin{aligned}
\lim_{h\to 0}\|\varepsilon\frac{C_{ts}}{1-C_{ts}}\|_{\mathcal{L}^1}&=\lim_{h\to 0}\mathrm{Tr}\left[\varepsilon f\left(H+\frac{\varepsilon}{\beta}(\nu_C^{-1}-tsa(0))\right)\right]\\
&=\frac{\nu_C}{1-t\nu_C sa(0)}+s\int_{\mathbb{R}^{2d}}\frac{e^{-\beta\alpha(X)}}{1-e^{-\beta\alpha(X)}}\frac{dX}{(2\pi)^d},
\end{aligned}$$

the term II in the above brackets satisfies

$$\|II\|_{\mathcal{L}^1}=\mathcal{O}(1),\quad\|II\|=\mathcal{O}(\varepsilon h^{-1})=o(h^0),$$

$$\left\|II-\frac{C_{ts}}{1-C_{ts}}(1-\Pi_0^h)(1-\widetilde{B}_{ts})(1-\Pi_0^h)\right\|_{\mathcal{L}^1}=o(h^0).$$

Again all these estimates are uniform with respect to $t \in [0,1]$, owing to the uniformity of the estimates in Proposition 5.6 with respect to $c = \frac{1}{\beta}(\nu_C^{-1} - tsa(0))$. By expanding the Neumann series $(1 + I + II)^{-1} = \sum_{k=0}^{\infty}(-1)^k (I + II)^k$ we deduce

$$\left[1 + \frac{C_{ts}}{1 - C_{ts}}(1 - \widetilde{B}_{ts})\right]^{-1} = 1 - \frac{C_{ts}}{1 - C_{ts}}(1 - \Pi_0^h)(1 - \widetilde{B}_{ts})(1 - \Pi_0^h) + R_h,$$

with $\|R_h\|_{\mathcal{L}^1} = o(h^0)$. With $\|\varepsilon(1 - C_{ts})^{-1}\| = \mathcal{O}(1)$ we finally obtain

$$\begin{aligned}&\varepsilon s[(1 - C_{ts})^{-1} - (1 - C_{ts}\widetilde{B}_{ts})^{-1}]\\ &\quad = \frac{s\varepsilon C_{ts}}{1 - C_{ts}}(1 - \Pi_0^h)(1 - \widetilde{B}_{ts})(1 - \Pi_0^h)(1 - C_{ts})^{-1} + R_h', \quad \|R_h'\|_{\mathcal{L}^1} = o(h^0),\end{aligned}$$

while $\|\varepsilon C_{ts}(1 - C_{ts})^{-1}\|_{\mathcal{L}^1} = \mathcal{O}(1)$, $\|1 - \widetilde{B}\| = \mathcal{O}(\varepsilon)$ and $\|(1 - \Pi_0^h)(1 - C_{ts})^{-1}\| = \mathcal{O}(h^{-1})$.

With $4\|a^{W,h}\| \leq C_a$, the remainder term tends to 0 as $h \to 0$ and we have proved, for all $s \in (-r_a, r_a)$,

$$\lim_{h \to 0} \Phi_{a,h}(s) = \Phi_{a,0}(s) = \frac{1}{1 - s\nu_C a(0)} \exp\left[s \int_{\mathbb{R}^{2d}} \frac{e^{-\beta\alpha(X)}}{1 - e^{-\beta\alpha(X)}} a(X) \frac{dX}{(2\pi)^d}\right].$$

By expanding the generating function according to Proposition 4.4, we obtain

$$\lim_{h \to 0} \operatorname{Tr}[\varrho_\varepsilon((a^{W,h})^{\otimes p})^{\text{Wick}}] = \sum_{k=0}^{p} \frac{1}{(p-k)!} \nu_C^k a(0)^k \int_{\mathbb{R}^{2d(p-k)}} a^{\otimes(p-k)}\, d\nu(\beta)^{\otimes p-k}.$$

with

$$d\nu(\beta) = \frac{e^{-\beta\alpha(X)}}{1 - e^{-\beta\alpha(X)}} \frac{dX}{(2\pi)^d}.$$

The possibility to take $a \in S(1, dX^2)$ means that our quantization is adapted to all the $\gamma_h^{(p)}$.

Now in order to identify the weak*-limits of the $\gamma_h^{(p)}$ we compute the Wigner measure associated with $\varrho_{\varepsilon(h)}$. Remember, see (28) and (29),

$$\operatorname{Tr}[\varrho_\varepsilon W(\sqrt{2}\pi f)] = \exp\left[-\frac{\varepsilon\pi^2}{2}\left\langle f, \frac{1 + e^{-\beta(H + \frac{\varepsilon}{\beta\nu_C})}}{1 - e^{-\beta(H + \frac{\varepsilon}{\beta\nu_C})}} f\right\rangle\right].$$

By using the orthonormal basis of eigenvectors $(\psi_j^h)_{j \in \mathbb{N}}$ of H with associated eigenvalues λ_j^h, $\lambda_0^h = 0$, $\lambda_j^h \geq ch$ for $j > 0$, we obtain

$$\log(\operatorname{Tr}[\varrho_{\varepsilon(h)} W(\sqrt{2}\pi f)]) = -\pi^2 \nu_C |\langle f, \psi_0^h\rangle|^2 + \mathcal{O}(\varepsilon h^{-1}).$$

With $\|\psi_0^h - \psi_0\|_{L^2} = o(h)$, $\psi_0(x) = \pi^{-\frac{d}{4}} U_T e^{-\frac{x^2}{2}}$, we obtain, after decomposing $f = f_0\psi_0 \oplus^\perp f'$,

$$\int_{L^2} e^{2i\pi \operatorname{Re}\langle f,z\rangle}\, d\mu(z) = \lim_{h\to 0} \operatorname{Tr}[\varrho_{\varepsilon(h)} W(\sqrt{2}\pi f)] = e^{-\pi^2 \nu_C |f_0|^2}.$$

We deduce, as in [Ammari and Nier 2008, Section 7.5; 2011, Section 4.4],

$$\mathcal{M}(\varrho_{\varepsilon(h)}, h \in \mathcal{E}) = \left\{ \left(\frac{e^{-\frac{|z_0|^2}{\nu_C}}}{\pi \nu_C} L(dz_0) \right) \otimes \delta_0(z') \right\} \quad (z = z_0\psi_0 \oplus^\perp z'),$$

and

$$\gamma_0^{(p)} = p!\nu_C^p |\psi_0^{\otimes p}\rangle\langle\psi_0^{\otimes p}| \quad \text{for all } p \in \mathbb{N}.$$

The fact that $\nu_{(I)}^{(p)} \equiv 0$ for all $p \in \mathbb{N}$, now comes from

$$\operatorname{Tr}[\gamma_0^{(p)}] = p!\, \nu_C^p = \nu^{(p)}(\{0\}). \qquad \square$$

Appendix A. Multiscale measures

We now recall facts about multiscale measures, introduced in [Fermanian-Kammerer and Gérard 2002; Fermanian Kammerer 2005]. For this we need a new class of symbols. Let $D', D'', D''' \in \mathbb{N}$ be such that $D' + D'' + D''' = D$ and set

$$F = \{X = (x', x'', x''', \xi', \xi'', \xi''') \in \mathbb{R}^{2D} : x' = 0,\ x'' = \xi'' = 0\}.$$

The class of symbols $S_F^{(2)}$ is defined as the set of

$$(X, Y) \to a(X, Y) \in \mathcal{C}^\infty(\mathbb{R}^{2D} \times \mathbb{R}^{D'+2D''})$$

(note that $\mathbb{R}^{D'+2D''} \cong F^\perp$, hence the notation $S_F^{(2)}$) such that

- there exists $C > 0$ such that for all $Y \in \mathbb{R}^{D'+2D''}$, we have $a(\cdot, Y) \in \mathcal{C}_0^\infty(B(0, C))$;
- there exists a function $a_\infty \in \mathcal{C}_0^\infty(\mathbb{R}^{2D} \times \mathbb{S}^{D'+2D''-1})$ such that $a(X, R\omega) \to a_\infty(X, \omega)$ as $R \to \infty$ in $\mathcal{C}^\infty(\mathbb{R}^{2D} \times \mathbb{S}^{D'+2D''-1})$.

Those symbols are quantized according to

$$a^{(2),h} = a_h^{W,h}, \quad a_h(X) = a\left(X, \frac{x'}{h^{\frac{1}{2}}}, \frac{X''}{h^{\frac{1}{2}}}\right) \quad X = (x', x'', x''', \xi', \xi'', \xi''').$$

Theorem 0.1 in [Fermanian Kammerer 2005], which also considers the case when $(x'/h^{\frac{1}{2}}, X''/h^{\frac{1}{2}})$ is replaced by $(x'/h^s, X''/h^s)$, $s < \frac{1}{2}$, says the following.

Proposition A.1. *Let $(\gamma_h)_{h\in\mathcal{E}}$ be a bounded family of nonnegative trace-class operators on $L^2(\mathbb{R}^{2D})$ with $\lim_{h\to 0} \operatorname{Tr}[\gamma_h] < +\infty$. There exist $\mathcal{E}' \subset \mathcal{E}$, $0 \in \bar{\mathcal{E}}'$, with*

$\mathcal{M}(\gamma_h, h \in \mathcal{E}') = \{\nu\}$, *a nonnegative measure* $\nu_{(I)}$ *on* $F \times \mathbb{S}^{D'+2D''-1}$ *and a* $\mathcal{L}^1(L^2(\mathbb{R}^{2D''}))$*-measure* m *on* $F \times \mathbb{R}^{D'}$ *such that the convergence*

$$\lim_{\substack{h\in\mathcal{E}'\\ h\to 0}} \mathrm{Tr}[\gamma_h a^{(2),h}] = \int_{\mathbb{R}^{2D}\setminus F} a_\infty\Big(X, \frac{(x', X'')}{|(x', X'')|}\Big)\, d\nu(X) + \int_{F\times\mathbb{S}^{D'+2D''-1}} a_\infty(X,\omega)\, d\nu_{(I)}(X,\omega) + \mathrm{Tr}\Big[\int_{F\times\mathbb{R}^{D'}} a(X, x', z, D_z)\, dm(X, x')\Big]$$

holds for all $a \in S_F^{(2)}$.

Remark A.2. With this scaling and when $a^{W,h} = a^W(x, hD_x) = a(x, hD_x) + O(h)$, $t = 0$, Fermanian Kammerer [2005] checked the equivariance by the semiclassical Egorov theorem. Hence, this construction is naturally extended to the case when $T^*\mathbb{R}^D$ is replaced by T^*M and F is replaced by a submanifold of $T^*\mathbb{R}^D$ on which the symplectic form has constant rank.

In Proposition 3.5 we use the simple case of the above result when $D' = D''' = 0$ and $D'' = D$. Note that in this case $F \times \mathbb{R}^{D'} = \{0\}$ and the trace-class-valued measure is nothing but a trace-class operator γ_0.

Appendix B. Wigner measures in the bosonic case and condition (PI)

Bosonic mean-field analysis is like semiclassical analysis in infinite dimension. Let $\mathscr{Z}$ be a separable complex Hilbert space and $\Gamma_+(\mathscr{Z})$ be the associated bosonic Fock space. With the scaled CCR relations

$$[a_+(g), a_+^*(f)] = \varepsilon\langle g, f\rangle, \quad [a_+(g), a_+(f)] = [a_+^*(g), a_+^*(f)] = 0$$

and after setting

$$\Phi(f) = \frac{a_+(f) + a_+^*(f)}{\sqrt{2}}, \quad W(f) = e^{i\Phi(h)}, \tag{28}$$

mean-field Wigner measures were introduced in [Ammari and Nier 2008]. Actually the parameter ε^{-1} represents the typical number of particles. Let $(\varrho_\varepsilon)_{\varepsilon\in\mathcal{E}}$, $0 \in \bar{\mathcal{E}}$, be a family of normal states (normalized nonnegative trace-class operators) in $\Gamma_+(\mathscr{Z})$. Under the sole uniform estimate $\mathrm{Tr}[\varrho_\varepsilon(1+N)^\delta] \le C_\delta$ for some $\delta > 0$, Wigner measures are defined as Borel probability measures on $\mathscr{Z}$ and characterized by their characteristic function as follows: $\mu \in \mathcal{M}(\varrho_\varepsilon, \varepsilon \in \mathcal{E})$ if and only if there exists $\mathcal{E}' \subset \mathcal{E}$, $0 \in \bar{\mathcal{E}}'$, such that,

$$\text{for all } f \in \mathscr{Z}, \quad \lim_{\substack{\varepsilon\in\mathcal{E}'\\ \varepsilon\to 0}} \mathrm{Tr}[\varrho_\varepsilon W(\sqrt{2}\pi f)] = \int_{\mathscr{Z}} e^{2i\pi \,\mathrm{Re}\langle f,z\rangle}\, d\mu(z). \tag{29}$$

Assuming $\mathrm{Tr}[\varrho_\varepsilon N_+^k] \le C^k$ for all $k \in \mathbb{N}$ (or as in Hypothesis 4.1, $\mathrm{Tr}[\varrho_\varepsilon e^{cN_+}] \le C$), $\mathcal{M}(\varrho_\varepsilon, \varepsilon \in \mathcal{E}) = \{\mu\}$ implies

$$\lim_{\varepsilon\to 0} \mathrm{Tr}[\varrho_\varepsilon \tilde{b}^{\mathrm{Wick}}] = \int_{\mathscr{Z}} \langle z^{\otimes p}, \tilde{b} z^{\otimes p}\rangle \, d\mu(z) \tag{30}$$

holds for all *compact* $\tilde{b} \in \mathcal{L}^\infty(\mathcal{S}_+^p \mathscr{Z}^{\otimes p})$. In particular with the definition of non-normalized reduced density matrices we obtain,

$$\text{for all } p \in \mathbb{N}, \quad w^*\text{-}\lim_{\varepsilon\to 0} \gamma_\varepsilon^{(p)} = \gamma_0^{(p)} = \int_{\mathscr{Z}} |z^{\otimes p}\rangle\langle z^{\otimes p}| \, d\mu(z).$$

This w^*-limit can be transformed to a $\| \; \|_{\mathcal{L}^1}$ if and only if the restriction to compact $\tilde{b}$ in (30) can be removed. It actually suffices to check that (30) holds for $\tilde{b} \in \mathcal{L}^\infty(\mathcal{S}_+^p \mathscr{Z}^{\otimes p})$ and $\tilde{b} = \mathrm{Id}_{\mathcal{S}_+^p \mathscr{Z}^{\otimes p}}$, as shows the following result.

Proposition B.1. *For a family* $(\varrho_\varepsilon)_{\varepsilon\in\mathcal{E}}$ *in* $\mathcal{L}^1(\mathcal{H})$, $0 \in \bar{\mathcal{E}}$, *such that* $\varrho_\varepsilon \ge 0$, $\mathrm{Tr}[\varrho_\varepsilon] = 1$, $\mathcal{M}(\varrho_\varepsilon, \varepsilon \in \mathcal{E}) = \{\mu\}$, *the conditions* (PI) *and* (P) *are equivalent*:

$$\left[(\mathrm{PI}): \quad \textit{for all } \alpha \in \mathbb{N}, \quad \lim_{\varepsilon\to 0} \mathrm{Tr}[\varrho_\varepsilon \boldsymbol{N}^\alpha] = \int_{\mathscr{Z}} |z|^{2\alpha} \, d\mu(z) < \infty\right]$$
$$\iff \left[(\mathrm{P}): \quad \textit{for all } b \in \mathcal{P}_{\mathrm{alg}}(\mathscr{Z}), \quad \lim_{\varepsilon\to 0} \mathrm{Tr}[\varrho_\varepsilon b^{\mathrm{Wick}}] = \int_{\mathscr{Z}} b \, d\mu\right],$$

where

$$\mathcal{P}_{p,q}(\mathscr{Z}) = \{b : \mathscr{Z} \ni z \mapsto b(z) = \langle z^{\otimes q}, \tilde{b} z^{\otimes p}\rangle \in \mathbb{C} : \tilde{b} \in \mathcal{L}(\mathcal{S}_+^p \mathscr{Z}^{\otimes p}; \mathcal{S}_+^q \mathscr{Z}^{\otimes q})\},$$

and $\mathcal{P}_{\mathrm{alg}}(\mathscr{Z}) = \oplus^{\mathrm{alg}}_{p,q\in\mathbb{N}} \mathcal{P}_{p,q}(\mathscr{Z})$.

We give below the proof, which rectifies a minor mistake in [Ammari and Nier 2011].

Proof. For $\alpha \in \mathbb{N}^*$, we have $(|z|^{2\alpha})^{\mathrm{Wick}} = \boldsymbol{N}(\boldsymbol{N} - \varepsilon) \cdots (\boldsymbol{N} - (\alpha - 1)\varepsilon)$. Hence the condition (PI) is equivalent to

$$(\mathrm{PI})': \quad \text{for all } \alpha \in \mathbb{N}, \quad \lim_{\varepsilon\to 0} \mathrm{Tr}[\varrho_\varepsilon (|z|^{2\alpha})^{\mathrm{Wick}}] = \int_{\mathscr{Z}} |z|^{2\alpha} \, d\mu(z) < \infty.$$

Hence the condition (PI) is a particular case of (P) and it is sufficient to prove $(\mathrm{PI})' \Rightarrow (\mathrm{P})$. From now, assume $(\mathrm{PI})'$.

We want to prove (P) for a general $b \in \mathcal{P}_{\mathrm{alg}}(\mathscr{Z}) = \bigoplus^{\mathrm{alg}}_{p,q\in\mathbb{N}} \mathcal{P}_{p,q}(\mathscr{Z})$. Let us first consider the "diagonal" case $b \in \mathcal{P}_{p,p}(\mathscr{Z})$, $p \in \mathbb{N}^*$. Using the decomposition $\tilde{b} = \tilde{b}_{R,+} - \tilde{b}_{R,-} + i\tilde{b}_{I,+} - i\tilde{b}_{I,-}$ with all the $\tilde{b}_\bullet \ge 0$ we can assume $\tilde{b} \ge 0$. For such a $\tilde{b}$, there exists a nondecreasing sequence $(\tilde{b}_n)_{n\ge 0}$ of nonnegative compact operators in $\mathcal{L}^\infty(\mathcal{S}_+^p \mathscr{Z})^{\otimes p}$ such that $\lim_{n\to\infty} \tilde{b}_n = \tilde{b}$ in the weak operator topology. Recall from [Ammari and Nier 2011, Proposition 2.9] that the convergence in the (P) condition always holds when the kernel $\tilde{b}$ is compact; thus,

$$\text{for all } n \in \mathbb{N}, \quad \int_{\mathscr{Z}} b_n \, d\mu = \lim_{\varepsilon \to 0} \operatorname{Tr}[\varrho_\varepsilon \, b_n^{\text{Wick}}] \leq \liminf_{\varepsilon \to 0} \operatorname{Tr}[\varrho_\varepsilon \, b^{\text{Wick}}].$$

Using $b_n(z) = \langle z^{\otimes p}, \tilde{b}_n z^{\otimes p} \rangle \to \langle z^{\otimes p}, \tilde{b} z^{\otimes p} \rangle = b(z)$ as $n \to \infty$ and Fatou's lemma yield

$$\int_{\mathscr{Z}} b \, d\mu \leq \liminf_{\varepsilon \to 0} \operatorname{Tr}[\varrho_\varepsilon b^{\text{Wick}}]. \tag{31}$$

The same arguments with $\tilde{b}$ replaced by $|b|_{\mathcal{P}_{p,p}} \operatorname{Id}_{\mathcal{S}_+^p \mathscr{Z}^{\otimes p}} - \tilde{b} \geq 0$ provide

$$\liminf_{\varepsilon \to 0} \operatorname{Tr}[\varrho_\varepsilon (|\tilde{b}|_{\mathcal{S}_+^p \mathcal{Z}^{\otimes p}} |z|^{2p} - b(z))^{\text{Wick}}] \geq \int (|\tilde{b}|_{\mathcal{S}_+^p \mathcal{Z}^{\otimes p}} |z|^{2p} - b(z)) \, d\mu(z).$$

With $(\mathrm{PI})'$ condition, the $|z|^{2p}$ terms can be removed on both sides and thus

$$\limsup_{\varepsilon \to 0} \operatorname{Tr}[\varrho_\varepsilon b^{\text{Wick}}] \leq \int_{\mathscr{Z}} b \, d\mu. \tag{32}$$

The inequalities (31) and (32) show that the convergence in the (P) condition holds for all $b \in \mathcal{P}_{p,p}(\mathscr{Z})$ such that $\tilde{b} \geq 0$, and hence for all $b \in \mathcal{P}_{p,p}(\mathscr{Z})$.

We now consider the general case $b \in \mathcal{P}_{p,q}(\mathscr{Z})$. There exists a sequence of compact operators $\tilde{b}_n \in \mathcal{L}^\infty(\mathcal{S}_+^p \mathscr{Z}^{\otimes p}, \mathcal{S}_+^q \mathscr{Z}^{\otimes q})$ such that,

$$\text{for all } n \in \mathbb{N}, \quad |b_n|_{\mathcal{P}_{p,q}} = |\tilde{b}_n|_{\mathcal{L}(\mathcal{S}_+^p \mathscr{Z}^{\otimes p}, \mathcal{S}_+^q \mathscr{Z}^{\otimes q})} \leq |\tilde{b}|_{\mathcal{L}(\mathcal{S}_+^p \mathscr{Z}^{\otimes p}, \mathcal{S}_+^q \mathscr{Z}^{\otimes q})} = |b|_{\mathcal{P}_{p,q}}$$

and,

$$\text{for all } z \in \mathscr{Z}, \quad \lim_{n \to \infty} b_n(z) = \lim_{n \to \infty} \langle z^{\otimes q}, \, \tilde{b}_n z^{\otimes p} \rangle = \langle z^{\otimes q}, \, \tilde{b} z^{\otimes p} \rangle = b(z).$$

For any fixed $n \in \mathbb{N}$,

$$\begin{aligned} \limsup_{\varepsilon \to 0} \left| \operatorname{Tr}[\varrho_\varepsilon b^{\text{Wick}}] - \int_{\mathscr{Z}} b(z) \, d\mu(z) \right| &\leq \limsup_{\varepsilon \to 0} \left| \operatorname{Tr}[\varrho_\varepsilon (b^{\text{Wick}} - b_n^{\text{Wick}})] \right| \\ &\quad + \limsup_{\varepsilon \to 0} \left| \operatorname{Tr}[\varrho_\varepsilon b_n^{\text{Wick}}] - \int_{\mathscr{Z}} b_n \, d\mu \right| + \int_{\mathscr{Z}} |b_n - b| \, d\mu, \end{aligned} \tag{33}$$

where the second term of the right-hand side vanishes because $\tilde{b}_n$ is a fixed compact operator. Using the Cauchy–Schwarz inequality with $\operatorname{Tr}[\varrho_\varepsilon] = 1$ gives

$$\left| \operatorname{Tr}[\varrho_\varepsilon (b^{\text{Wick}} - b_n^{\text{Wick}})] \right| \leq \operatorname{Tr}[\varrho_\varepsilon (b^{\text{Wick}} - b_n^{\text{Wick}})(b^{\text{Wick},*} - b_n^{\text{Wick},*})]^{\frac{1}{2}}.$$

From the proved result when $p = q$, we deduce

$$\limsup_{\varepsilon \to 0} \left| \operatorname{Tr}[\varrho_\varepsilon (b^{\text{Wick}} - b_n^{\text{Wick}})] \right| \leq \left[\int_{\mathscr{Z}} |b - b_n|^2 \, d\mu(z) \right]^{\frac{1}{2}}. \tag{34}$$

With $\int_{\mathscr{Z}} |z|^{r(p+q)}\, d\mu(z) < \infty$ and,

$$\text{for all } n \in \mathbb{N}, \quad \text{for all } z \in \mathscr{Z}, \quad |b(z) - b_n(z)|^r \leq (2|b|_{\mathcal{P}_{p,q}})^r |z|^{r(p+q)},$$

Lebesgue's convergence theorem yields

$$\lim_{n\to\infty} \int_{\mathscr{Z}} |b - b_n|^r \, d\mu = 0 \tag{35}$$

for $r \in \{1, 2\}$. Combining (33), (34) and (35) proves (P) for any $b \in \mathcal{P}_{p,q}(\mathscr{Z})$. □

Appendix C. The composition formula of Wick quantized operators

We give an algebraic proof for the composition formula (4) of two Wick quantized operators on a finite- or infinite-dimensional separable complex Hilbert space $\mathscr{Z}$. This proof holds in both the bosonic and fermionic cases. It uses only the definition of the Wick quantization, and it involves neither creation and annihilation operators, nor the canonical commutation or anticommutation relations.

We define $[\![m, n]\!] := \{m, \ldots, n\}$ for $m \leq n \in \mathbb{N}$. The action of the symmetric group $\mathfrak{S}_{[\![1,n]\!]}$ on product vectors in $\mathscr{Z}^{\otimes n}$, $\sigma \cdot (z_1 \otimes \cdots \otimes z_n) = z_{\sigma_1} \otimes \cdots \otimes z_{\sigma_n}$, $z_j \in \mathscr{Z}$, is extended to $\mathscr{Z}^{\otimes n}$ by linearity and density. With this notation,

$$\mathcal{S}^n_{\pm} = \frac{1}{n!} \sum_{\mathfrak{S}_{[\![1,n]\!]}} s_{\pm}(\sigma)\, \sigma \,\cdot\, .$$

We begin with a preliminary lemma on a special set of permutations.

Lemma C.1. *Let $k, p, q, K \in \mathbb{N}$ such that $k \in [\![\max\{0, p + q - K\}, \min\{p, q\}]\!]$, and*

$$\mathfrak{S}(k) := \big\{\sigma \in \mathfrak{S}_{[\![1,K]\!]} \;\big|\; \mathrm{card}\big(\sigma([\![p - k + 1, p - k + q]\!]) \cap [\![1, p]\!]\big) = k\big\}.$$

(1) *The cardinal of $\mathfrak{S}(k)$ is*

$$\mathrm{card}\, \mathfrak{S}(k) = \binom{q}{k}\binom{p}{k} k! \frac{(K - q)!\,(K - p)!}{(K - (q + p - k))!}.$$

(2) *Any permutation $\sigma \in \mathfrak{S}(k)$ can be factorized as $\sigma = \sigma^{(1)}\sigma^{(2)}\sigma^{(3)}\sigma^{(4)}$, where*

$$\sigma^{(1)} \in \mathfrak{S}_{[\![1,p]\!]}, \qquad \sigma^{(3)} \in \mathfrak{S}_{[\![p-k+1,p-k+q]\!]},$$
$$\sigma^{(2)} \in \mathfrak{S}_{[\![p+1,K]\!]}, \quad \sigma^{(4)} \in \mathfrak{S}_{[\![1,K]\!]\setminus[\![p-k+1,p-k+q]\!]}.$$

Note that:

- There is no uniqueness of such a decomposition.
- For $A \subset B$ an element of $\mathfrak{S}_A$ is identified with the corresponding element of $\mathfrak{S}_B$ which is the identity on $B \setminus A$.
- The permutations $\sigma^{(1)}$ and $\sigma^{(2)}$ commute, and so do $\sigma^{(3)}$ and $\sigma^{(4)}$.

Proof. (1) We count the number of permutations in $\mathfrak{S}(k)$. We first choose k integers out of $[\![p-k+1, p-k+q]\!]$ and k integers out of $[\![1, p]\!]$. There are $\binom{q}{k}\binom{p}{k}$ such possible choices and $k!$ possible permutations for each of these choices. Then the remaining $q-k$ integers of $[\![p-k+1, p-k+q]\!]$ have to be sent in $[\![p+1, K]\!]$. There are $(q-k)!\binom{K-p}{q-k}$ possibilities for that. In the same way we have $(p-k)!\binom{K-q}{p-k}$ possibilities for the remaining integers of $[\![1, p]\!]$ that come from $[\![1, K]\!] \setminus [\![p-k+1, p-k+q]\!]$. Finally the $K-k-(q-k)-(p-k)$ remaining integers on both sides can be permuted in $(K-q-p+k)!$ different ways, so that

$$\operatorname{card}\mathfrak{S}(k) = \binom{q}{k}\binom{p}{k}k!\,(q-k)!\binom{K-p}{q-k}(p-k)!\binom{K-q}{p-k}(K-q-p+k)!$$

and this gives the result.

(2) Let $A=\sigma^{-1}([\![1,p]\!])\cap[\![p-k+1,p-k+q]\!]$. There exists $\sigma^{(3)}\in\mathfrak{S}_{[\![p-k+1,p-k+q]\!]}$ such that $\sigma^{(3)}(A) = [\![p-k+1, p]\!]$. Then

$$\sigma\,\sigma^{(3)-1}([\![p-k+1, p]\!]) = \sigma(A) \subseteq [\![1, p]\!].$$

Hence there exists $\sigma^{(1)} \in \mathfrak{S}_{[\![1,p]\!]}$ such that $\sigma^{(1)}(j) = \sigma\,\sigma^{(3)-1}(j)$ on $[\![p-k+1, p]\!]$. Similarly, there exists $\sigma^{(2)} \in \mathfrak{S}_{[\![p+1,K]\!]}$ such that $\sigma^{(2)}(j) = \sigma\,\sigma^{(3)-1}(j)$ on $[\![p+1, p-k+q]\!]$. Note that $\sigma^{(1)}$ and $\sigma^{(2)}$ commute. Finally, we set $\sigma^{(4)} = \sigma^{(2)-1}\sigma^{(1)-1}\sigma\sigma^{(3)-1}$. By construction, $\sigma^{(4)}(j) = j$ for $j \in [\![p-k+1, p-k+q]\!]$, hence $\sigma^{(4)} \in \mathfrak{S}_{[\![1,K]\!]\setminus[\![p-k+1,p-k+q]\!]}$ and $\sigma = \sigma^{(1)}\sigma^{(2)}\sigma^{(3)}\sigma^{(4)}$ (as $\sigma^{(4)}$ and $\sigma^{(3)}$ commute). □

Notation 1. On $\mathcal{L}(\mathscr{Z}^{\otimes p}; \mathscr{Z}^{\otimes q})$, the equivalence relation $\cong$ is defined by

$$A \cong B \quad \Longleftrightarrow \quad \mathcal{S}_{\pm}^{q}\, A\, \mathcal{S}_{\pm}^{p,*} = \mathcal{S}_{\pm}^{q}\, B\, \mathcal{S}_{\pm}^{p,*}.$$

Lemma C.2. *Let $\tilde{b}_j \in \mathcal{L}(\mathcal{S}_{\pm}^{p_j}\, \mathscr{Z}^{\otimes p_j}; \mathcal{S}_{\pm}^{q_j}\, \mathscr{Z}^{\otimes q_j})$ and n_j such that $n_1 + p_1 = n_2 + q_2 =: K$. Then*

$$(\tilde{b}_1 \otimes \mathrm{Id}^{\otimes n_1})\mathcal{S}_{\pm}^{K,*}\mathcal{S}_{\pm}^{K}(\tilde{b}_2 \otimes \mathrm{Id}^{\otimes n_2}) \cong \sum_k (\pm 1)^{(p_2+q_2)(k-p_1)} \frac{n_2!\,n_1!}{K'!\,K!\,k!}\,(\tilde{b}_1 \sharp^k \tilde{b}_2) \otimes \mathrm{Id}^{\otimes K'},$$

where $k \in [\![\max\{0, p_1 + q_2 - K\}, \min\{p_1, q_2\}]\!]$, and $K' = K - q_2 - p_1 + k$.

Proof. Using the partition $\mathfrak{S}_{[\![1,K]\!]} = \bigsqcup_k \tilde{\mathfrak{S}}(k)$ into subsets

$$\tilde{\mathfrak{S}}(k) := \big\{\sigma \in \mathfrak{S}_{[\![1,K]\!]} \;\big|\; \operatorname{card}\big(\sigma([\![1, q_2]\!]) \cap [\![1, p_1]\!]\big) = k\big\}$$

for $k \in [\![\max\{0, p_1 + q_2 - K\}, \min\{p_1, q_2\}]\!]$ yields

$$(\tilde{b}_1\otimes\mathrm{Id}^{\otimes n_1})\mathcal{S}_{\pm}^{K,*}\mathcal{S}_{\pm}^{K}(\tilde{b}_2\otimes\mathrm{Id}^{\otimes n_2}) = \frac{1}{K!}\sum_k \sum_{\tilde{\sigma}\in\tilde{\mathfrak{S}}(k)} (\tilde{b}_1\otimes\mathrm{Id}^{\otimes n_1})s_{\pm}(\tilde{\sigma})\tilde{\sigma}\cdot(\tilde{b}_2\otimes\mathrm{Id}^{\otimes n_2}).$$

We fix k and $\tilde\sigma \in \tilde{\mathfrak{S}}(k)$. A cyclic permutation $\tau_r := (1\,2\,3\,\cdots\,r)$ acting on $\mathcal{Z}^{\otimes r}$ defines the shift operator $\tau_r\,\cdot\, = (1\,2\,3\,\cdots\,r)\,\cdot$ and then $\sigma := \tilde\sigma\,\tau_K^{k-p_1}$ is in $\mathfrak{S}(k)$ (with $p = p_1$ and $q = q_2$) and

$$
\begin{aligned}
&(\tilde b_1\otimes \mathrm{Id}^{\otimes n_1})\, s_\pm(\tilde\sigma)\,\tilde\sigma\tau_K^{k-p_1}\,\tau_K^{p_1-k}\cdot(\tilde b_2\otimes\mathrm{Id}^{\otimes n_2})\,\tau_{p_2+n_2}^{k-p_1}\tau_{p_2+n_2}^{p_1-k}\cdot\\
&\ \cong(\tilde b_1\otimes \mathrm{Id}^{\otimes n_1})\, s_\pm(\sigma)\,\sigma\cdot(\pm1)^{K(k-p_1)}(\mathrm{Id}^{\otimes p_1-k}\otimes\tilde b_2\otimes\mathrm{Id}^{\otimes K'})(\pm1)^{(p_2+n_2)(k-p_1)}\\
&\ \cong(\pm1)^{(K+p_2+n_2)(k-p_1)}(\tilde b_1\otimes \mathrm{Id}^{\otimes n_1})s_\pm(\sigma)\sigma\cdot(\mathrm{Id}^{\otimes p_1-k}\otimes\tilde b_2\otimes\mathrm{Id}^{\otimes K'})
\end{aligned}
$$

holds for operators in $\mathcal{L}(\mathscr{Z}^{\otimes q_1+n_1};\mathscr{Z}^{\otimes p_2+n_2})$. We used

$$
s_\pm(\sigma)=s_\pm(\tilde\sigma)s_\pm(\tau_K^{k-p_1})=s_\pm(\tilde\sigma)(\pm1)^{K(k-p_1)}
$$

and

$$
(\tau_{p_2+n_2}^{p_1-k}\cdot)\circ\mathcal{S}_\pm^{p_2+n_2}=(\pm1)^{(p_2+n_2)(p_1-k)}\mathcal{S}_\pm^{p_2+n_2}.
$$

Owing to the factorization $\sigma=\sigma^{(1)}\sigma^{(2)}\sigma^{(3)}\sigma^{(4)}$ of Lemma C.1 with $\sigma^{(i)}\sigma^{(i+1)}=\sigma^{(i+1)}\sigma^{(i)}$ for $i\in\{1,3\}$, we get

$$
\begin{aligned}
&(\tilde b_1\otimes \mathrm{Id}^{\otimes n_1})s_\pm(\sigma)\sigma\cdot(\mathrm{Id}^{\otimes p_1-k}\otimes\tilde b_2\otimes\mathrm{Id}^{\otimes K'})\\
&\ \cong(\tilde b_1\otimes \mathrm{Id}^{\otimes n_1})s_\pm(\sigma)(\sigma^{(1)}\sigma^{(2)}\sigma^{(3)}\sigma^{(4)})\cdot(\mathrm{Id}^{\otimes p_1-k}\otimes\tilde b_2\otimes\mathrm{Id}^{\otimes K'})\\
&\ \cong s_\pm(\sigma)((b_1\,\sigma^{(1)}\cdot)\otimes\mathrm{Id}^{\otimes n_1}\sigma^{(2)}\cdot)\,\sigma^{(4)}\cdot(\mathrm{Id}^{\otimes p_1-k}\otimes(\sigma^{(3)}\cdot\tilde b_2)\otimes\mathrm{Id}^{\otimes K'})\\
&\ \cong s_\pm(\sigma)(\tilde b_1 s_\pm(\sigma^{(1)})\otimes s_\pm(\sigma^{(2)})\mathrm{Id}^{\otimes n_1})s_\pm(\sigma^{(4)})(\mathrm{Id}^{\otimes p_1-k}\otimes s_\pm(\sigma^{(3)})\tilde b_2\otimes\mathrm{Id}^{\otimes K'})\\
&\ \cong(\tilde b_1\otimes \mathrm{Id}^{\otimes n_1})\,(\mathrm{Id}^{\otimes p_1-k}\otimes\tilde b_2\otimes\mathrm{Id}^{\otimes K'})\\
&\ \cong[(\tilde b_1\otimes\mathrm{Id}^{\otimes q_2-k})(\mathrm{Id}^{\otimes p_1-k}\otimes\tilde b_2)]\otimes\mathrm{Id}^{\otimes K'}\\
&\ \cong\left(\frac{p_1!}{(p_1-k)!}\frac{q_2!}{(q_2-k)!}\right)^{-1}(\tilde b_1\sharp^k\tilde b_2)\otimes\mathrm{Id}^{\otimes K'}.
\end{aligned}
$$

We conclude with the first statement of Lemma C.1 which counts the terms in $\sum_{\tilde\sigma\in\tilde{\mathfrak{S}}(k)}$ because $\mathrm{card}(\tilde{\mathfrak{S}}(k))=\mathrm{card}(\mathfrak{S}(k))$. □

Proof of Proposition 2.2. For n_1, n_2 such that $n_1+p_1=n_2+q_2=:K$, using Lemma C.2,

$$
\begin{aligned}
&\varepsilon^{-\frac{p_1+q_1+p_2+q_2}{2}}\times\tilde b_1^{\mathrm{Wick}}\tilde b_2^{\mathrm{Wick}}\big|_{\mathcal{S}_\pm^{n_2+p_2}\mathscr{Z}^{\otimes n_2+p_2}}\\
&\quad=\frac{\sqrt{K!\,(n_1+q_1)!}}{n_1!}\,\frac{\sqrt{(n_2+p_2)!\,K!}}{n_2!}\\
&\qquad\qquad\cdot\mathcal{S}_\pm^{q_1+n_1}(\tilde b_1\otimes\mathrm{Id}^{\otimes n_1})\mathcal{S}_\pm^{p_1+n_1,*}\mathcal{S}_\pm^{p_2+q_2}(\tilde b_2\otimes\mathrm{Id}^{\otimes n_2})\mathcal{S}_\pm^{p_2+n_2,*}
\end{aligned}
$$

$$= \sum_k (\pm 1)^{(p_2+q_2)(k-p_1)} \frac{\sqrt{(n_1+q_1)!\,(n_2+p_2)!}}{n_1!\,n_2!}\, K!\, \frac{n_2!\,n_1!}{K'!\,K!\,k!} \cdot \mathcal{S}_\pm^{q_1+n_1}((\tilde{b}_1\sharp^k\tilde{b}_2)\otimes \mathrm{Id}^{\otimes K'})\mathcal{S}_\pm^{p_2+n_2,*}$$

$$= \sum_k (\pm 1)^{(p_2+q_2)(k-p_1)} \frac{\sqrt{(q_2+q_1-k+K')!\,(p_2+p_1-k+K')!}}{K'!\,k!} \cdot \mathcal{S}_\pm^{q_1+n_1}((\tilde{b}_1\sharp^k\tilde{b}_2)\otimes \mathrm{Id}^{\otimes K'})\mathcal{S}_\pm^{p_2+n_2,*},$$

where $K' := K - q_2 - p_1 + k$.

With $p_2 + n_2 = p_2 + p_1 - k + K'$ and $q_1 + n_1 = q_2 + q_1 - k + K'$, we thus obtain the equality of operators

$$\tilde{b}_1^{\mathrm{Wick}}\tilde{b}_2^{\mathrm{Wick}} = \sum_k (\pm 1)^{(p_2+q_2)(k-p_1)} \frac{\varepsilon^k}{k!} (\tilde{b}_1\sharp^k\tilde{b}_2)^{\mathrm{Wick}}$$

restricted to $\mathcal{S}_\pm^{n_2+p_2}\mathscr{Z}^{\otimes n_2+p_2}$. □

Appendix D. A general formula for $\mathrm{Tr}[\Gamma_\pm(C)]$

The following result about traces of the second quantized operator $\Gamma_\pm(C)$ is often presented for self-adjoint trace-class operators, although it is valid without self-adjointness. We recall here the general version for the sake of completeness. It relies on a simple holomorphy argument and can be compared with Lidskii's theorem, which says that for any trace-class operator T, we have $\mathrm{Tr}[T] = \sum_{\lambda\in\sigma(T)}\lambda$.

Lemma D.1. *For any trace-class operator $C \in \mathcal{L}^1(\mathscr{Z})$ (which is assumed to be a strict contraction in the bosonic case, $\pm = +$), its second quantized version $\Gamma_\pm(C)$ is trace-class in $\Gamma_\pm(\mathscr{Z})$ and*

$$\mathrm{Tr}[\Gamma_\pm(C)] = \exp(\mp\,\mathrm{Tr}[\log(1 \mp C)]).$$

Proof. When $C = C^* \in \mathcal{L}^1(\mathscr{Z})$ using an orthonormal basis of eigenvectors $(e_n)_{n\in\mathbb{N}}$ in $\mathscr{Z}$ with the corresponding eigenvalues $(\lambda_n)_{n\in\mathbb{N}}$, and

$$\Gamma_\pm(\mathscr{Z}) \cong \bigotimes_{n\in\mathbb{N}} \Gamma_\pm(\mathbb{C}e_n),$$

(the infinite tensor product of Hilbert spaces with a stabilizing sequence $u_n = \Omega_n$ with $\Omega_n \in \Gamma_\pm(\mathbb{C}e_n)$ the vacuum vector), we obtain

- in the bosonic case with $\|C\| < 1$,

$$\mathrm{Tr}[\Gamma_+(C)] = \prod_{n\in\mathbb{N}} \mathrm{Tr}[\Gamma_+(\lambda_n \mathrm{Id}_{\mathbb{C}})] = \prod_{n\in\mathbb{N}} \frac{1}{1-\lambda_n} = \exp\Big(-\sum_{n\in\mathbb{N}} \log(1-\lambda_n)\Big)$$
$$= \exp(-\,\mathrm{Tr}[\log(1-C)]),$$

• in the fermionic case,

$$\begin{aligned}\mathrm{Tr}[\Gamma_-(C)] &= \prod_{n\in\mathbb{N}} \mathrm{Tr}[\Gamma_-(\lambda_n \mathrm{Id}_{\mathbb{C}})] = \prod_{n\in\mathbb{N}} (1+\lambda_n) = \exp\Big(+\sum_{n\in\mathbb{N}} \log(1+\lambda_n)\Big)\\ &= \exp(\mathrm{Tr}[\log(1+C)]).\end{aligned}$$

The functoriality of $\Gamma_\pm$ for the polar decomposition $C = U|C|$ is given by $\Gamma_\pm(C) = \Gamma_\pm(U)\Gamma_\pm(|C|)$, while $\|C\| < 1 \Leftrightarrow \||C|\| < 1$ in the bosonic case. Hence $\Gamma_\pm(C)$ is trace-class when $C \in \mathcal{L}^1(\mathscr{Z})$ (and $\|C\| < 1$ in the bosonic case).

Set $\mathcal{C} = \mathcal{L}^1(\mathscr{Z})$ in the fermionic case and $\mathcal{C} = \mathcal{L}^1(\mathscr{Z}) \cap \{C \in \mathcal{L}(\mathscr{Z}) : \|C\| < 1\}$ in the bosonic case. In both cases $\mathcal{C}$ is an open convex set on which the two sides of the equality are holomorphic functions. Actually the holomorphy of the left-hand side comes from series expansion

$$\mathrm{Tr}[\Gamma_\pm(C)] = \sum_{n=0}^{\infty} \mathrm{Tr}[\mathcal{S}_\pm^n C^{\otimes n} \mathcal{S}_\pm^{n,*}],$$

which converges uniformly in

$$B(C_0, \delta_{C_0}) = \{C \in \mathcal{L}^1(\mathscr{Z}) : \|C - C_0\|_{\mathcal{L}^1(\mathscr{Z})} < \delta_{C_0}\}$$

for $\delta_{C_0} > 0$ small enough, for any $C_0 \in \mathcal{L}^1(\mathscr{Z})$ (satisfying additionally $\|C_0\| < 1$ in the bosonic case). Actually the estimate $\|C\|_{\mathcal{L}^1(\mathscr{Z})} \le A$ (and $\|C\| \le \varrho$ with $\varrho < 1$ in the bosonic case) implies $\||C|\|_{\mathcal{L}^1(\mathscr{Z})} \le A$ (and $\||C|\| \le \varrho$ in the bosonic case). Now the inequality

$$\left|\mathrm{Tr}[\mathcal{S}_\pm^n C^{\otimes n} \mathcal{S}_\pm^{n,*}]\right| \le \mathrm{Tr}[\mathcal{S}_\pm^n |C|^{\otimes n} \mathcal{S}_\pm^{n,*}],$$

and the formula in the self-adjoint case with

$$\sum_{n=0}^{\infty} \mathrm{Tr}[\mathcal{S}_-^n |C|^{\otimes n} \mathcal{S}_-^{n,*}] \le \exp(A) \quad \text{(fermions)}$$

or

$$\sum_{n=0}^{\infty} \mathrm{Tr}[\mathcal{S}_+^n |C|^{\otimes n} \mathcal{S}_+^{n,*}] \le \exp\left(\frac{A}{1-\varrho}\right) \quad \text{(bosons)},$$

ensures the uniform convergence of the series.

For any $C \in \mathcal{C}$, we know C and $\mathrm{Re}\, C = \frac{1}{2}(C + C^*)$ belong to $\mathcal{C}$ so that $C(s) = \mathrm{Re}\, C + is\, \mathrm{Im}\, C$ belongs to $\mathcal{C}$ when $s \in \omega_0 = (-\delta, \delta) + i(-\delta, \delta)$ and when $s \in \omega_1 = (1-\delta, 1+\delta) + i(-\delta, \delta)$ for $\delta > 0$ small enough. By the convexity of $\mathcal{C}$, we have $C(s) \in \mathcal{C}$ for all $s \in \omega = (-\delta, 1+\delta) + i(-\delta, \delta)$. When $s \in i(-\delta, \delta)$, $C(s)$ is self-adjoint and the equality holds. The holomorphy of both sides with respect to $s \in \omega$ implies that the equality holds true for all $s \in \omega$, in particular when $s = 1$. □

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A nonlinear estimate of the life span of solutions of the three dimensional Navier–Stokes equations

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The purpose of this article is to establish bounds from below for the life span of regular solutions to the incompressible Navier–Stokes system, which involve norms not only of the initial data, but also of nonlinear functions of the initial data. We provide examples showing that those bounds are significant improvements to the one provided by the classical fixed point argument. One of the important ingredients is the use of a scale-invariant energy estimate.

1. Introduction

In this article our aim is to give bounds from below for the life span of solutions to the incompressible Navier–Stokes system in the whole space $\mathbb{R}^3$. We are not interested here in the regularity of the initial data: we focus on obtaining bounds from below for the life span associated with regular initial data. Here regular means that the initial data belongs to the intersection of all Sobolev spaces of nonnegative index. Thus all the solutions we consider are regular ones, as long as they exist.

Let us recall the incompressible Navier–Stokes system, together with some of its basic features. The incompressible Navier–Stokes system is the following:

$$\text{(NS)}\qquad \begin{aligned} &\partial_t u - \Delta u + u\cdot\nabla u = -\nabla p,\\ &\operatorname{div} u = 0 \quad\text{and}\quad u_{|t=0} = u_0, \end{aligned}$$

where u is a three dimensional, time-dependent vector field and p is the pressure, determined by the incompressibility condition $\operatorname{div} u = 0$:

$$-\Delta p = \operatorname{div}(u\cdot\nabla u) = \sum_{1\leq i,j\leq 3} \partial_i\partial_j(u^i u^j).$$

This system has two fundamental properties related to its physical origin:

- scaling invariance,
- dissipation of kinetic energy.

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The scaling property is the fact that if a function u satisfies (NS) on a time interval $[0,T]$ with the initial data u_0, then the function u_λ defined by

$$u_\lambda(t,x) \stackrel{\text{def}}{=} \lambda u(\lambda^2 t, \lambda x)$$

satisfies (NS) on the time interval $[0,\lambda^{-2}T]$ with the initial data $\lambda u_0(\lambda\,\cdot)$. This property is far from being a characteristic property of the system (NS). It is indeed satisfied by all systems of the form

$$\text{(GNS)} \qquad \begin{aligned} &\partial_t u - \Delta u + Q(u,u) = 0 \quad \text{with} \quad Q^i(u,u) \stackrel{\text{def}}{=} \sum_{1\le j,k\le 3} A^i_{j,k}(D)(u^j u^k),\\ &u_{|t=0} = u_0, \end{aligned}$$

where the $A^i_{j,k}(D)$ are smooth homogeneous Fourier multipliers of order 1. Indeed denoting by $\mathbb{P}$ the projection onto divergence free vector fields

$$\mathbb{P} \stackrel{\text{def}}{=} \mathrm{Id} - (\partial_i \partial_j \Delta^{-1})_{ij},$$

the Navier–Stokes system takes the form

$$\begin{aligned} &\partial_t u - \Delta u + \mathbb{P}\,\mathrm{div}(u\otimes u) = 0,\\ &u_{|t=0} = u_0, \end{aligned}$$

which is of the type (GNS). For this class of systems, the following result holds. The definition of homogeneous Sobolev spaces $\dot H^s$ is recalled in the Appendix.

Proposition 1.1. *Let u_0 be a regular three-dimensional vector field. A positive time T exists such that a unique regular solution to (GNS) exists on $[0,T]$. Let $T^\star(u_0)$ be the maximal time of existence of this regular solution. Then, for any γ in the interval $]0,\frac12[$, a constant c_γ exists such that*

$$T^\star(u_0) \ge c_\gamma \|u_0\|^{-\frac{1}{\gamma}}_{\dot H^{\frac12+2\gamma}}. \tag{1}$$

In the case when $\gamma = \frac14$ for the particular case of (NS), this type of result goes back to the seminal work of J. Leray [1934]. Let us point out that the same type of result can be proved for the $L^{3+6\gamma/(1-2\gamma)}$ norm.

Proof. This result is obtained by a scaling argument. Let us define the following function

$$\underline{T}_{\dot H^{\frac12+2\gamma}}(r) \stackrel{\text{def}}{=} \inf\big\{T^\star(u_0) \mid \|u_0\|_{\dot H^{\frac12+2\gamma}} = r\big\}.$$

We assume that at least one smooth initial data u_0 develops singularities, which means exactly that $T^\star(u_0)$ is finite. Let us mention that this lower bound is in fact a minimum (see [Poulon 2015]). Actually the function $\underline{T}_{\dot H^{\frac12+2\gamma}}$ may be computed using a scaling argument. Observe that

$$\|u_0\|_{\dot H^{\frac12+2\gamma}} = r \iff \|r^{-\frac{1}{2\gamma}} u_0(r^{-\frac{1}{2\gamma}}\cdot)\|_{\dot H^{\frac12+2\gamma}} = 1.$$

As we have $T^\star(u_0) = r^{-\frac{1}{\gamma}} T^\star\big(r^{-\frac{1}{2\gamma}} u_0(r^{-\frac{1}{2\gamma}}\cdot)\big)$, we infer that $\underline{T}_{\dot H^{\frac12+2\gamma}}(r) = r^{-\frac{1}{\gamma}} \underline{T}_{\dot H^{\frac12+2\gamma}}(1)$ and thus that

$$T^\star(u_0) \geq c_\gamma \|u_0\|_{\dot H^{\frac12+2\gamma}}^{-\frac{1}{\gamma}} \quad \text{with} \quad c_\gamma \stackrel{\text{def}}{=} \underline{T}_{\dot H^{\frac12+2\gamma}}(1)\,.$$

The proposition is proved. □

Now let us investigate the optimality of such a result, in particular concerning the norm appearing in the lower bound (1). Useful results and definitions concerning Besov spaces are recalled in the Appendix; the Besov norms of particular interest in this text are the $\dot B^{-1}_{\infty,2}$ norm which is given by

$$\|a\|_{\dot B^{-1}_{\infty,2}} \stackrel{\text{def}}{=} \left(\int_0^\infty \|e^{t\Delta}a\|^2_{L^\infty}\,dt\right)^{\frac12}$$

and the Besov norms $\dot B^{-\sigma}_{\infty,\infty}$ for $\sigma > 0$, which are

$$\|a\|_{\dot B^{-\sigma}_{\infty,\infty}} \stackrel{\text{def}}{=} \sup_{t>0} t^{\frac{\sigma}{2}} \|e^{t\Delta}a\|_{L^\infty}.$$

It has been known since [Fujita and Kato 1964] that a smooth initial data in $\dot H^{\frac12}$ (corresponding of course to the limit case $\gamma = 0$ in Proposition 1.1) generates a smooth solution for some time $T > 0$. Let us point out that in dimension 3, the following inequality holds

$$\|a\|_{\dot B^{-1}_{\infty,2}} \lesssim \|a\|_{\dot H^{\frac12}}.$$

The norms $\dot B^{-\sigma}_{\infty,\infty}$ are the smallest norms invariant by translation and having a given scaling. More precisely, we have the following result:

Proposition 1.2 [Meyer 1997, Lemma 9]. *Let $d \geq 1$ and let $(E, \|\cdot\|_E)$ be a normed space continuously included in $\mathcal{S}'(\mathbb{R}^d)$, the space of tempered distributions on $\mathbb{R}^d$. Assume that E is stable by translation and by dilation, and that a constant C_0 exists such that*

$$\forall (\lambda, e) \in \,]0,\infty[\, \times \mathbb{R}^d, \qquad \forall a \in E, \quad \|a(\lambda\cdot - e)\|_E \leq C_0 \lambda^{-\sigma} \|a\|_E\,.$$

Then a constant C_1 exists such that

$$\forall a \in E, \quad \|a\|_{\dot B^{-\alpha}_{\infty,\infty}} \leq C_1 \|a\|_E.$$

Proof. Let us simply observe that, as E is continuously included in $\mathcal{S}'(\mathbb{R}^d)$, a constant C exists such that for all a in E,

$$|\langle a, e^{-|\cdot|^2}\rangle| \leq C\|a\|_E\,.$$

Then by invariance by translation and dilation of E, we infer immediately that

$$\|e^{t\Delta}a\|_{L^\infty} \le C_1 t^{-\frac{\sigma}{2}} \|a\|_E,$$

which proves the proposition. □

Now let us state a first improvement to Proposition 1.1 where the life span is bounded from below in terms of the $\dot{B}^{-1+2\gamma}_{\infty,\infty}$ norm of the initial data.

Theorem 1.3. *With the notation of Proposition 1.1, for any γ in the interval $\left]0, \frac{1}{2}\right[$, a constant c'_γ exists such that*

$$T^\star(u_0) \ge T_{\mathrm{FP}}(u_0) \stackrel{\mathrm{def}}{=} c'_\gamma \|u_0\|^{-\frac{1}{\gamma}}_{\dot{B}^{-1+2\gamma}_{\infty,\infty}}. \tag{2}$$

This theorem is proved in Section 2; the proof relies on a fixed point theorem in a space included in the space of L^2 in time functions, with values in L^∞.

Let us also recall that if a scaling 0 norm of a regular initial data is small, then the solution of (NS) associated with u_0 is global. This a consequence of the Koch and Tataru theorem [2001], which can be translated as follows in the context of smooth solutions.

Theorem 1.4. *A constant c_0 exists such that for any regular initial data u_0 satisfying*

$$\|u_0\|_{\mathrm{BMO}^{-1}} \stackrel{\mathrm{def}}{=} \sup_{t>0} t^{\frac{1}{2}} \|e^{t\Delta}u_0\|_{L^\infty} + \left(\sup_{\substack{x\in\mathbb{R}^3\\ R>0}} \frac{1}{R^3} \int_0^{R^2}\int_{B(x,R)} |e^{t\Delta}u_0(y)|^2\,dy\,dt \right)^{\frac{1}{2}} \le c_0,$$

the associate solution of (GNS) is globally regular.

Let us remark that

$$\|u_0\|_{\dot{B}^{-1}_{\infty,\infty}} \le \|u_0\|_{\mathrm{BMO}^{-1}} \le \|u_0\|_{\dot{B}^{-1}_{\infty,2}}.$$

We shall explain in Section 2 how to deduce Theorem 1.4 from the Koch and Tataru theorem [2001].

The previous results are valid for the whole class of systems (GNS). Now let us present the second main feature of the incompressible Navier–Stokes system, which is not shared by all systems under the form (GNS) as it relies on a special structure of the nonlinear term (which must be skew-symmetric in L^2): the dissipation estimate for the kinetic energy. For regular solutions of (NS) it holds that

$$\frac{1}{2}\frac{d}{dt}\|u(t)\|^2_{L^2} + \|\nabla u(t)\|^2_{L^2} = 0,$$

which gives by integration in time

$$\forall t \geq 0, \quad \mathcal{E}\big(u(t)\big) \stackrel{\text{def}}{=} \tfrac{1}{2}\|u(t)\|_{L^2}^2 + \int_0^t \|\nabla u(t')\|_{L^2}\, dt' = \tfrac{1}{2}\|u_0\|_{L^2}^2. \tag{3}$$

T. Tao [2016] pointed out that the energy estimate is not enough to prevent possible singularities from appearing. Our purpose here is to investigate if this energy estimate can improve the lower bound (2) on the life span for regular initial data. We recall indeed that for smooth initial data, all Leray solutions — meaning solutions in the sense of distributions satisfying the energy inequality

$$\mathcal{E}\big(u(t)\big) \leq \tfrac{1}{2}\|u_0\|_{L^2}^2 \tag{4}$$

coincide with the smooth solution as long as the latter exists.

What we shall use here is a rescaled version of the energy dissipation inequality in the spirit of [Chemin and Planchon 2012], on the fluctuation $w \stackrel{\text{def}}{=} u - u_{\mathrm{L}}$ with $u_{\mathrm{L}}(t) \stackrel{\text{def}}{=} e^{t\Delta}u_0$.

Proposition 1.5. *Let u be a regular solution of (NS) associated with some initial data u_0. Then the fluctuation w satisfies, for any positive t*

$$\mathcal{E}\Big(\frac{w(t)}{t^{\frac{1}{4}}}\Big) + \int_0^t \frac{\|w(t')\|_{L^2}^2}{t'^{\frac{3}{2}}}\, dt' \lesssim Q_{\mathrm{L}}^0 \exp \|u_0\|_{\dot{B}^{-1}_{\infty,2}}^2$$
$$\text{with } Q_{\mathrm{L}}^0 \stackrel{\text{def}}{=} \int_0^\infty t^{\frac{1}{2}} \|\mathbb{P}(u_{\mathrm{L}}\cdot\nabla u_{\mathrm{L}})(t)\|_{L^2}^2\, dt.$$

Our main result is then the following:

Theorem 1.6. *There is a constant $C > 0$ such that the following holds. For any regular initial data of (NS),*

$$T^*(u_0) > T_{\mathrm{L}}(u_0), \tag{5}$$

where

$$T_{\mathrm{L}}(u_0) \stackrel{\text{def}}{=} C(Q_{\mathrm{L}}^0)^{-2}\Big(\|\partial_3 u_0\|^2_{\dot{B}^{-\frac{3}{2}}_{\infty,\infty}} Q_{\mathrm{L}}^0 + \sqrt{Q_{\mathrm{L}}^0 Q_{\mathrm{L}}^1}\Big)^{-2} \exp(-4\|u_0\|^2_{\dot{B}^{-1}_{\infty,2}}),$$
$$\text{with } Q_{\mathrm{L}}^1 \stackrel{\text{def}}{=} \int_0^\infty t^{\frac{3}{2}} \big\|\partial_3^2\big(\mathbb{P}(u_{\mathrm{L}}\cdot\nabla u_{\mathrm{L}})\big)(t)\big\|_{L^2}^2\, dt\,.$$

The main two features of this result are that:

- the statement involves nonlinear quantities associated with the initial data, namely norms of $\mathbb{P}(u_{\mathrm{L}}\cdot\nabla u_{\mathrm{L}})$;
- one particular (arbitrary) direction plays a specific role.

This theorem is proved in Section 4.

The following theorem shows that the lower bound on $T^*(u_0)$ in Theorem 1.6 is, for some classes of initial data, a significant improvement.

Theorem 1.7. *Let* (γ, η) *be in* $\big]0, \frac{1}{2}\big[\times]0,1[$. *There is a constant* C *and a family* $(u_{0,\varepsilon})_{\varepsilon\in]0,1[}$ *of regular initial data such that, with the notation of Theorems* 1.3 *and* 1.6,

$$T_{\mathrm{FP}}(u_{0,\varepsilon}) = C\varepsilon^2 |\log\varepsilon|^{-\frac{1}{\gamma}} \quad \textit{and} \quad T_{\mathrm{L}}(u_{0,\varepsilon}) \geq C\varepsilon^{-2+\eta}.$$

This theorem is proved in Section 5. The family $(u_{0,\varepsilon})_{\varepsilon\in]0,1[}$ is closely related to the family used in [Chemin and Gallagher 2009] to exhibit families of initial data which do not obey the hypothesis of the Koch and Tataru theorem and which nevertheless generate global smooth solutions. However it is too large to satisfy the assumptions of Theorem 2 in [Chemin and Gallagher 2009] so it is not known if the associated solution is global.

In the following we shall denote by C a constant which may change from line to line, and we shall sometimes write $A \lesssim B$ for $A \leq CB$.

2. Proof of Theorem 1.3

Let u_0 be a smooth vector field and let us solve (GNS) by means of a fixed point method. We define the bilinear operator B by

$$\partial_t B(u,v) - \Delta B(u,v) = -\tfrac{1}{2}\big(Q(u,v)+Q(v,u)\big), \quad \text{and} \quad B(u,v)|_{t=0} = 0. \tag{6}$$

One can decompose the solution u to (GNS) into

$$u = u_{\mathrm{L}} + B(u,u).$$

Resorting to the Littlewood–Paley decomposition defined in the Appendix, let us define for any real number γ and any time $T > 0$, the quantity

$$\|f\|_{E_T^\gamma} \stackrel{\text{def}}{=} \sup_{j\in\mathbb{Z}} 2^{-j(1-2\gamma)}\big(\|\Delta_j f\|_{L^\infty([0,T]\times\mathbb{R}^3)} + 2^{2j}\|\Delta_j f\|_{L^1([0,T];L^\infty(\mathbb{R}^3))}\big).$$

Using Lemma 2.1 of [Chemin 1999] it is easy to see that

$$\|u_{\mathrm{L}}\|_{E_\infty^\gamma} \lesssim \|u_0\|_{\dot B^{-1+2\gamma}_{\infty,\infty}},$$

so Theorem 1.3 will follow from the fact that B maps $E_T^\gamma \times E_T^\gamma$ into E_T^γ with the following estimate:

$$\|B(u,v)\|_{E_T^\gamma} \leq C_\gamma T^\gamma \|u\|_{E_T^\gamma}\|v\|_{E_T^\gamma}. \tag{7}$$

So let us prove (7). Using again Lemma 2.1 of [Chemin 1999] along with the fact that the $A^i_{k,\ell}(D)$ are smooth homogeneous Fourier multipliers of order 1, we have

$$\|\Delta_j B(u,v)(t)\|_{L^\infty} \lesssim \int_0^t e^{-c2^{2j(t-t')}} 2^j \big\|\Delta_j\big(u(t')\otimes v(t') + v(t')\otimes u(t')\big)\big\|_{L^\infty}\,dt'.$$

We then decompose (componentwise) the product $u \otimes v$ following Bony's paraproduct algorithm: for all functions a and b the support of the Fourier transform of $S_{j'+1}a\Delta_{j'}b$ and $S_{j'}b\Delta_{j'}a$ is included in a ball $2^{j'}B$ where B is a fixed ball of $\mathbb{R}^3$, so one can write for some fixed constant $c > 0$

$$ab = \sum_{2^{j'} \geq c2^j} \big(S_{j'+1}a\Delta_{j'}b + \Delta_{j'}aS_{j'}b\big),$$

so thanks to Young's inequality in time one can write

$$2^{-j(1-2\gamma)}\big(\|\Delta_j B(u,v)\|_{L^\infty([0,T]\times\mathbb{R}^3)} + 2^{2j}\|\Delta_j B(u,v)\|_{L^1([0,T];L^\infty(\mathbb{R}^3))}\big) \lesssim \mathcal{B}_j^1(u,v) + \mathcal{B}_j^2(u,v), \quad (8)$$

with

$$\begin{aligned}
\mathcal{B}_j^1(u,v) &\stackrel{\text{def}}{=} 2^{2j\gamma} \sum_{2^{j'} \geq \max\{c2^j, T^{-\frac{1}{2}}\}} \|S_{j'+1}u\|_{L^\infty([0,T]\times\mathbb{R}^3)}\|\Delta_{j'}v\|_{L^1([0,T];L^\infty(\mathbb{R}^3))} \\
&\quad + 2^{2j\gamma} \sum_{c2^j \leq 2^{j'} < T^{-\frac{1}{2}}} \|S_{j'+1}u\|_{L^\infty([0,T]\times\mathbb{R}^3)}\|\Delta_{j'}v\|_{L^1([0,T];L^\infty(\mathbb{R}^3))}, \\
\mathcal{B}_j^2(u,v) &\stackrel{\text{def}}{=} 2^{2j\gamma} \sum_{2^{j'} \geq \max\{c2^j, T^{-\frac{1}{2}}\}} \|S_{j'}v\|_{L^\infty([0,T]\times\mathbb{R}^3)}\|\Delta_{j'}u\|_{L^1([0,T];L^\infty(\mathbb{R}^3))} \\
&\quad + 2^{2j\gamma} \sum_{c2^j \leq 2^{j'} < T^{-\frac{1}{2}}} \|S_{j'}v\|_{L^\infty([0,T]\times\mathbb{R}^3)}\|\Delta_{j'}u\|_{L^1([0,T];L^\infty(\mathbb{R}^3))}.
\end{aligned}$$

In each of the sums over $c2^j \leq 2^{j'} < T^{-\frac{1}{2}}$ we write

$$\|f\|_{L^1([0,T];L^\infty(\mathbb{R}^3))} \leq T\|f\|_{L^\infty([0,T]\times\mathbb{R}^3)}$$

and we can estimate the two terms $\mathcal{B}_j^1(u,v)$ and $\mathcal{B}_j^2(u,v)$ in the same way: for $\ell \in \{1,2\}$ it holds that

$$\begin{aligned}
\mathcal{B}_j^\ell(u,v) &\leq \|u\|_{E_T^\gamma}\|v\|_{E_T^\gamma}\Bigg(2^{2j\gamma} \sum_{2^{j'} \geq \max\{c2^j, T^{-\frac{1}{2}}\}} 2^{-4j'\gamma} \\
&\qquad + T2^{2j(1-\gamma)} \sum_{c \leq 2^{j'-j} < (2^{2j}T)^{-\frac{1}{2}}} 2^{2(j'-j)(1-2\gamma)}\Bigg) \\
&\leq \|u\|_{E_T^\gamma}\|v\|_{E_T^\gamma}\Bigg(T^\gamma + T2^{2j(1-\gamma)} \sum_{c \leq 2^{j'-j} < (2^{2j}T)^{-\frac{1}{2}}} 2^{2(j'-j)(1-2\gamma)}\Bigg).
\end{aligned}$$

Once it is noticed that

$$T2^{2j(1-\gamma)} \sum_{c\leq 2^{j'-j}<(2^{2j}T)^{-\frac{1}{2}}} 2^{2(j'-j)(1-2\gamma)} \leq \mathbf{1}_{\{2^{2j}T\leq C\}}(T2^{2j})^{\gamma}2^{-2j\gamma} \lesssim T^{\gamma},$$

the estimate (7) is proved and Theorem 1.3 follows. □

3. Proof of Theorem 1.4

As the solutions given by the Fujita and Kato theorem [1964] and the Koch and Tataru theorem [2001] are unique in their own class, they are unique in the intersection and thus coincide as long as the Fujita–Kato solution exists. Thus Theorem 1.4 is a question of propagation of regularity, which is provided by the following lemma (which proves the theorem).

Lemma 3.1. *A constant c_0 exists which satisfies the following. Let u be a regular solution of* (GNS) *on* $[0,T[$ *associated with a regular initial data u_0 such that*

$$\|u\|_{\mathrm{K}} \stackrel{\mathrm{def}}{=} \sup_{t\in[0,T[} t^{\frac{1}{2}}\|u(t)\|_{L^\infty} \leq c_0\,.$$

Then $T^\star(u_0) > T$.

Proof. The proof is based on a paralinearization argument (see [Chemin 1999]). Observe that for any T less than $T^\star(u_0)$, u is a solution on $[0,T[$ of the *linear* equation

$$\text{(PGNS)} \qquad \begin{aligned} \partial_t v - \Delta v + \mathcal{Q}(u,v) &= 0,\\ v_{|t=0} &= u_0, \end{aligned}$$

$$\text{with} \quad \mathcal{Q}(u,v) \stackrel{\mathrm{def}}{=} \sum_{j\in\mathbb{Z}} Q(S_{j+1}u,\Delta_j v) + \sum_{j\in\mathbb{Z}} Q(\Delta_j v, S_j u).$$

In the same spirit as (6), let us define $\mathrm{PB}(u,v)$ by

$$\partial_t \mathrm{PB}(u,v) - \Delta \mathrm{PB}(u,v) = -\mathcal{Q}(u,v) \quad \text{and} \quad \mathrm{PB}(u,v)|_{t=0} = 0. \tag{9}$$

A solution of (PGNS) is a solution of

$$v = u_{\mathrm{L}} + \mathrm{PB}(u,v).$$

Let us introduce the space F_T of continuous functions with values in $\dot H^{\frac{1}{2}}$, which are elements of $L^4([0,T];\dot H^1)$, equipped with the norm

$$\|v\|_{F_T} \stackrel{\mathrm{def}}{=} \Big(\sum_{j\in\mathbb{Z}} 2^j \|\Delta_j v\|^2_{L^\infty([0,T[;L^2)}\Big)^{\frac{1}{2}} + \|v\|_{L^4([0,T[;\dot H^1)}.$$

Notice that the first part of the norm was introduced in [Chemin and Lerner 1995] and is a larger norm than the supremum in time of the $\dot H^{\frac12}$ norm. Moreover it holds that

$$\|u_{\rm L}\|_{F_T} \lesssim \|u_0\|_{\dot H^{\frac12}}.$$

Let us temporarily assume the following inequality:

$$\|{\rm PB}(u,v)\|_{F_T} \lesssim \|u\|_{\rm K}\|v\|_{F_T}\,. \tag{10}$$

Then it is obvious that if $\|u\|_{\rm K}$ is small enough for some time $[0,T[$, the linear equation (PGNS) has a unique solution in F_T (in the distribution sense) which satisfies in particular, if c_0 is small enough,

$$\|v\|_{F_T} \le C\|u_0\|_{\dot H^{\frac12}} + \tfrac12\|v\|_{F_T}.$$

As u is a regular solution of (PGNS), it therefore satisfies

$$\forall t<T,\quad \|u\|_{L^4([0,t];\dot H^1)} \le 2C\|u_0\|_{\dot H^{\frac12}},$$

which implies that $T^\star(u_0)>T$, so the lemma is proved provided we prove inequality (10).

Let us observe that for any j in $\mathbb{Z}$,

$$\partial_t\Delta_j{\rm PB}(u,v)-\Delta\Delta_j{\rm PB}(u,v) = -\Delta_j\,\mathcal{Q}(u,v)\,. \tag{11}$$

By definition of $\mathcal{Q}$, we have

$$\begin{aligned}&\big\|\Delta_j\,\mathcal{Q}(u,v)(t)\|_{L^2}\\ &\le\sum_{j'\in\mathbb{Z}}\ \sum_{1\le i,k,\ell\le 3}\big(\|\Delta_j A^i_{k,\ell}(D)(S_{j'+1}u\Delta_{j'}v)\|_{L^2}+\|\Delta_j A^i_{k,\ell}(D)(\Delta_{j'}vS_{j'}u)\|_{L^2}\big).\end{aligned}$$

As the $A^i_{k,\ell}(D)$ are smooth homogeneous Fourier multipliers of order 1, we infer that for some fixed nonnegative integer N_0

$$\begin{aligned}&\|\Delta_j\,\mathcal{Q}(u,v)(t)\|_{L^2}\\ &\qquad\lesssim 2^j\sum_{j'\ge j-N_0}\big(\|S_{j'+1}u(t)\Delta_{j'}v(t)\|_{L^2}+\|\Delta_{j'}v(t)S_{j'}u(t)\|_{L^2}\big)\\ &\qquad\lesssim 2^j\sum_{j'\ge j-N_0}\big(\|S_{j'+1}u(t)\|_{L^\infty}\|\Delta_{j'}v(t)\|_{L^2}+\|\Delta_{j'}v(t)\|_{L^2}\|S_{j'}u(t)\|_{L^\infty}\big)\\ &\qquad\lesssim 2^j\|u(t)\|_{L^\infty}\sum_{j'\ge j-N_0}\|\Delta_{j'}v(t)\|_{L^2}.\end{aligned}$$

Using relation (11) and the definition of the norm on F_T, we infer that

$$\begin{aligned}\|\Delta_j \mathrm{PB}(u,v)(t)\|_{L^2} &\leq \int_0^t e^{-c2^{2j}(t-t')}\|\Delta_j \mathcal{Q}(u,v)(t')\|_{L^2}\,dt'\\ &\lesssim 2^j \int_0^t e^{-c2^{2j}(t-t')}\|u(t')\|_{L^\infty} \sum_{j'\geq j-N_0} \|\Delta_{j'} v(t')\|_{L^2}\,dt'\\ &\lesssim 2^j \|u\|_{\mathrm{K}}\|v\|_{F_T} \sum_{j'\geq j-N_0} c_{j'} 2^{-\frac{j'}{2}} \int_0^t e^{-c2^{2j}(t-t')}\frac{1}{\sqrt{t'}}\,dt',\end{aligned}$$

where $(c_j)_{j\in\mathbb{Z}}$ denotes a generic element of the sphere of $\ell^2(\mathbb{Z})$. Thus we have, for all t less than T,

$$2^{\frac{j}{2}}\|\Delta_j \mathrm{PB}(u,v)(t)\|_{L^2} \lesssim \|u\|_{\mathrm{K}}\|v\|_{F_T} \sum_{j'\geq j-N_0} c_{j'} 2^{-\frac{j'-j}{2}} \int_0^t 2^j e^{-c2^{2j}(t-t')}\frac{1}{\sqrt{t'}}\,dt'.$$

Thanks to Young's inequality, we have $\displaystyle\sum_{j'\geq j-N_0} c_{j'} 2^{-\frac{j'-j}{2}} \lesssim c_j$ and we deduce that

$$2^{\frac{j}{2}}\|\Delta_j \mathrm{PB}(u,v)(t)\|_{L^2} \lesssim c_j \|u\|_{\mathrm{K}}\|v\|_{F_T} \int_0^t 2^j e^{-c2^{2j}(t-t')}\frac{1}{\sqrt{t'}}\,dt'. \tag{12}$$

As we have

$$\int_0^t 2^j e^{-c2^{2j}(t-t')}\frac{1}{\sqrt{t'}}\,dt' \lesssim \int_0^t \frac{1}{\sqrt{t-t'}}\frac{1}{\sqrt{t'}}\,dt',$$

we infer finally that

$$\sum_{j\in\mathbb{Z}} 2^j \|\Delta_j \mathrm{PB}(u,v)\|^2_{L^\infty([0,T];L^2)} \lesssim \|u\|^2_{\mathrm{K}}\|v\|^2_{F_T}. \tag{13}$$

Moreover returning to inequality (12), we have

$$2^j\|\Delta_j \mathrm{PB}(u,v)\|_{L^4([0,T];L^2)} \lesssim c_j \|u\|_{\mathrm{K}}\|v\|_{F_T} \left\| \int_0^t 2^{\frac{3j}{2}} e^{-c2^{2j}(t-t')}\frac{1}{\sqrt{t'}}\,dt'\right\|_{L^4(\mathbb{R}^+)}.$$

The Hardy–Littlewood–Sobolev inequality implies that

$$\left\| \int_0^t 2^{\frac{3j}{2}} e^{-c2^{2j}(t-t')}\frac{1}{\sqrt{t'}}\,dt'\right\|_{L^4(\mathbb{R}^+)} \lesssim 1.$$

Since thanks to the Minkowski inequality we have

$$\|\mathrm{PB}(u,v)\|^2_{L^4([0,T];\dot H^1)} \leq \sum_{j\in\mathbb{Z}} 2^{2j}\|\Delta_j \mathrm{PB}(u,v)\|^2_{L^4([0,T];L^2)},$$

and together with inequality (13) this concludes the proof of inequality (10) and thus the proof of Lemma 3.1. □

4. Proof of Theorem 1.6

The plan of the proof of Theorem 1.6 is the following: as previously we look for the solution of (NS) in the form

$$u = u_{\mathrm{L}} + w,$$

where we recall that $u_{\mathrm{L}}(t) = e^{t\Delta}u_0$. Moreover we recall that the solution u satisfies the energy inequality (4). By construction, the fluctuation w satisfies

$$\text{(NSF)}\quad \partial_t w - \Delta w + (u_{\mathrm{L}} + w)\cdot\nabla w + w\cdot\nabla u_{\mathrm{L}} = -u_{\mathrm{L}}\cdot\nabla u_{\mathrm{L}} - \nabla p, \quad \operatorname{div} w = 0.$$

Let us prove that the life span of w satisfies the lower bound (5). The first step of the proof consists in proving Proposition 1.5, stated in the introduction. This is achieved in Section 4A. The next step is the proof of a similar energy estimate on $\partial_3 w$ — that contrary to the scaled energy estimate of Proposition 1.5, the next result is useful in general only locally in time. It is proved in Section 4B.

Proposition 4.1. *With the notation of Proposition 1.5 and Theorem 1.6, the fluctuation w satisfies the following estimate*:

$$\mathcal{E}(\partial_3 w)(t) \lesssim \biggl(Q_{\mathrm{L}}^0 \biggl(t^{\frac12} \sup_{t'\in(0,t)} \|\partial_3 w(t)\|_{L^2}^4 + \|\partial_3 u_0\|^2_{\dot B^{-\frac32}_{\infty,\infty}} \biggr) + \sqrt{Q_{\mathrm{L}}^0 Q_{\mathrm{L}}^1} \biggr) \exp(2\|u_0\|^2_{\dot B^{-1}_{\infty,2}}).$$

Combining both propositions, one can conclude the proof of Theorem 1.6. This is performed in Section 4C.

4A. ***The rescaled energy estimate on the fluctuation: proof of Proposition 1.5.*** An L^2 energy estimate on (NSF) gives

$$\frac12 \frac{d}{dt}\|w(t)\|_{L^2}^2 + \|\nabla w(t)\|_{L^2}^2 = -\sum_{1\le j,k\le 3} \int_{\mathbb{R}^3} w^j \partial_j u_{\mathrm{L}}^k w^k(t,x)\,dx - \bigl(\mathbb{P}(u_{\mathrm{L}}\cdot\nabla u_{\mathrm{L}})|w\bigr)(t)\,.$$

From this, after an integration by parts and using the fact that the divergence of w is zero, we infer that

$$\frac12\frac{d}{dt}\biggl(\frac{\|w(t)\|_{L^2}^2}{t^{\frac12}}\biggr) + \frac{\|w(t)\|_{L^2}^2}{2t^{\frac32}} + \frac{\|\nabla w(t)\|_{L^2}^2}{t^{\frac12}} \le \frac{\|w(t)\|_{L^2}\|u_{\mathrm{L}}(t)\|_{L^\infty}\|\nabla w(t)\|_{L^2}}{t^{\frac12}} + \frac{\|\mathbb{P}(u_{\mathrm{L}}\cdot\nabla u_{\mathrm{L}})(t)\|_{L^2}\|w(t)\|_{L^2}}{t^{\frac12}}\,.$$

Let us observe that

$$\frac{\|\mathbb{P}(u_{\mathrm{L}}\cdot\nabla u_{\mathrm{L}})(t)\|_{L^2}\|w(t)\|_{L^2}}{t^{\frac12}} = t^{\frac14}\|\mathbb{P}(u_{\mathrm{L}}\cdot\nabla u_{\mathrm{L}})(t)\|_{L^2}\frac{\|w(t)\|_{L^2}}{t^{\frac34}}\,.$$

Using a convexity inequality, we infer that

$$\frac{d}{dt}\Big(\frac{\|w(t)\|_{L^2}^2}{t^{\frac12}}\Big)+\frac{\|w(t)\|_{L^2}^2}{2t^{\frac32}}+\frac{\|\nabla w(t)\|_{L^2}^2}{t^{\frac12}} \leq \frac{\|w(t)\|_{L^2}^2\|u_{\rm L}(t)\|_{L^\infty}^2}{t^{\frac12}}+t^{\frac12}\|u_{\rm L}(t)\cdot\nabla u_{\rm L}(t)\|_{L^2}^2.$$

Thus we deduce that

$$\begin{aligned}\frac{d}{dt}\Big(\frac{\|w(t)\|_{L^2}^2}{t^{\frac12}}\exp\Big(-\int_0^t\|u_{\rm L}(t')\|_{L^\infty}^2\,dt'\Big)\Big)&\\ +\exp\Big(-\int_0^t\|u_{\rm L}(t')\|_{L^\infty}^2\,dt'\Big)\Big(\frac{\|w(t)\|_{L^2}^2}{2t^{\frac32}}+\frac{\|\nabla w(t)\|_{L^2}^2}{t^{\frac12}}\Big)&\\ \leq \exp\Big(-\int_0^t\|u_{\rm L}(t')\|_{L^\infty}^2\,dt'\Big)t^{\frac12}\|\mathbb{P}(u_{\rm L}\cdot\nabla u_{\rm L})(t)\|_{L^2}^2,&\end{aligned}$$

from which we infer by the definition of the $\dot B^{-1}_{\infty,2}$ norm and of $Q^0_{\rm L}$ that

$$\forall t\geq 0,\quad \frac{\|w(t)\|_{L^2}^2}{t^{\frac12}}+\int_0^t\Big(\frac{\|w(t')\|_{L^2}^2}{2t'^{\frac32}}+\frac{\|\nabla w(t)\|_{L^2}^2}{t'^{\frac12}}\Big)dt'\leq Q^0_{\rm L}\exp\|u_0\|^2_{\dot B^{-1}_{\infty,2}}. \tag{14}$$

Proposition 1.5 follows. □

4B. ***Proof of Proposition 4.1.*** Now let us investigate the evolution of $\partial_3 w$ in L^2. Applying the partial differentiation ∂_3 to (NSF), we get

$$\begin{aligned}\partial_t\partial_3 w-\Delta\partial_3 w+(u_{\rm L}+w)\cdot\nabla\partial_3 w+\partial_3 w\cdot\nabla u_{\rm L}&\\ =-\partial_3 u_{\rm L}\cdot\nabla w-\partial_3 w\cdot\nabla w-w\cdot\nabla\partial_3 u_{\rm L}-\partial_3(u_{\rm L}\cdot\nabla u_{\rm L})-\nabla\partial_3 p.&\end{aligned} \tag{15}$$

The difficult terms to estimate are those which do not contain explicitly $\partial_3 w$. So let us define

$$(a)\stackrel{\rm def}{=}-\big(\partial_3 u_{\rm L}\cdot\nabla w|\partial_3 w\big)_{L^2},\quad (b)\stackrel{\rm def}{=}-\big(w\cdot\nabla\partial_3 u_{\rm L}|\partial_3 w\big)_{L^2},$$
$$(c)\stackrel{\rm def}{=}-\big(\partial_3(u_{\rm L}\cdot\nabla u_{\rm L})|\partial_3 w\big)_{L^2}.$$

The third term is the easiest. By integration by parts and using the Cauchy–Schwarz inequality along with (14) we have

$$\begin{aligned}\Big|\int_0^\infty(c)(t)\,dt\Big|&=\Big|\int_0^\infty\int_{\mathbb{R}^3}\partial_3^2\big(\mathbb{P}(u_{\rm L}\cdot\nabla u_{\rm L})(t,x)\big)\cdot w(t,x)\,dx\,dt\Big|\\ &\leq\Big(\int_0^\infty t^{\frac32}\big\|\partial_3^2\mathbb{P}(u_{\rm L}\cdot\nabla u_{\rm L})(t)\big\|_{L^2}^2\,dt\Big)^{\frac12}\Big(\int_0^\infty\frac{\|w(t)\|_{L^2}^2}{t^{\frac32}}\,dt\Big)^{\frac12}\\ &\leq\sqrt{Q^0_{\rm L}Q^1_{\rm L}}\exp\big(\tfrac12\|u_0\|^2_{\dot B^{-1}_{\infty,2}}\big).\end{aligned}$$

Now let us estimate the contribution of (a) and (b). By integration by parts, we get, thanks to the divergence free condition on u_{L},

$$(a) = \big(\partial_3 u_{\mathrm{L}} \otimes w | \nabla \partial_3 w\big)_{L^2} \quad \text{and} \quad (b) = \big(w \otimes \partial_3 u_{\mathrm{L}} | \nabla \partial_3 w\big)_{L^2}.$$

The two terms can be estimated exactly in the same way since they are both of the form

$$\int_{\mathbb{R}^3} w(t,x) \partial_3 u_{\mathrm{L}}(t,x) \nabla \partial_3 w(t,x)\, dx.$$

We have

$$\begin{aligned}\left|\int_{\mathbb{R}^3} w(t,x) \partial_3 u_{\mathrm{L}}(t,x) \nabla \partial_3 w(t,x)\, dx\right| &\\ &\leq \|w(t)\|_{L^2} \|\partial_3 u_{\mathrm{L}}(t)\|_{L^\infty} \|\nabla \partial_3 w\|_{L^2}\\ &\leq \tfrac{1}{100} \|\nabla \partial_3 w\|_{L^2}^2 + 100 \|w(t)\|_{L^2}^2 \|\partial_3 u_{\mathrm{L}}(t)\|_{L^\infty}^2.\end{aligned}$$

The first term will be absorbed by the Laplacian. The second term can be understood as a source term. By time integration, we get indeed

$$\begin{aligned}\int_0^T \|w(t)\|_{L^2}^2 \|\partial_3 u_{\mathrm{L}}(t)\|_{L^\infty}^2\, dt &\leq \int_0^T \frac{\|w(t)\|_{L^2}^2}{t^{\frac{3}{2}}} \big(t^{\frac{3}{4}} \|\partial_3 u_{\mathrm{L}}(t)\|_{L^\infty}\big)^2\, dt\\ &\leq \|\partial_3 u_0\|_{\dot{B}^{-\frac{3}{2}}_{\infty,\infty}}^2 \int_0^\infty \frac{\|w(t)\|_{L^2}^2}{t^{\frac{3}{2}}}\, dt,\end{aligned}$$

so it follows, thanks to Proposition 1.5, that

$$\begin{aligned}\int_0^T \int_{\mathbb{R}^3} w(t,x) \partial_3 u_{\mathrm{L}}(t,x) \nabla \partial_3 w(t,x)\, dx\, dt &\\ &\leq \tfrac{1}{100} \int_0^T \|\nabla \partial_3 w(t)\|_{L^2}^2\, dt + C \|\partial_3 u_0\|_{\dot{B}^{-\frac{3}{2}}_{\infty,\infty}}^2 \mathcal{Q}_{\mathrm{L}}^0 \exp \|u_0\|_{\dot{B}^{-1}_{\infty,2}}^2.\end{aligned}$$

The contribution of the quadratic term in (15) is estimated as follows: Writing, for any function a,

$$\|a\|_{L^p_{\mathrm{h}} L^q_{\mathrm{v}}} \stackrel{\text{def}}{=} \left(\int \|a(x_1,x_2,\cdot)\|_{L^q(\mathbb{R})}^p\, dx_1\, dx_2\right)^{\frac{1}{p}},$$

we have by Hölder's inequality

$$\begin{aligned}\left|\int_{\mathbb{R}^3} \partial_3 w(t,x) \cdot \nabla w(t,x) \partial_3 w(t,x)\, dx\right| &\\ &\leq \|\partial_3 w(t)\|_{L^2_{\mathrm{v}} L^4_{\mathrm{h}}}^2 \|\nabla w\|_{L^\infty_{\mathrm{v}} L^2_{\mathrm{h}}}\\ &\leq \|\partial_3 w(t)\|_{L^2} \|\nabla_{\mathrm{h}} \partial_3 w(t)\|_{L^2} \|\nabla w(t)\|_{L^2}^{\frac{1}{2}} \|\nabla \partial_3 w(t)\|_{L^2}^{\frac{1}{2}},\end{aligned}$$

where we have used the inequalities

$$\|a\|_{L^\infty_{\rm v}L^2_{\rm h}} \lesssim \|\partial_3 a\|_{L^2}^{\frac12}\|a\|_{L^2}^{\frac12} \quad \text{and} \quad \|a\|_{L^2_{\rm v}L^4_{\rm h}} \lesssim \|a\|_{L^2}^{\frac12}\|\nabla_{\rm h} a\|_{L^2}^{\frac12} \tag{16}$$

with $\nabla_{\rm h} \stackrel{\rm def}{=} (\partial_1, \partial_2)$. The first inequality comes from

$$\begin{aligned}\|a(\cdot, x_3)\|_{L^2_{\rm h}}^2 &= \tfrac12 \int_{-\infty}^{x_3} \big(\partial_3 a(\cdot\,, z)|a(\cdot\,, z)\big)_{L^2_{\rm h}}\, dz \\ &\leq \tfrac12 \int_{\mathbb{R}} \|\partial_3 a(\cdot\,, z)\|_{L^2_{\rm h}} \|a(\cdot\,, z)\|_{L^2_{\rm h}}\, dz \\ &\leq \|\partial_3 a\|_{L^2}\|a\|_{L^2},\end{aligned}$$

while the second simply comes from the embedding $\dot H^{\frac12}_{\rm h} \subset L^4_{\rm h}$ and an interpolation. By Young's inequality it follows that

$$\begin{aligned}&\left|\int_{\mathbb{R}^3} \partial_3 w(t,x)\cdot\nabla w(t,x)\partial_3 w(t,x)\, dx\right| \\ &\qquad\leq \tfrac{1}{100}\|\nabla\partial_3 w\|_{L^2}^2 + C\|\nabla w(t)\|_{L^2}^2\|\partial_3 w(t)\|_{L^2}^4 \\ &\qquad\leq \tfrac{1}{100}\|\nabla\partial_3 w(t)\|_{L^2}^2 + \Big(\sup_{t'\in[0,t]}\|\partial_3 w(t')\|_{L^2}^4\Big) t^{\frac12}\frac{\|\nabla w(t)\|_{L^2}^2}{t^{\frac12}},\end{aligned}$$

from which we infer by Proposition 1.5 that

$$\begin{aligned}&\left|\int_{\mathbb{R}^3} \partial_3 w(t,x)\cdot\nabla w(t,x)\partial_3 w(t,x)\, dx\right| \\ &\qquad\leq \tfrac{1}{100}\|\nabla\partial_3 w(t)\|_{L^2}^2 + \Big(\sup_{t'\in[0,t]}\|\partial_3 w(t')\|_{L^2}^4\Big) t^{\frac12} Q^0_{\rm L} \exp\|u_0\|^2_{\dot B^{-1}_{\infty,2}}.\end{aligned}$$

Finally, after an integration by parts we find

$$\begin{aligned}&\int_{\mathbb{R}^3} \partial_3 w(t,x)\cdot\nabla u_{\rm L}(t,x)\partial_3 w(t,x)\, dx \\ &\qquad\leq \|\partial_3 w(t)\|_{L^2}\|u_{\rm L}(t)\|_{L^\infty}\|\nabla\partial_3 w(t)\|_{L^2} \\ &\qquad\leq \tfrac{1}{100}\|\nabla\partial_3 w(t)\|_{L^2}^2 + C\|\partial_3 w(t)\|_{L^2}^2\|u_{\rm L}(t)\|_{L^\infty}^2,\end{aligned}$$

so plugging all these estimates together we infer thanks to Gronwall's inequality that

$$\begin{aligned}&\sup_{t\in[0,T]}\|\partial_3 w(t)\|_{L^2}^2 + \int_0^T \|\nabla\partial_3 w(t)\|_{L^2}^2\, dt \\ &\lesssim \Big(T^{\frac12} Q^0_{\rm L} \sup_{t'\in[0,t]}\|\partial_3 w(t')\|_{L^2}^4 + \|\partial_3 u_0\|^2_{\dot B^{-\frac32}_{\infty,\infty}} Q^0_{\rm L} + \sqrt{Q^0_{\rm L} Q^1_{\rm L}}\Big)\exp\big(2\|u_0\|^2_{\dot B^{-1}_{\infty,2}}\big).\end{aligned}$$

Proposition 4.1 is proved. □

4C. *End of the proof of Theorem 1.6.*

4C1. *Control of the fluctuation.* To make notation lighter let us set

$$M_{\mathrm{L}} \stackrel{\text{def}}{=} \big(\|\partial_3 u_0\|^2_{\dot{B}^{-\frac{3}{2}}_{\infty,\infty}} Q^0_{\mathrm{L}} + \sqrt{Q^0_{\mathrm{L}} Q^1_{\mathrm{L}}}\big) \exp(2\|u_0\|^2_{\dot{B}^{-1}_{\infty,2}}).$$

Proposition 4.1 provides the existence of a constant K such that the following a priori estimate holds

$$\sup_{t\in[0,T]} \|\partial_3 w(t)\|^2_{L^2} + \int_0^T \|\nabla\partial_3 w(t)\|^2_{L^2}\,dt \\ \leq K T^{\frac{1}{2}} Q^0_{\mathrm{L}} \sup_{t\in[0,T]} \|\partial_3 w(t)\|^4_{L^2} \exp(2\|u_0\|^2_{\dot{B}^{-1}_{\infty,2}}) + K M_{\mathrm{L}}.$$

Let T^* be the maximal time of existence of u, hence of w, and recalling that $w(t=0)=0$, set T_1 to be the maximal time T for which

$$\sup_{t\in[0,T]} \|\partial_3 w(t)\|^2_{L^2} \leq 2KM_{\mathrm{L}}.$$

Then on $[0, T_1]$ it holds that

$$\sup_{t\in[0,T]} \|\partial_3 w(t)\|^2_{L^2} + \int_0^T \|\nabla\partial_3 w(t)\|^2_{L^2}\,dt \leq 4K^3 T_1^{\frac{1}{2}} Q^0_{\mathrm{L}} M^2_{\mathrm{L}} + KM_{\mathrm{L}} \\ \leq KM_L\big(1 + 4K^2 T_1^{\frac{1}{2}} Q^0_{\mathrm{L}} M_{\mathrm{L}}\big).$$

This implies that

$$T_1 \geq T_* \quad \text{with} \quad T_* \stackrel{\text{def}}{=} \left(\frac{1}{8K^2 Q^0_{\mathrm{L}} M_{\mathrm{L}}}\right)^2,$$

and on $[0, T_*]$ it holds that

$$\sup_{t\in[0,T]} \|\partial_3 w(t)\|^2_{L^2} + \int_0^T \|\nabla\partial_3 w(t)\|^2_{L^2}\,dt \leq \tfrac{3}{2} K M_{\mathrm{L}}. \tag{17}$$

4C2. *End of the proof of the theorem.* Under the assumptions of Theorem 1.6 we know that there exists a unique solution u to (NS) on some time interval $[0, T^*[$, which satisfies the energy estimate. Let us prove that this time interval contains $[0, T_*]$. Since the initial data u_0 belongs to L^2, we may assume that u is a global Leray solution, meaning that

$$\forall t \geq 0, \quad \mathcal{E}(u(t)) \leq \tfrac{1}{2}\|u_0\|^2_{L^2}. \tag{18}$$

Moreover one clearly has

$$\sup_{t\geq 0} \|\partial_3 u_{\mathrm{L}}(t)\|^2_{L^2} + \int_0^\infty \|\nabla\partial_3 u_{\mathrm{L}}(t)\|^2_{L^2}\,dt \leq \|\partial_3 u_0\|^2_{L^2},$$

so together with (17) this implies that on $[0, T_*]$,

$$\sup_{t\in[0,T]} \|\partial_3 w(t)\|_{L^2}^2 + \int_0^T \|\nabla\partial_3 u(t)\|_{L^2}^2\,dt \lesssim \|\partial_3 u_0\|_{L^2}^2 + M_{\mathrm{L}}. \tag{19}$$

Let us prove that these estimates provide a control on u in $\dot H^1$ on $[0, T_*]$. After differentiation of (NS) with respect to the horizontal variables and an energy estimate, we get for any ℓ in $\{1, 2\}$ and after an integration by parts

$$\begin{aligned}\frac12\frac{d}{dt}\|\partial_\ell u(t)\|_{L^2}^2 + \|\nabla\partial_\ell u(t)\|_{L^2}^2 &= -\int_{\mathbb{R}^3} \partial_\ell(u\cdot\nabla u)\cdot\partial_\ell u\,(t,x)\,dx\\ &\le \|u\|_{L^\infty_{\mathrm{v}}L^4_{\mathrm{h}}}\|\nabla u(t)\|_{L^2_{\mathrm{v}}L^4_{\mathrm{h}}}\|\partial_\ell^2 u(t)\|_{L^2}.\end{aligned}$$

Similarly to (16) we have

$$\|u\|_{L^\infty_{\mathrm{v}}L^4_{\mathrm{h}}}^2 \lesssim \|u\|^2_{L^\infty_{\mathrm{v}}\dot H_{\mathrm{h}}^{\frac12}} \lesssim \int_{-\infty}^{x_3} \big(\partial_3 u(\cdot,z)|u(\cdot,z)\big)_{\dot H_{\mathrm{h}}^{\frac12}}\,dz \lesssim \|\partial_3 u\|_{L^2}\|\nabla_{\mathrm{h}} u\|_{L^2},$$

so using (16) we infer that

$$\begin{aligned}&\left|\int_{\mathbb{R}^3} \partial_\ell(u\cdot\nabla u)\cdot\partial_\ell u(t,x)\,dx\right|\\ &\qquad\le C\|\partial_3 u(t)\|_{L^2}^{\frac12}\|\nabla_{\mathrm{h}} u(t)\|_{L^2}^{\frac12}\|\nabla u(t)\|_{L^2}^{\frac12}\|\nabla\nabla_{\mathrm{h}} u(t)\|_{L^2}^{\frac12}\|\partial_\ell^2 u(t)\|_{L^2}\\ &\qquad\le \tfrac{1}{100}\|\nabla\nabla_{\mathrm{h}} u(t)\|_{L^2}^2 + C\|\partial_3 u\|_{L^2}^2\|\nabla_{\mathrm{h}} u\|_{L^2}^2\|\nabla u(t)\|_{L^2}^2.\end{aligned}$$

We obtain

$$\frac{d}{dt}\|\nabla_{\mathrm{h}} u(t)\|_{L^2}^2 + \|\nabla\nabla_{\mathrm{h}} u(t)\|_{L^2}^2 \lesssim \|\partial_3 u\|_{L^2}^2\|\nabla_{\mathrm{h}} u\|_{L^2}^2\|\nabla u(t)\|_{L^2}^2,$$

and Gronwall's inequality implies that

$$\begin{aligned}&\|\nabla_{\mathrm{h}} u(t)\|_{L^2}^2 + \int_0^t \|\nabla\nabla_{\mathrm{h}} u(t')\|_{L^2}^2\,dt'\\ &\qquad\le \|\nabla_{\mathrm{h}} u_0\|_{L^2}^2 \exp\Big(\int_0^t \|\partial_3 u(t')\|_{L^2}^2\|\nabla u(t')\|_{L^2}^2 dt'\Big).\end{aligned}$$

The fact that we control $\|\nabla u\|_{L^2_t(L^2_x)}$ and $\|\partial_3 u\|_{L^\infty_t(L^2_x)}$ thanks to (18) and (19) implies that on $[0, T_*]$ we have

$$\sup_{t\in[0,T]} \|\nabla u(t)\|_{L^2}^2 + \int_0^T \|\nabla^2 u(t)\|_{L^2}^2\,dt \le \|\nabla u_0\|_{L^2}^2 \exp\big(\|u_0\|_{L^2}(KM_{\mathrm{L}})^{\frac12}\big).$$

This means that there is a unique, smooth solution at least on $[0, T_*]$, completing the proof of Theorem 1.6. □

5. Comparison of both life spans: proof of Theorem 1.7

Let us introduce the notation

$$f_\varepsilon(x_1,x_2,x_3) \stackrel{\text{def}}{=} \cos\Big(\frac{x_1}{\varepsilon}\Big) f\Big(x_1,\frac{x_2}{\varepsilon^\alpha},x_3\Big),$$

where ε is a given number, assumed to be small, and α is a fixed parameter in the open interval $]0,1[$. We assume the initial data is given by the following expression

$$u_{0,\varepsilon}(x) = \frac{A_\varepsilon}{\varepsilon}\big(0,\varepsilon^\alpha(-\partial_3\phi)_\varepsilon,(\partial_2\phi)_\varepsilon\big), \tag{20}$$

where ϕ is a smooth compactly supported function and the parameter $A_\varepsilon \gg 1$ will be tuned later.

Let us recall that Lemma 3.1 of [Chemin and Gallagher 2009] claims in particular that

$$\forall \sigma>0,\quad \|f_\varepsilon\|_{\dot B^{-\sigma}_{p,1}} \le C_\sigma \varepsilon^{\sigma+\frac{\alpha}{p}} \quad\text{and}\quad \|f_\varepsilon\|_{\dot B^{-\sigma}_{\infty,\infty}} \ge c_\sigma\varepsilon^{\sigma}. \tag{21}$$

This implies that

$$\begin{gathered}\|u_{0,\varepsilon}\|_{\dot B^{-1+2\gamma}_{\infty,\infty}} \lesssim A_\varepsilon \varepsilon^{-2\gamma},\quad \|u_{0,\varepsilon}\|_{\dot B^{-1}_{\infty,\infty}} \sim \|u_{0,\varepsilon}\|_{\dot B^{-1}_{\infty,2}} \sim A_\varepsilon,\\ \text{and}\quad \|\partial_3 u_{0,\varepsilon}\|_{\dot B^{-\frac{3}{2}}_{\infty,\infty}} \lesssim A_\varepsilon \varepsilon^{\frac12}.\end{gathered} \tag{22}$$

With the notation of Theorem 1.3 it therefore holds that

$$T_{\mathrm{FP}}(u_{0,\varepsilon}) \ge C\varepsilon^2 A_\varepsilon^{-\frac{1}{\gamma}}.$$

Let us now compute $T_{\mathrm{L}}(u_{0,\varepsilon})$. Recalling that $u_{\mathrm{L}}(t) = e^{t\Delta}u_{0,\varepsilon}$, we can write

$$\begin{aligned} u^1_L\partial_1 u^1_L + u^2_L\partial_2 u^1_L &= \Big(\frac{A_\varepsilon}{\varepsilon}\Big)^2 e^{t\Delta} f_\varepsilon e^{t\Delta} g_\varepsilon,\\ u^1_L\partial_1 u^2_L + u^2_L\partial_2 u^2_L &= \Big(\frac{A_\varepsilon}{\varepsilon}\Big)^2 e^{t\Delta} \widetilde f_\varepsilon e^{t\Delta} \widetilde g_\varepsilon.\end{aligned}$$

where f, g, $\widetilde f$, $\widetilde g$ are smooth compactly supported functions. Now let us estimate

$$\int_0^\infty t^{\frac12}\big\|e^{t\Delta} f_\varepsilon\, e^{t\Delta} g_\varepsilon\big\|^2_{L^2}\,dt.$$

for f and g given smooth compactly supported functions. We write

$$\begin{aligned}\int_0^\infty t^{\frac12}\|e^{t\Delta} f_\varepsilon e^{t\Delta} g_\varepsilon\|^2_{L^2}\,dt &= \int_0^\infty t^{\frac32}\|e^{t\Delta} f_\varepsilon\, e^{t\Delta} g_\varepsilon\|^2_{L^2}\,\frac{dt}{t}\\ &\le \int_0^\infty (t^{\frac38}\|e^{t\Delta} f_\varepsilon\|_{L^4})^2 (t^{\frac38}\|e^{t\Delta} g_\varepsilon\|)^2_{L^4}\,\frac{dt}{t},\end{aligned}$$

thanks to the Hölder inequality. The Cauchy–Schwarz inequality and the definition of Besov norms imply that

$$\int_0^\infty t^{\frac12}\|e^{t\Delta}f_\varepsilon e^{t\Delta}g_\varepsilon\|_{L^2}^2\,dt \le \Big(\int_0^\infty \big(t^{\frac38}\|e^{t\Delta}f_\varepsilon\|_{L^4}\big)^4\,\frac{dt}{t}\Big)^{\frac12}\Big(\int_0^\infty \big(t^{\frac38}\|e^{t\Delta}g_\varepsilon\|_{L^4}\big)^4\,\frac{dt}{t}\Big)^{\frac12} \le \|f_\varepsilon\|^2_{\dot B^{-\frac34}_{4,4}}\|g_\varepsilon\|^2_{\dot B^{-\frac34}_{4,4}}.$$

It is easy to check that

$$\|f_\varepsilon\|_{\dot B^{-\frac34}_{4,4}} \lesssim \varepsilon^{\frac{3+\alpha}{4}},$$

so it follows (since $\mathbb{P}$ is a homogeneous Fourier multiplier of order 0) that

$$Q_{\mathrm L}^0 \lesssim A_\varepsilon^4\varepsilon^{\alpha-1}. \tag{23}$$

For the initial data (20), differentiations with respect to the vertical variable ∂_3 have no real influence on the term $u_{\mathrm L}(t)\cdot\nabla u_{\mathrm L}(t)$. Indeed, we have

$$\partial_3^2\big(u_{\mathrm L}(t)\cdot\nabla u_{\mathrm L}(t)\big) = \partial_3^2 u_{\mathrm L}(t)\cdot\nabla u_{\mathrm L}(t) + 2\partial_3 u_{\mathrm L}(t)\cdot\partial_3\nabla u_{\mathrm L}(t) + u_{\mathrm L}(t)\cdot\partial_3^2\nabla u_{\mathrm L}(t),$$

and it is then obvious that $\partial_3^2\big(u_{\mathrm L}(t)\cdot\nabla u_{\mathrm L}(t)\big)$ is a sum of term of the type

$$\Big(\frac{A_\varepsilon}{\varepsilon}\Big)^2 e^{t\Delta}f_\varepsilon e^{t\Delta}g_\varepsilon.$$

Then following the lines used to estimate the term Q_L^0, we write

$$\int_0^\infty t^{\frac32}\|e^{t\Delta}f_\varepsilon e^{t\Delta}g_\varepsilon\|_{L^2}^2\,dt \le \Big(\int_0^\infty (t^{\frac58}\|e^{t\Delta}f_\varepsilon\|_{L^4})^4\,\frac{dt}{t}\Big)^{\frac12}\Big(\int_0^\infty (t^{\frac58}\|e^{t\Delta}g_\varepsilon\|_{L^4})^4\,\frac{dt}{t}\Big)^{\frac12} \le \|f_\varepsilon\|^2_{\dot B^{-\frac54}_{4,4}}\|g_\varepsilon\|^2_{\dot B^{-\frac54}_{4,4}}.$$

It is easy to check that

$$\|f_\varepsilon\|_{\dot B^{-\frac54}_{4,4}} \lesssim \varepsilon^{\frac{5+\alpha}{4}},$$

so it follows that

$$Q_{\mathrm L}^1 \lesssim A_\varepsilon^4\varepsilon^{\alpha+1}.$$

Together with (22) and (23), we infer that

$$\begin{aligned}Q^0_{\mathrm{L}}\big(\|\partial_3 u_0\|^2_{\dot B^{-\frac32}_{\infty,\infty}} Q^0_{\mathrm{L}}+\sqrt{Q^0_{\mathrm{L}}Q^1_{\mathrm{L}}}\big)\exp(4\|u_0\|^2_{\dot B^{-1}_{\infty,2}})&\\ &\lesssim A^4_\varepsilon \varepsilon^{\alpha-1}(A^6_\varepsilon\varepsilon^\alpha+A^4_\varepsilon\varepsilon^\alpha)\exp(C_0A^2_\varepsilon)\\ &\lesssim A^{10}_\varepsilon\varepsilon^{2\alpha-1}\exp(C_0A^2_\varepsilon)\end{aligned}$$

because A_ε is larger than 1. Let us choose some κ in $]0,\eta[$ and then

$$A_\varepsilon \overset{\text{def}}{=} \Big(\frac{C_0}{-\kappa\log\varepsilon}\Big)^{\frac12}.$$

Then with the notation of Theorem 1.6 we have

$$T_{\mathrm{L}} = CA_\varepsilon^{-20}\varepsilon^{2(1-2\alpha+\kappa)}.$$

Let us choose κ' in $]\kappa,\eta[$. By definition of A_ε we get that

$$T_L \geq C\varepsilon^{2(1-2\alpha+\kappa')}.$$

Choosing $\alpha = 1-(\eta-\kappa')/4$ concludes the proof of Theorem 1.7. □

Appendix: A Littlewood–Paley toolbox

Let us recall some well-known results on Littlewood–Paley theory (see for instance [Bahouri et al. 2011] for more details).

Definition A.1. Let $\phi\in\mathcal{S}(\mathbb{R}^3)$ be such that $\widehat\phi(\xi)=1$ for $|\xi|\leq 1$ and $\widehat\phi(\xi)=0$ for $|\xi|>2$. We define, for $j\in\mathbb{Z}$, the function $\phi_j(x)\overset{\text{def}}{=}2^{3j}\phi(2^jx)$, and the Littlewood–Paley operators

$$S_j \overset{\text{def}}{=} \phi_j * \cdot \quad\text{and}\quad \Delta_j \overset{\text{def}}{=} S_{j+1}-S_j.$$

Homogeneous Sobolev spaces are defined by the norm

$$\|a\|_{\dot H^s} \overset{\text{def}}{=} \Big(\sum_{j\in\mathbb{Z}} 2^{2js}\|\Delta_j a\|^2_{L^2}\Big)^{\frac12}.$$

This norm is equivalent to

$$\|a\|_{\dot H^s} \sim \Big(\int_{\mathbb{R}^3}|\xi|^{2s}|\mathcal{F}a(\xi)|^2\,d\xi\Big)^{\frac12},$$

where $\mathcal{F}$ is the Fourier transform. Finally let us recall the definition of Besov norms of negative index.

Definition A.2. Let σ be a positive real number and (p,q) in $[1,\infty]^2$. Let us define the homogeneous Besov norm $\|\cdot\|_{\dot B^{-\sigma}_{p,q}}$ by

$$\|a\|_{\dot B^{-\sigma}_{p,q}} = \big\| t^{\frac{\sigma}{2}} \|e^{t\Delta}a\|_{L^p} \big\|_{L^q(\mathbb{R}^+;\frac{dt}{t})}.$$

Let us mention that thanks to the properties of the heat flow, for $p_1 \le p_2$ and $q_1 \le q_2$, we have the following inequality, valid for any regular function a

$$\|a\|_{\dot B^{-\sigma-3(\frac{1}{p_1}-\frac{1}{p_2})}_{p_2,q}} \lesssim \|a\|_{\dot B^{-\sigma}_{p_1,q}} \quad \text{and} \quad \|a\|_{\dot B^{-\sigma}_{p,q_2}} \lesssim \|a\|_{\dot B^{-\sigma}_{p,q_1}}.$$

An equivalent definition using the Littlewood–Paley decomposition is

$$\|a\|_{\dot B^{-\sigma}_{p,q}} \sim \Big(\sum_{j\in\mathbb{Z}} 2^{-j\sigma q}\|\Delta_j a\|^q_{L^p}\Big)^{\frac{1}{q}}.$$

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