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ABSTRACT. By using the pseudo-metric introduced in [F. Golse, T. Paul: Archive for Rational Mech. Anal. **223** (2017) 57–94], which is an analogue of the Wasserstein distance of exponent 2 between a quantum density operator and a classical (phase-space) density, we prove that the convergence of time splitting algorithms for the von Neumann equation of quantum dynamics is uniform in the Planck constant $\hbar$. We obtain explicit uniform in $\hbar$ error estimates for the first order Lie-Trotter, and the second order Strang splitting methods.

1. Introduction

One of the main challenges in quantum dynamics and high frequency waves is that one needs to numerically resolve the small wave length which is computationally prohibitive [1, 7, 16, 14]. When a numerical method is developed one would like to know its mesh strategy, namely, the dependence of the time step and mesh size on the wave length $\hbar$ (for a misuse of notation in this article we will not distinguish the difference between the reduced Planck constant $\hbar$ and the wave length).

Finite difference schemes for the Schrödinger equation typically require both time step and mesh size in the semiclassical regime (i.e. for $\hbar \ll 1$) to be of order $O(\hbar)$ (see [19]), or even $o(\hbar)$. On the other hand, the time splitting spectral method can improve the time step to be of order $O(1)$ if only the physical observables are of interest [2]. An important mathematical object to understand these mesh strategies is the Wigner transform [21], which is a convenient tool to study the semiclassical limit of the Schrödinger equation [8, 18]. In fact, the mesh strategy of $\Delta t = O(1)$, for the time step Δt, of the time-splitting spectral method can only be understood in the Wigner framework, and not in terms of the wave function [2].

Since the solution to the Schrödinger equation is oscillatory with wave length of order $\hbar$, if one uses a standard metric, such as the L^2 or Sobolev norm, one would end up with an numerical error of order $O((\Delta t/\hbar)^m)$ for some integer m which depends on the order of the method. This will not allow one to see an $\hbar$ independent mesh strategy. The argument of an $\hbar$ independent time-step strategy in [2] for the time splitting discretization to the linear Schrödinger equation, which was also useful in establishing a similar mesh strategy for the nonlinear Erhenfest dynamics [6], was made at a formal level without quantifying the numerical error. One would be interested in finding a suitable metric which allows one to establish

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such a mesh strategy at the *rigorous* level. In the present paper, we use the pseudo-metric introduced in [10] to establish a uniform (in $\hbar$) error estimate of the time splitting methods for the von Neumann equation (which describes the evolution of mixed quantum states, and reduces to the Schrödinger equation in the case of pure quantum states [4]) in the semiclassical regime.

Our final results (Theorems 3.1 and 3.2) are stated in terms of the Monge-Kantorovich, or Wasserstein distance of exponent 2 between the Husimi transforms of the density operator and of its numerical approximation. Indeed, quantum particles are expected to become localized on phase-space trajectories in the classical limit. Since Monge-Kantorovich, or Wasserstein distances metrize the weak topology of Borel probability measures on phase-space (see Theorem 7.12 in [20]), they are expected to be the appropriate metrics to compare the phase-space densities of quantum particles in the classical limit. Besides, the Husimi transform is the most natural procedure for associating a classical phase-space probability density to a quantum density operator in a way that is compatible with the classical limit: see for instance Theorem III.1 (1) in [18].

Nevertheless, the definition of the Husimi transform is intimately related to the notion of Schrödinger coherent states (plane waves with Gaussian envelope), and there is some arbitrariness in this choice. Non-Gaussian wave packets can also be used to define generalized Husimi transforms, in terms of which our error analysis can also be formulated, following [11]. To avoid this arbitrariness, we think it useful to have a formulation of our uniform in $\hbar$ error bounds directly in terms of density operators, and not in terms of their Husimi transforms. This formulation is slightly more involved than the one in terms of Husimi transforms, and for this reason, is relegated in Appendix B.

2. A Pseudo-Metric for the Classical Limit

Definition 2.1. *A density operator on* $\mathfrak{H} := L^2(\mathbf{R}^d)$ *is an operator* $R \in \mathcal{L}(\mathfrak{H})$ *such that*

$$R = R^* \geq 0\,, \quad \operatorname{trace}_{\mathfrak{H}}(R) = 1\,.$$

The set of all density operators on $\mathfrak{H}$ *will be denoted by* $\mathcal{D}(\mathfrak{H})$.

In the definition above, the notation $\mathcal{L}(\mathfrak{H})$ designates the algebra of bounded linear operators defined on $\mathfrak{H}$, and $\|T\|$ is the operator norm of $T \in \mathcal{L}(\mathfrak{H})$. Henceforth, we also denote by $\mathcal{L}^p(\mathfrak{H})$ for all $p \geq 1$ the two-sided ideal of $\mathcal{L}(\mathfrak{H})$ whose elements are the operators $T \in \mathcal{L}(\mathfrak{H})$ such that $|T|^p = (T^*T)^{p/2}$ is a trace-class operator on $\mathfrak{H}$. The Schatten norm of exponent p is denoted $\|T\|_p$ for all $T \in \mathcal{L}^p(\mathfrak{H})$. For instance $\mathcal{L}^1(\mathfrak{H})$ and $\mathcal{L}^2(\mathfrak{H})$ are respectively the sets of trace-class and of Hilbert-Schmidt operators on $\mathfrak{H}$, and $\|\cdot\|_1$ and $\|\cdot\|_2$ designate respectively the trace norm and the Hilbert-Schmidt norm. The notation $\operatorname{trace}_{\mathfrak{H}}(T)$ designates the trace of $T \in \mathcal{L}^1(\mathfrak{H})$.

We denote by $\mathcal{D}^2(\mathfrak{H})$ the set of density operators on $\mathfrak{H}$ such that

$$\operatorname{trace}_{\mathfrak{H}}(R^{1/2}(-\hbar^2\Delta_y + |y|^2)R^{1/2}) < \infty\,. \tag{1}$$

If $R \in \mathcal{D}^2(\mathfrak{H})$, one has

$$\operatorname{trace}_{\mathfrak{H}}((-\hbar^2\Delta_y + |y|^2)^{1/2}R(-\hbar^2\Delta_y + |y|^2)^{1/2}) = \operatorname{trace}_{\mathfrak{H}}(R^{1/2}(-\hbar^2\Delta_y + |y|^2)R^{1/2}) < \infty \tag{2}$$

as can be seen from the lemma below (applied to $A = \lambda^2|y|^2 - \hbar^2\Delta_y$ and $T = R$).

Lemma 2.2. *Let $T \in \mathcal{L}(\mathfrak{H})$ satisfy $T = T^* \geq 0$, and let A be an unbounded operator on $\mathfrak{H}$ such that $A = A^* \geq 0$. Then*

$$\operatorname{trace}_{\mathfrak{H}}(T^{1/2}AT^{1/2}) = \operatorname{trace}_{\mathfrak{H}}(A^{1/2}TA^{1/2}) \in [0, +\infty] .$$

Proof. The definition of $T^{1/2}$ and $A^{1/2}$ can be found in Theorem 3.35 in chapter V, §3 of [17], together with the fact that $A^{1/2}$ and $T^{1/2}$ are self-adjoint.

If $\operatorname{trace}_{\mathfrak{H}}(T^{1/2}AT^{1/2}) < \infty$, then $A^{1/2}T^{1/2} \in \mathcal{L}^2(\mathfrak{H})$ and the equality holds by formula (1.26) in chapter X, §1 of [17].

If $\operatorname{trace}_{\mathfrak{H}}(T^{1/2}AT^{1/2}) = \infty$, then $\operatorname{trace}_{\mathfrak{H}}(A^{1/2}TA^{1/2}) = +\infty$, for otherwise $T^{1/2}A^{1/2}$ and its adjoint $A^{1/2}T^{1/2}$ would belong to $\mathcal{L}^2(\mathfrak{H})$, so that $T^{1/2}AT^{1/2} \in \mathcal{L}^1(\mathfrak{H})$, which would be in contradiction with the assumption that $\operatorname{trace}_{\mathfrak{H}}(T^{1/2}AT^{1/2}) = \infty$. □

Definition 2.3. *Let $f \equiv f(x,\xi)$ be a probability density on $\mathbf{R}^{2d}$ and let $R \in \mathcal{D}(\mathfrak{H})$. A coupling of f and R is a measurable operator-valued function $(x,\xi) \mapsto Q(x,\xi)$ such that, for a.e. $(x,\xi) \in \mathbf{R}^d \times \mathbf{R}^d$,*

$$Q(x,\xi) = Q(x,\xi)^* \geq 0 , \quad \operatorname{trace}_{\mathfrak{H}}(Q(x,\xi)) = f(x,\xi) , \quad \iint_{\mathbf{R}^d\times\mathbf{R}^d} Q(x,\xi)dxd\xi = R .$$

The second condition above implies that $Q(x,\xi) \in \mathcal{L}^1(\mathfrak{H})$ for a.e. $(x,\xi) \in \mathbf{R}^d\times\mathbf{R}^d$. Since $\mathcal{L}^1(\mathfrak{H})$ is separable, the notion of strong and weak measurability are equivalent for Q. The set of couplings of f and R is denoted by $\mathcal{C}(f,R)$. Notice that the operator-valued function $(x,\xi) \mapsto f(x,\xi)R$ belongs to $\mathcal{C}(f,R)$.

In [10], one considers the following "pseudometric".

Definition 2.4. *For each probability density f on $\mathbf{R}^d \times \mathbf{R}^d$ satisfying*

$$\iint_{\mathbf{R}^d\times\mathbf{R}^d} (|x|^2 + |\xi|^2) f(x,\xi)dxd\xi < \infty \tag{3}$$

and each $R \in \mathcal{D}^2(\mathfrak{H})$, set

$$E_\hbar(f,R) := \inf_{Q\in\mathcal{C}(f,R)} \left(\iint_{\mathbf{R}^d\times\mathbf{R}^d} \operatorname{trace}_{\mathfrak{H}}(Q(x,\xi)^{1/2} c(x,\xi,y,\hbar D_y) Q(x,\xi)^{1/2}) dxd\xi \right)^{1/2} ,$$

where the quantum transportation cost is the quadratic differential operator in y, parametrized by $(x,\xi) \in \mathbf{R}^d \times \mathbf{R}^d$:

$$c(x,\xi,y,\hbar D_y) := |x-y|^2 + |\xi - \hbar D_y|^2 , \quad D_y := -i\nabla_y .$$

Since $c(x,\xi,y,\hbar D_y) = c(x,\xi,y,\hbar D_y)^* \leq 2(|x|^2 + |\xi|^2) + 2c(0,0,y,\hbar D_y)$, any coupling $Q \in \mathcal{C}(f,R)$ satisfies

$$\begin{aligned} &\operatorname{trace}_{\mathfrak{H}}(Q(x,\xi)^{1/2} c(x,\xi,y,\hbar D_y) Q(x,\xi)^{1/2}) \\ &\leq 2(|x|^2 + |\xi|^2) \operatorname{trace}_{\mathfrak{H}}(Q(x,\xi)) + 2 \operatorname{trace}_{\mathfrak{H}}(Q(x,\xi)^{1/2} c(0,0,y,\hbar D_y) Q(x,\xi)^{1/2}) \\ &= 2(|x|^2 + |\xi|^2) f(x,\xi) + 2 \operatorname{trace}_{\mathfrak{H}}(c(0,0,y,\hbar D_y)^{1/2} Q(x,\xi) c(0,0,y,\hbar D_y)^{1/2}) \end{aligned}$$

for a.e. $(x,\xi) \in \mathbf{R}^d \times \mathbf{R}^d$. Hence

$$\begin{aligned} \iint_{\mathbf{R}^{2d}} \operatorname{trace}_{\mathfrak{H}}(Q(x,\xi)^{\frac12} c(x,\xi,y,\hbar D_y) Q(x,\xi)^{\frac12}) dxd\xi &\leq 2 \iint_{\mathbf{R}^{2d}} (|x|^2 + |\xi|^2) f(x,\xi) dxd\xi \\ &+ 2 \operatorname{trace}_{\mathfrak{H}}(c(0,0,y,\hbar D_y)^{\frac12} R c(0,0,y,\hbar D_y)^{\frac12}) < \infty \end{aligned}$$

by (2) provided that f satisfies (3) and $R\in\mathcal{D}^2(\mathfrak{H})$. This argument uses Lemma 2.2 with $T=Q(x,\xi)$ and $A=c(0,0,y,\hbar D_y)$ before it is known that

$$\operatorname{trace}_{\mathfrak{H}}(Q(x,\xi)^{1/2}c(0,0,y,\hbar D_y)Q(x,\xi)^{1/2})<\infty\qquad\text{for a.e. }(x,\xi)\in\mathbf{R}^d\times\mathbf{R}^d\,.$$

Let $R\in\mathcal{D}(\mathfrak{H})$. The Wigner transform of R is

$$W_\hbar(R)(x,\xi):=\tfrac{1}{(2\pi)^d}\int_{\mathbf{R}^d}r(x+\tfrac12\hbar y,x-\tfrac12\hbar y)e^{-i\xi\cdot y}dy\,,\tag{4}$$

where $r\equiv r(x,y)$ is the integral kernel of R. It is a well known fact that $W_\hbar(R)$ is real-valued (since $R=R^*$). It is also well known that $W_\hbar(R)$ is not necessarily nonnegative a.e. on $\mathbf{R}^d\times\mathbf{R}^d$. For instance, if $r(X,Y)=\psi(X)\overline{\psi(Y)}$ with ψ odd, one has

$$W_\hbar(R)(0,0)=-\tfrac{1}{(2\pi)^d}\int_{\mathbf{R}^d}|\psi(\tfrac12\hbar y)|^2dy<0\,.$$

The Husimi transform of R henceforth denoted $\tilde W_\hbar(R)$ is defined in terms of its Wigner transform by the formula

$$\tilde W_\hbar(R):=e^{\hbar\Delta_{x,\xi}/4}W_\hbar(R)\,.\tag{5}$$

Finally, we recall the definition of a Töplitz operator. The family of Schrödinger coherent states is

$$|q,p\rangle(x):=(\pi\hbar)^{-d/4}e^{-|x-q|^2/2\hbar}e^{ip\cdot(x-q/2)/\hbar}\,,\qquad x,q,p\in\mathbf{R}^d\,.$$

Let μ be a positive Borel measure on $\mathbf{R}^d\times\mathbf{R}^d$; the Töplitz operator with symbol μ is

$$\operatorname{OP}^T_\hbar(\mu):=\tfrac{1}{(2\pi\hbar)^d}\int_{\mathbf{R}^d\times\mathbf{R}^d}|q,p\rangle\langle q,p|\mu(dqdp)\,.$$

One easily checks that, if μ is the Lebesgue measure (denoted by 1), then

$$\operatorname{OP}^T_\hbar(1)=I\,.$$

Moreover, one easily checks that, if μ is a Borel probability measure on $\mathbf{R}^d\times\mathbf{R}^d$, then $\operatorname{OP}^T_\hbar((2\pi\hbar)^d\mu)\in\mathcal{D}(\mathfrak{H})$. In addition, if μ has finite second order moment as in (3), then one has $\operatorname{OP}^T_\hbar((2\pi\hbar)^d\mu)\in\mathcal{D}^2(\mathfrak{H})$. One could also use non-Gaussian wave-packets, but we shall avoid this in the present paper: see the remarks following Proposition 2.6.

The pseudo-metric $E_\hbar$ is obviously reminiscent of distances used in the context of optimal transport. Henceforth, we denote by $\operatorname{dist}_{\mathrm{MK},2}$ the Monge-Kantorovich, or Wasserstein distance with exponent 2 defined on the set of Borel probability measures satisfying the finite second order moment condition (3) (see chapter 7 in [20]), whose definition is recalled below.

Definition 2.5. *For all ρ and ρ', Borel probability measures on $\mathbf{R}^{2d}$, we set*

$$\operatorname{dist}_{\mathrm{MK},2}(\rho,\rho'):=\inf_{\pi\in\Pi(\rho,\rho')}\left(\int_{\mathbf{R}^{2d}}(|q-q'|^2+|p-p'|^2)\pi(dqdpdq'dp')\right)^{1/2}\,,$$

where $\Pi(\rho,\rho')$ designates the set of couplings of ρ and ρ'. More precisely, $\Pi(\rho,\rho')$ is the set of Borel probability measures on $\mathbf{R}^{2d}\times\mathbf{R}^{2d}$ with first and second marginals ρ and ρ' resp., i.e. such that

$$\begin{aligned}\int_{\mathbf{R}^{2d}\times\mathbf{R}^{2d}}&(\phi(q,p)+\phi'(q',p'))\pi(dqdpdq'dp')\\&=\int_{\mathbf{R}^{2d}}\phi(q,p)\rho(dqdp)+\int_{\mathbf{R}^{2d}}\phi'(q',p')\rho'(dq'dp')\end{aligned}$$

for all $\phi, \phi' \in C_b(\mathbf{R}^{2d})$.

The proposition below explains precisely how the somewhat mysterious pseudo-metric $E_\hbar$ compares to the better known Monge-Kantorovich, or Wasserstein distance $\operatorname{dist}_{\mathrm{MK},2}$. This proposition is Theorem 2.4 in [10], and its proof can be found in section 3 of [10].

Proposition 2.6. *Let* $R \in \mathcal{D}^2(\mathfrak{H})$ *and let* f *be a probability distribution on* $\mathbf{R}^d \times \mathbf{R}^d$ *with finite second order moment* (3).
(a) One has

$$E_\hbar(f,R)^2 \geq d\hbar\,.$$

(b) One has

$$E_\hbar(f,R)^2 \geq \operatorname{dist}_{\mathrm{MK},2}(f,\tilde{W}_\hbar(R))^2 - d\hbar$$

(c) For each Borel probability measure μ *on* $\mathbf{R}^d \times \mathbf{R}^d$ *with finite second order moment as in* (3), *one has*

$$E_\hbar(f,\mathrm{OP}_\hbar^T((2\pi\hbar)^d\mu))^2 \leq \operatorname{dist}_{\mathrm{MK},2}(f,\mu)^2 + d\hbar\,.$$

The pseudo-metric $E_\hbar$ can be used to obtain a quantitative formulation of the classical limit of quantum mechanics, as explained in [10]. We start from a Töplitz initial density operator, which is evolved under the von Neumann and time-splitting dynamics, and we compare the exact solution with its numerical approximation at time $t > 0$. Choosing a Töplitz operator as initial data has the following advantage: the symbol of the initial density operator is the best approximation of this quantum density by a classical density in terms of the $E_\hbar$ pseudo-distance, as shown by Proposition 2.6 (a) and (c). The evolved exact and approximate density operators at time t are in general no longer Töplitz operators, but their Husimi transforms can be compared by means of the lower bound in Proposition 2.6 (b). Statement (b) in Proposition 2.6 is another reason for using the distance $\operatorname{dist}_{\mathrm{MK},2}$ between the Husimi transforms of the exact and the numerical solutions in this context, in addition to the motivations already mentioned in the last paragraph of section 1.

As mentioned above, one can define notions analogous to Töplitz operators and Husimi transforms in terms of non-Gaussian wave-packets instead of the Schrödinger, Gaussian coherent states introduced above. The analysis in the present paper can be adapted to this more general setting, with some modifications. While Proposition 2.6 (a) holds without modifications, statements (b) and (c) should be modified by following closely the proofs of Theorems 2.2 and 3.1 in [11].

Henceforth, we denote by V a real-valued function satisfying

$$V^- \in L^{d/2}(\mathbf{R}^d)\,, \quad \text{and} \quad V \in C^{1,1}(\mathbf{R}^d)\,. \tag{6}$$

(Here, the notation V^- designates the function $x \mapsto V^-(x) := \max(-V(x),0)$.)

Let $\lambda \geq 0$, and set

$$H_\lambda(x,\xi) := \tfrac{1}{2}\lambda|\xi|^2 + V(x)\,.$$

(From the physical point of view, the parameter $\lambda \geq 0$ which appears in the definition of the Hamiltonian H_λ can be thought of as the reciprocal mass of the particle whose dynamics is defined in terms of the Hamiltonian flow associated to H_λ, whose definition is recalled below. In the present paper, the parameter λ is used only as a convenient notation for defining the various time-splitting algorithms considered.)

Since V satisfies the second condition in (6), we deduce from the Cauchy-Lipschitz theorem that the Hamiltonian H_λ generates a globally defined flow denoted

$$(X(t;x,\xi),\Xi(t;x,\xi))$$

on $\mathbf{R}^d\times\mathbf{R}^d$. In other words, $t\mapsto(X(t;x,\xi),\Xi(t;x,\xi))$ is the solution to the Cauchy problem

$$\dot{X}=\lambda\Xi\,,\quad \dot{\Xi}=-\nabla V(X)\,,\qquad (X(0;x,\xi),\Xi(0;x,\xi))=(x,\xi)\,.$$

Equivalently, for each probability distribution f^{in} on $\mathbf{R}^d\times\mathbf{R}^d$ satisfying (3), the function $f^{in}\circ\Phi_{-t}$, where Φ_t is the map $(x,\xi)\mapsto\Phi_t(x,\xi):=(X(t;x,\xi),\Xi(t;x,\xi))$, is the solution to the Cauchy problem for the Liouville equation

$$\partial_t f+\{H_\lambda,f\}=0\,,\qquad f\big|_{t=0}=f^{in}\,. \tag{7}$$

Here, the notation $\{\cdot,\cdot\}$ designates the Poisson bracket defined on $\mathbf{R}^d\times\mathbf{R}^d$ by the relations

$$\{x_j,x_k\}=\{\xi_j,\xi_k\}=0\,,\quad \{\xi_j,x_k\}=\delta_{jk}\,.$$

Likewise consider the quantum Hamiltonian

$$\mathcal{H}_\lambda:=-\tfrac{1}{2}\hbar^2\lambda\Delta_y+V(y)\,.$$

The parameter λ that appears in the definition of the operator $\mathcal{H}_\lambda$ has the same meaning, and is used similarly as in the classical setting.

The first condition in (6) implies that $\mathcal{H}_\lambda$ has a self-adjoint extension (still denoted by $\mathcal{H}_\lambda$) on $\mathfrak{H}$ (see Lemma 4.8b in chapter VI, §4 of [17]). By the Stone theorem, $U(t):=e^{it\mathcal{H}_\lambda/\hbar}$ is a unitary group on $\mathfrak{H}$, and, for each $R^{in}\in\mathcal{D}(\mathfrak{H})$, the density operator $R(t):=U^*(t)R^{in}U(t)$ is the generalized solution to the Cauchy problem for the von Neumann equation

$$i\hbar\partial_t R=[\mathcal{H}_\lambda,R]\,,\qquad R\big|_{t=0}=R^{in}\,. \tag{8}$$

Theorem 2.7. *Let $R^{in}\in\mathcal{D}^2(\mathfrak{H})$ and let f^{in} be a probability density on $\mathbf{R}^d\times\mathbf{R}^d$ satisfying* (3)*. Then*

$$E_\hbar(f^{in}\circ\Phi_{-t},U(t)^*R^{in}U(t))\le E_\hbar(f^{in},R^{in})\exp\left(\tfrac{1}{2}t(\lambda+\max(1,\operatorname{Lip}(\nabla V)^2))\right)\,.$$

This is a straightforward variant of Theorem 2.7 in [10] with an external potential and without interaction potential (i.e. in the special case $N=n=1$). The parameter $\lambda\ge 0$ appearing in the statement above is the other (unessential) difference with the situation discussed in [10]. The interested reader is referred to Appendix A for a proof of Theorem 2.7.

3. Main Results

The simple time-splitting method for the von Neumann equation is

$$\begin{cases} R_\hbar^0=R_\hbar^{in}\,,\\ i\hbar\partial_t A_\hbar=[-\tfrac{1}{2}\hbar^2\Delta_x,A_\hbar]\,, & A_\hbar\big|_{t=0}=R_\hbar^n\,,\qquad n\in\mathbf{N}\,,\\ i\hbar\partial_t B_\hbar=[V(x),B_\hbar]\,, & B_\hbar\big|_{t=0}=A_\hbar(\Delta t)\,,\\ R_\hbar^{n+1}=B_\hbar(\Delta t)\,. \end{cases} \tag{9}$$

Theorem 3.1. *Let V satisfy* (6)*, and assume that $R^{in} \in \mathcal{D}^2(\mathfrak{H})$ is a Töplitz operator on $\mathfrak{H}$. Let $t \mapsto R_\hbar(t)$ be the solution of the Cauchy problem* (8)*, and let $R_\hbar^n$ be the sequence of density operators constructed by the simple splitting method* (9)*. Let $T > 0$, and pick a time step $\Delta t \in (0, \frac{1}{2})$. Then, for each $n = 0, \ldots, [T/\Delta t]$, the simple splitting method satisfies the following error estimate, stated in terms of the quadratic Monge-Kantorovich or Wasserstein distance between the Husimi functions of the approximate and the exact quantum density operators:*

$$\begin{aligned} &\operatorname{dist}_{\mathrm{MK},2}(\tilde{W}_\hbar(R^n), \tilde{W}_\hbar(R(n\Delta t))) \\ &\le C_T \Delta t + 2\sqrt{d\hbar}\left(1 + \exp\left(\tfrac{1}{2}T(1 + \max(1, \operatorname{Lip}(\nabla V)^2))\right)\right), \end{aligned}$$

where the constant C_T depends only on T, $\nabla V(0)$ and $\operatorname{Lip}(\nabla V)$, and is defined in formula (14) *below.*

Instead of the simple splitting method, one can instead consider the Strang splitting method

$$(10) \qquad \begin{cases} R_\hbar^0 = R_\hbar^{in}\,, \\ i\hbar\partial_t A_\hbar = [-\frac{1}{2}\hbar^2\Delta_x, A_\hbar]\,, & A_\hbar\big|_{t=0} = R_\hbar^n\,, \\ i\hbar\partial_t B_\hbar = [V(x), B_\hbar]\,, & B_\hbar\big|_{t=0} = A_\hbar(\frac{1}{2}\Delta t)\,, \qquad n \in \mathbf{N}\,, \\ i\hbar\partial_t G_\hbar = [-\frac{1}{2}\hbar^2\Delta_x, G_\hbar]\,, & G_\hbar\big|_{t=0} = B_\hbar(\Delta t)\,, \\ R_\hbar^{n+1} = G_\hbar(\frac{1}{2}\Delta t)\,. \end{cases}$$

Strang splitting is a second order (in Δt) method, so that the convergence rate obtained in the previous theorem can be improved as indicated below.

Theorem 3.2. *Let V satisfy* (6) *and*

$$\nabla^m V \in L^\infty(\mathbf{R}^d)\,, \quad m = 1, 2, 3\,.$$

Let $R^{in} \in \mathcal{D}^2(\mathfrak{H})$ be a Töplitz operator on $\mathfrak{H}$, and let $t \mapsto R_\hbar(t)$ be the solution of the Cauchy problem (8)*. On the other hand, let $R_\hbar^n$ be the sequence of density operators constructed by the Strang splitting method* (10)*. Let $T > 0$, and pick a time step $\Delta t \in (0, \frac{1}{2})$. Then, for each $n = 0, \ldots, [T/\Delta t]$, the Strang splitting method satisfies the following error estimate, stated in terms of the quadratic Monge-Kantorovich or Wasserstein distance between the Husimi functions of the approximate and the exact quantum density operators:*

$$\begin{aligned} &\operatorname{dist}_{\mathrm{MK},2}(\tilde{W}_\hbar(R^n), \tilde{W}_\hbar(R(n\Delta t))) \\ &\le D_T \Delta t^2 + 2\sqrt{d\hbar}\left(1 + \exp\left(\tfrac{1}{2}T(1 + \max(1, \operatorname{Lip}(\nabla V)^2))\right)\right), \end{aligned}$$

where the constant D_T depends only on T and $\|\nabla^m V\|_{L^\infty}$ for $m = 1, 2, 3$, and is defined in formula (17) *below.*

Our strategy is the following. First, Theorem 2.7 gives the error between the solution of the von Neumann solution (8) and that of the classical Liouville equation (7). Then we obtain an analogous error between the time split von Neumann and the time split Liouville. Finally we estimate the time splitting error of the classical Liouville equation, measured in distance $\operatorname{dist}_{MK2}$. Then a triangle type inequality leads to the results in Theorem 3.1 and 3.2. This strategy is best illustrated by Figure 1.

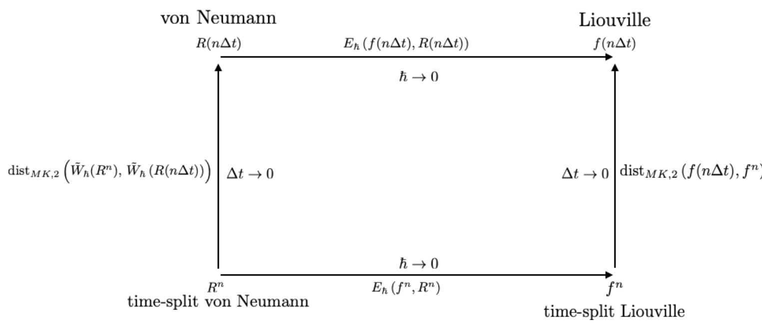

FIGURE 1. The limits $\Delta t \to 0$ and $\hbar \to 0$.

The error estimates Theorems 3.1 and 3.2 do not provide a uniform in $\hbar$ error estimate, since they contain an $O(\hbar^{1/2})$ term in their right hand side. In particular, these error estimates are useful only in the vanishing $\hbar$ limit. Yet these two theorems contain all the new information on the time splitting methods for quantum dynamics in the semiclassical regime that can be obtained with our approach. Besides, these two theorems are of independent interest, and lead to better convergence rates that the uniform error estimate given below in the vanishing $\hbar$ regime. In contrast, a classical L^2 norm estimate gives an error of order $O(\Delta t/\hbar)^m$ [1] (for some positive integer m that depends on the order of the splitting), which blows up as $\hbar \to 0$.

In order to obtain uniform in $\hbar$ error estimates for the simple and the Strang splitting methods, we need to optimize these estimates with the error estimates for the time splitting method in the case of the Schrödinger equation with fixed $\hbar$ (or equivalently for $\hbar = 1$). Such error estimates have been studied in detail and can be found for instance in [5]. The idea of combining and optimizing the error estimates in the asymptotic (macroscopic) regime and the microscopic regime is often used in numerical methods for kinetic and hyperbolic equations involving multiple scales, a computational methodology known as Asymptotic-Preserving Schemes [9, 15].

Our final uniform error estimate will be formulated in terms of an optimal transport distance denoted dist_1, already used in [12] (see formula (13) in [12]). All the convergence statements in Theorems 3.1 and 3.2 are ultimately formulated in terms of the Monge-Kantorovich-Wasserstein distance $\mathrm{dist}_{\mathrm{MK},2}$, to which the "pseudo-metric" $E_\hbar$ can be conveniently compared (see Proposition 2.6), the uniform in $\hbar$ error estimates stated below as Corollaries 3.4 and 3.5 are all based on some optimization procedure comparing the L^1 and the $\mathrm{dist}_{\mathrm{MK},2}$ distances between the Husimi transforms of the exact and of the approximate solutions of the quantum dynamical problem. This optimization procedure is precisely the reason for using the distance dist_1, a weaker variant of the Monge-Kantorovich-Wasserstein distance of exponent 1, with a transportation cost that is truncated at infinity. The definition of dist_1 is recalled below for the reader's convenience.

Definition 3.3. *For all ρ and ρ', Borel probability measures on $\mathbf{R}^{2d}$, we set*

$$\text{dist}_1(\rho,\rho') := \inf_{\pi\in\Pi(\rho,\rho')}\int_{\mathbf{R}^{2d}} \min(1,\sqrt{|q-q'|^2+|p-p'|^2})\pi(dqdpdq'dp')\,.$$

Here, the notation $\Pi(\rho,\rho')$ designates the set of couplings of ρ,ρ' already used to define the Monge-Kantorovich-Wasserstein distance $\text{dist}_{\text{MK},2}$ (Definition 2.5).

Our uniform estimates for the simple splitting method is given in the following statement, which is a consequence of Theorem 3.1 and of the error estimate in Theorem 2 of [5].

Corollary 3.4. *Let $V\in C^2(\mathbf{R}^d)$ satisfy (6), and let $R^{in}=\text{OP}_\hbar^T((2\pi\hbar)^d\mu^{in})$, where μ^{in} is a Borel probability measure on $\mathbf{R}^{2d}$ such that*

$$\int_{\mathbf{R}^{2d}}(|q|^2+|p|^2)\mu^{in}(dqdp)<\infty\,.$$

Let $t\mapsto R_\hbar(t)$ be the solution of the Cauchy problem (8), and let $R_\hbar^n$ be the sequence of density operators constructed by the simple splitting method (10). Let $T>0$, and pick a time step $\Delta t\in(0,\frac{1}{2})$. Then, for each $n=0,\dots,[T/\Delta t]$, the simple splitting method satisfies the following uniform in $\hbar$ error estimate:

$$\text{dist}_1(\tilde{W}_\hbar(R_\hbar^n),\tilde{W}_\hbar(R_\hbar(n\Delta t)))\le 2C[T,V,\mu^{in}]\Delta t^{1/3}\,,$$

where $C[T,V,\mu^{in}]$ is defined in (21). In particular, the constant $C[T,V,\mu^{in}]$ is independent of $\hbar$.

Likewise, Theorem 3.2 and the error estimate in Theorem 3 of [5] lead to the following statement.

Corollary 3.5. *Let $V\in W^{4,\infty}(\mathbf{R}^d)$ satisfy (6), and let $R^{in}=\text{OP}_\hbar^T((2\pi\hbar)^d\mu^{in})$, where μ^{in} is a Borel probability measure on $\mathbf{R}^{2d}$ such that*

$$\int_{\mathbf{R}^{2d}}(|q|^2+|p|^2)\mu^{in}(dqdp)<\infty\,.$$

Let $t\mapsto R_\hbar(t)$ be the solution of the Cauchy problem (8), and let $R_\hbar^n$ be the sequence of density operators constructed by the Strang splitting method (9). Let $T>0$, and pick a time step $\Delta t\in(0,\frac{1}{2})$. Then, for each $n=0,\dots,[T/\Delta t]$, the simple splitting method satisfies the following uniform in $\hbar$ error estimate:

$$\text{dist}_1(\tilde{W}_\hbar(R_\hbar^n),\tilde{W}_\hbar(R_\hbar(n\Delta t)))\le 2D[T,V,\mu^{in}]\Delta t^{2/3}\,,$$

where $D[T,V,\mu^{in}]$ is defined in (23). In particular, the constant $D[T,V,\mu^{in}]$ is independent of $\hbar$.

As will be clear from the proofs, the uniform in $\hbar$ estimates obtained in these two corollaries involve the $O(\hbar^{1/2})$ term in the convergence rates in Theorems 3.1 and 3.2, and the nonuniform bounds in Theorems 2 and 3 resp. of [5]. The uniform error bounds in $\Delta t^{1/3}$ for the simple splitting and in $\Delta t^{2/3}$ for the Strang splitting are not expected to be sharp. These estimates involve the $d\hbar$ term that is a lower bound of $E_\hbar$ as explained in Proposition 2.6 (a), and that appears in the inequalities in Proposition 2.6 (b)-(c). Perhaps using metrics other than $E_\hbar$ to compare the quantum and classical dynamics could improve these uniform error bounds — but such metrics remain to be constructed at the time of this writing.

Specifically, the uniform $O(\Delta t^{1/3})$ error bound in Corollary 3.4 is obtained as the minimum of the $O(\hbar^{1/2})$ term in Theorem 3.1 and of the (nonuniform) $O(\Delta t/\hbar)$ error bound in Theorem 2 of [5]. This $O(\Delta t^{1/3})$ uniform error estimate corresponds to the "worst" possible distinguished asymptotic regime $\hbar \sim \Delta t^{2/3}$. Although the $O(\Delta t)$ term in Theorem 3.1 is smaller than the $O(\Delta t^{1/3})$ uniform error estimate in Corollary 3.4, the $O(\Delta t + \hbar^{1/2})$ error estimate in Theorem 3.1 is still of independent interest in all cases where $\hbar$ is small and satisfies $\hbar = O(\Delta t^2)$.

Likewise, the uniform $O(\Delta t^{2/3})$ error bound in Corollary 3.5 comes as the minimum of the $O(\hbar^{1/2})$ term in the convergence rates in Theorem 3.2 and of the (nonuniform) $O(\Delta t^2/\hbar^2)$ error bound in Theorem 3 of [5]. In this case, the "worst" possible distinguished asymptotic regime is $\hbar \sim \Delta t^{4/5}$. Here again, the $O(\Delta t^2)$ term in Theorem 3.2 is smaller than the $O(\Delta t^{2/3})$ uniform error estimate in Corollary 3.5. Nevertheless, the $O(\Delta t^2 + \hbar^{1/2})$ error estimate in Theorem 3.2 is of interest independently of the uniform $O(\Delta t^{2/3})$ bound in Corollary 3.5 whenever $\hbar$ is small and satisfies $\hbar = O(\Delta t^4)$. Observe that the Strang splitting method is of second order in time in that regime, for the quantum dynamics as well as for the classical dynamics.

The uniform in $\hbar$ error bounds obtained in Corollaries 3.4 and 3.5 are expected to carry over to the case of a time-dependent potential $V \equiv V(t,x)$, provided that $V(t,\cdot) \in C^{1,1}(\mathbf{R}^d)$ with $\sup_{0\le t\le T} \operatorname{Lip}(\nabla_x V(t,\cdot)) < \infty$ for each $T > 0$. For instance, Theorem 2.7 is easily seen to hold for such potentials (with essentially the same proof). Since our final results depend on Theorems 3 and 4 from [5], and this reference only treats the case of potentials that are independent of the time variable, we have chosen the same setting to avoid tedious verifications of the nonuniform in $\hbar$ error bounds analogous to Theorems 3 and 4 from [5] in the case of time-dependent potentials.

A more significant generalization of our results in Corollaries 3.4 and 3.5 would be to obtain analogous uniform in $\hbar$ error bounds for the full discretization of the von Neumann equation — that is to say, when the spatial derivatives are also discretized. Unfortunately, at the time of this writing, there does not exist any numerical method known to capture the correct physical solutions by using $\hbar$-independent spatial mesh sizes. Among direct solvers for the Schrödinger equation, the most competitive method dealing with highly oscillatory solutions is the time-splitting spectral method, which requires $O(\hbar)$ mesh size in order to capture the physical observables: see [2]. The Gaussian beam, or Gaussian wave packet type methods require the mesh size to be of order $O(\sqrt{\hbar})$: see [16]. Since the analysis developed in the paper is aimed at obtaining $\hbar$-independent error estimates, it is less scientifically interesting to apply it to $\hbar$-dependent spatial discretizations. This is the reason why the present paper focusses on the time-discretization and does not discuss the fully discretized (in the time and space variable) problem.

Finally, as mentioned in the introduction, one can also express all these error bounds directly in terms of some appropriate distance between the density operator that is the exact solution of the von Neumann equation and its time-split approximation. This metric on density operators, and the corresponding error bounds can be found in Appendix B.

4. The Simple Splitting Algorithm

4.1. **The Simple Splitting Algorithm for the von Neumann Equation in the Semiclassical Regime.**

In this subsection we estimate the error between the time split von Neumann and the time split Liouville equations. By analogy with the simple splitting method (9) for the von Neumann equation, consider the simple time-splitting method for the Liouville equation:

$$\begin{cases} f^0 = f^{in}\,, \\ \partial_t a + \{\tfrac{1}{2}|\xi|^2, a\} = 0\,, & a\big|_{t=0} = f^n\,, \qquad n \in \mathbf{N}\,, \\ \partial_t b + \{V(x), b\} = 0\,, & b\big|_{t=0} = a(\Delta t)\,, \\ f^{n+1} = b(\Delta t)\,. \end{cases}$$

Applying Theorem 2.7 to one time step of the free dynamics, i.e. with $V \equiv 0$ and $\lambda = 1$ shows that

$$E_\hbar(a(\Delta t), A_\hbar(\Delta t)) \le E_\hbar(f^n, R^n)\exp(\tfrac{1}{2}\Delta t)\,.$$

Next we apply the same Theorem 2.7 to the Hamiltonian dynamics defined by the potential V, with $\lambda = 0$: thus

$$\begin{aligned} E_\hbar(f^{n+1}, R^{n+1}) =& E_\hbar(b(\Delta t), B_\hbar(\Delta t)) \\ \le& E_\hbar(a(\Delta t), A_\hbar(\Delta t))\exp(\tfrac{1}{2}\Delta t \max(1, \mathrm{Lip}(\nabla V)^2))\,. \end{aligned}$$

Putting both estimates together shows that

$$E_\hbar(f^{n+1}, R^{n+1}) \le E_\hbar(f^n, R^n)\exp(\tfrac{1}{2}\Delta t(1 + \max(1, \mathrm{Lip}(\nabla V)^2)))\,.$$

Let $T > 0$; then for each $n = 0, \dots, [T/\Delta t] + 1$, one has

$$\begin{aligned} E_\hbar(f^n, R^n) \le& E_\hbar(f^{in}, R^{in})\exp(\tfrac{1}{2}n\Delta t(1 + \max(1, \mathrm{Lip}(\nabla V)^2))) \\ \le& E_\hbar(f^{in}, R^{in})\exp(\tfrac{1}{2}T(1 + \max(1, \mathrm{Lip}(\nabla V)^2)))\,. \end{aligned} \tag{11}$$

Observe that the amplification rate $\exp(\tfrac{1}{2}T(1+\max(1, \mathrm{Lip}(\nabla V)^2)))$ in this estimate is uniform in (i.e. independent of) $\hbar$. This is the key point in our analysis.

4.2. **The Simple Splitting Algorithm for the Liouville Equation.**

In this subsection, we estimate the distance between the classical Liouville equation and its time split approximation. While the error analysis for the simple splitting method is well known in general, its formulation in terms of $\mathrm{dist}_{\mathrm{MK},2}$ is perhaps less classical.

One expresses the solutions a and b of the kinetic and the potential part of the Liouville evolution as follows, by using the method of characteristics:

$$\begin{aligned} a(t, y, \eta) &= f^n(K_t(y, \eta)) && \text{where } K_t(y, \eta) := (y - t\eta, \eta)\,, \\ b(t, y, \eta) &= a(\Delta t, P_t(y, \eta)) && \text{where } P_t(y, \eta) := (y, \eta + t\nabla V(y))\,. \end{aligned}$$

Thus, one step of simple splitting corresponds to setting

$$f^{n+1}(y, \eta) = f^n \circ P_{\Delta t} \circ K_{\Delta t}(y, \eta) = f^n(y - \Delta t\eta, \eta + \Delta t\nabla V(y - \Delta t\eta))\,. \tag{12}$$

Since the transformation $P_{\Delta t}\circ K_{\Delta t}$ has Jacobian one, the formula (12) means that $f^{n+1}(y,\eta)dyd\eta$ is the image of the measure $f^n(y,\eta)dyd\eta$ by $P_{\Delta t}\circ K_{\Delta t}$. One finds

$$\begin{aligned}\operatorname{dist}_{\mathrm{MK},2}&(f^{in}\circ\Phi_{-(n+1)\Delta t}, f^{in}\circ(P_{\Delta t}\circ K_{\Delta t})^{n+1})^2\\ &\le\int|X(-\Delta t,x,\xi)-(y-\Delta t\eta)|^2q^n(dxd\xi dyd\eta)\\ &\quad+\int|\Xi(-\Delta t,x,\xi)-(\eta+\Delta t\nabla V(y-\Delta t\eta))|^2q^n(dxd\xi dyd\eta)\end{aligned}$$

where q^n is *any* coupling of $f(n\Delta t,\cdot,\cdot)$ and f^n. This makes it clear that finding an error bound in the metric $\operatorname{dist}_{\mathrm{MK},2}$ for a splitting method applied to the Liouville equation is mostly a question pertaining to the numerical analysis of ordinary differential equations. Our reference for such questions is [13].

First we seek to bound

$$|(X,\Xi)(-t,x,\xi)-(Y,H)(-t,y,\eta)|^2\,,$$

where

$$(Y,H)(-t,y,\eta)=P_t\circ K_t(y,\eta)=(y-t\eta,\eta+t\nabla V(y-t\eta))$$

is the numerical particle trajectory. As in the modified equation method described in chapter IX.4 of [13], we write dynamical equations for (Y,H). Inverting these relations, and denoting $Y_t:=Y(t;y,\eta)$ and $H_t:=H(t;y,\eta)$ for simplicity, one has

$$(y,\eta)=(Y_{-t}+t(H_{-t}-t\nabla V(Y_{-t})),H_{-t}-t\nabla V(Y_{-t}))\,.$$

Differentiating in time, we find that

$$\begin{aligned}\dot Y=&H+t(-\nabla V(Y)-t\nabla^2V(Y)\dot Y)+2t\nabla V(Y)+t^2\nabla^2V(Y)\dot Y\\ =&H+t\nabla V(Y)\,,\\ \dot H=&-\nabla V(Y)-t\nabla^2V(Y)\cdot H-t^2\nabla^2V(Y)\cdot\nabla V(Y)\,.\end{aligned}$$

Thus, we seek to compare the trajectories of the two following differential systems:

$$\begin{cases}\dot X=\Xi\,,\\ \dot\Xi=-\nabla V(X)\,,\end{cases}\qquad\text{and}\qquad\begin{cases}\dot Y=H+t\nabla V(Y)\,,\\ \dot H=-\nabla V(Y)-t\nabla^2V(Y)\cdot H-t^2\nabla^2V(Y)\cdot\nabla V(Y)\,.\end{cases}$$

Clearly

$$\begin{cases}\dfrac{d}{dt}|X-Y|^2\le|X-Y|^2+|\Xi-H|^2+|z(t)|^2+|X-Y|^2\,,\\ \dfrac{d}{dt}|\Xi-H|^2\le\|\nabla^2V\|_{L^\infty}(|X-Y|^2+|\Xi-H|^2)+|\zeta(t)|^2+|\Xi-H|^2\,,\end{cases}$$

with

$$\begin{cases}z(t):=t\nabla V(y+t\eta)\,,\\ \zeta(t)=-t\nabla^2V(y+t\eta)\cdot(\eta-t\nabla V(y+t\eta))-t^2\nabla^2V(y+t\eta)\cdot\nabla V(y+t\eta)\,.\end{cases}$$

Set $E:=|\nabla V(0)|$. Then, by the mean value inequality,

$$\begin{cases}|z(t)|\le|t|(E+\|\nabla^2V\|_{L^\infty}(|y|+|t||\eta|))\,,\\ |\zeta(t)|\le\|\nabla^2V\|_{L^\infty}|t|(|\eta|+|t|(E+\|\nabla^2V\|_{L^\infty}(|y|+|t||\eta|)))\\ \qquad\qquad+t^2\|\nabla^2V\|_{L^\infty}(E+\|\nabla^2V\|_{L^\infty}(|y|+t\eta))\,.\end{cases}$$

By Gronwall's inequality, setting $\Lambda := \max(1, E, \|\nabla^2 V\|_{L^\infty}))$, and assuming that $0 \le t \le \frac{1}{2}$ for simplicity, one has

$$|X - Y|^2(t) + |\Xi - H|^2(t) \le (|x-y|^2 + |\xi - \eta|^2) e^{(2+\Lambda)|t|} + \frac{e^{(2+\Lambda)|t|} - 1}{2+\Lambda} \tfrac{9}{4}\Lambda^2(\tfrac{1}{2} + \Lambda)^2 t^2 (1 + |y|^2 + |\eta|^2)\,.$$

Choosing at this point an *optimal* coupling q^n of $f(n\Delta t, \cdot, \cdot)$ and f^n (see Theorem 1.3 in [20] for the existence of an optimal coupling), one has

$$\begin{aligned}\mathrm{dist}_{\mathrm{MK},2}(f((n+1)\Delta t, \cdot, \cdot), f^{n+1})^2 &= \int (|X-Y|^2 + |\Xi - H|^2) q^{n+1}(dX d\Xi dY dH) \\ = \int (|X(-\Delta t; x, \xi) - Y(-\Delta t; y, \eta)|^2 &+ |\Xi(-\Delta t; x, \xi) - H(-\Delta t; y, \eta)|^2) q^n(dx d\xi dy d\eta) \\ &= \mathrm{dist}_{\mathrm{MK},2}(f(n\Delta t, \cdot, \cdot), f^n)^2 e^{(2+\Lambda)\Delta t} \\ &+ \tfrac{9}{4}\Lambda^2(\tfrac{1}{2} + \Lambda)^2 \Delta t^2 \frac{e^{(2+\Lambda)\Delta t} - 1}{2+\Lambda} \left(1 + \int (|y|^2 + |\eta|^2) f^n(y, \eta) dy d\eta\right)\end{aligned}$$

and we need to bound the last term in the right hand side. Since $f^n(y, \eta) dy d\eta$ is the image of the measure $f^{n-1}(y, \eta) dy d\eta$ by the transformation $P_{\Delta t} \circ K_{\Delta t}$, one has

$$\begin{aligned}\mu_n &:= \int (|y|^2 + |\eta|^2) f^n(y, \eta) dy d\eta \\ &= \int (|y + \Delta t \eta|^2 + |\eta - \Delta t \nabla V(y + \Delta t \eta)|^2) f^{n-1}(y, \eta) dy d\eta\end{aligned}$$

(by substitution in the left hand side), since

$$\begin{aligned}&|y + \Delta t \eta|^2 + |\eta - \Delta t \nabla V(y + \Delta t \eta)|^2 \\ &\le (|y|^2 + |\eta|^2)(1 + \Delta t)^2 (1 + 2\Lambda^2 \Delta t (1 + \Delta t)) + 2\Delta t (1 + \Delta t) E^2\,.\end{aligned}$$

We easily check that

$$\mu_n \le (1 + \Delta t + 2\Lambda^2 \Delta t (1 + \Delta t)^2)(1 + \Delta t)\mu_{n-1} + 2\Delta t (1 + \Delta t) E^2\,,$$

and since $1 + \alpha \le e^\alpha$,

$$\begin{aligned}\mu_n &\le (1 + \Delta t + 2\Lambda^2 \Delta t (1 + \Delta t)^2)^n (1 + \Delta t)^n \mu_0 \\ &+ 2\Delta t (1 + \Delta t) E^2 \frac{(1 + \Delta t + 2\Lambda^2 \Delta t (1 + \Delta t)^2)^n (1 + \Delta t)^n - 1}{(1 + \Delta t + 2\Lambda^2 \Delta t (1 + \Delta t)^2)(1 + \Delta t) - 1} \\ &\le \exp(2n\Delta t (1 + \Lambda^2 (1 + \Delta t)^2))\mu_0 \\ &+ 2(1 + \Delta t) E^2 \frac{\exp(2n\Delta t (1 + \Lambda^2 (1 + \Delta t)^2)) - 1}{1 + (1 + \Delta t)(1 + 2\Lambda^2 (1 + \Delta t)^2)}\,.\end{aligned}$$

Thus, we arrive at the inequality

$$\begin{aligned}\mathrm{dist}_{\mathrm{MK},2}&(f((n+1)\Delta t, \cdot, \cdot), f^{n+1})^2 \le \mathrm{dist}_{\mathrm{MK},2}(f(n\Delta t, \cdot, \cdot), f^n)^2 e^{(2+\Lambda)\Delta t} \\ &+ \tfrac{9}{4}\Lambda^2(\tfrac{1}{2} + \Lambda)^2 \Delta t^2 \frac{e^{(2+\Lambda)\Delta t} - 1}{2+\Lambda} \Bigg(1 + \exp(2n\Delta t (1 + \Lambda^2 (1 + \Delta t)^2))\mu_0 \\ &+ 2(1 + \Delta t) E \frac{\exp(2n\Delta t (1 + \Lambda^2 (1 + \Delta t)^2)) - 1}{1 + (1 + \Delta t)(1 + 2\Lambda^2 (1 + \Delta t)^2)}\Bigg).\end{aligned}$$

Iterating in n, we conclude that, for $n = 0, 1, \ldots, [T/\Delta t]$,

$$\mathrm{dist}_{\mathrm{MK},2}(f(n\Delta t, \cdot, \cdot), f^n) \le C_T \Delta t\,, \tag{13}$$

where

$$C_T^2 := \tfrac{9}{4}\Lambda^2(\tfrac{1}{2}+\Lambda)^2\frac{e^{(2+\Lambda)T}-1}{2+\Lambda}\Bigg(1+\exp(2T(1+\Lambda^2(1+\Delta t)^2))\mu_0 \\ +2(1+\Delta t)E\frac{\exp(2T(1+\Lambda^2(1+\Delta t)^2))-1}{1+(1+\Delta t)(1+2\Lambda^2(1+\Delta t)^2)}\Bigg). \tag{14}$$

4.3. **Error Estimate for the Simple Splitting Method.** By Theorem 2.7, for each $n=0,1,\ldots,[T/\Delta t]$, one has

$$E_\hbar(f(n\Delta t,\cdot,\cdot),R(n\Delta t))\le E_\hbar(f^{in},R^{in})\exp\left(\tfrac{1}{2}n\Delta t(1+\max(1,\mathrm{Lip}(\nabla V)^2))\right)$$

and in particular

$$E_\hbar(f(n\Delta t,\cdot,\cdot),R(n\Delta t))\le E_\hbar(f^{in},R^{in})\exp\left(\tfrac{1}{2}T(1+\max(1,\mathrm{Lip}(\nabla V)^2))\right). \tag{15}$$

Putting together (11), (13) and (15) shows that

$$E_\hbar(f^n,R^n)+\mathrm{dist}_{\mathrm{MK},2}(f(n\Delta t,\cdot,\cdot),f^n)+E_\hbar(f(n\Delta t,\cdot,\cdot),R(n\Delta t)) \\ \le 2E_\hbar(f^{in},R^{in})\exp\left(\tfrac{1}{2}T(1+\max(1,\mathrm{Lip}(\nabla V)^2))\right)+C_T\Delta t\,.$$

According to Proposition 2.6 (b) and using the triangle inequality for $\mathrm{dist}_{\mathrm{MK},2}$, we conclude that

$$\mathrm{dist}_{\mathrm{MK},2}(\tilde W_\hbar(R^n),\tilde W_\hbar(R(n\Delta t))) \\ \le 2E_\hbar(f^{in},R^{in})\exp\left(\tfrac{1}{2}T(1+\max(1,\mathrm{Lip}(\nabla V)^2))\right)+C_T\Delta t+2\sqrt{d\hbar}\,.$$

If R^{in} is the Töplitz operator with symbol $(2\pi\hbar)^d f^{in}$, this inequality and Proposition 2.6 (c) imply the desired inequality in Theorem 3.1.

5. The Strang Splitting Algorithm

In this subsection we estimate the error between the time split von Neumann and the time split Liouville equations. The Strang time-splitting method for the Liouville equation is

$$\begin{cases} f^0=f^{in}\,, & & \\ \partial_t a+\{\tfrac{1}{2}|\xi|^2,a\}=0\,, & a\big|_{t=0}=f^n\,, & \\ \partial_t b+\{V(x),b\}=0\,, & b\big|_{t=0}=a(\tfrac{1}{2}\Delta t)\,, & n\in\mathbf{N}\,, \\ \partial_t g+\{\tfrac{1}{2}|\xi|^2,g\}=0\,, & g\big|_{t=0}=b(n\Delta t)\,, & \\ f^{n+1}=g(\tfrac{1}{2}\Delta t)\,. & & \end{cases}$$

Applying Theorem 2.7 to one time step of the free dynamics, i.e. with $V\equiv 0$ and $\lambda=1$ shows that

$$E_\hbar(a(\tfrac{1}{2}\Delta t),A_\hbar(\tfrac{1}{2}\Delta t))\le E_\hbar(f^n,R^n)\exp(\tfrac{1}{4}\Delta t)\,.$$

Next we apply the same Theorem 2.7 to the Hamiltonian dynamics defined by the potential V, with $\lambda=0$: thus

$$E_\hbar(b(\Delta t),B_\hbar(\Delta t))\le E_\hbar(a(\tfrac{1}{2}\Delta t),A_\hbar(\tfrac{1}{2}\Delta t))\exp(\tfrac{1}{2}\Delta t\max(1,\mathrm{Lip}(\nabla V)^2))\,.$$

Finally, we apply again Theorem 2.7 to the last time step of the free dynamics, so that

$$\begin{aligned}E_\hbar(f^{n+1},R_\hbar^{n+1}) &= E_\hbar(g(\tfrac12\Delta t),G_\hbar(\tfrac12\Delta t)) \le E_\hbar(b(\Delta t),B_\hbar(\Delta t))\exp(\tfrac14\Delta t)\\ &\le E_\hbar(a(\tfrac12\Delta t),A_\hbar(\frac12\Delta t))\exp(\tfrac14\Delta t+\tfrac12\Delta t\max(1,\mathrm{Lip}(\nabla V)^2))\\ &\le E_\hbar(f^n,R^n)\exp(\tfrac14\Delta t+\tfrac12\Delta t\max(1,\mathrm{Lip}(\nabla V)^2)+\tfrac14\Delta t)\\ &= E_\hbar(f^n,R^n)\exp(\tfrac12\Delta t(1+\max(1,\mathrm{Lip}(\nabla V)^2))\,.\end{aligned}$$

Hence the uniform in $\hbar$ estimate (11) also holds for the Strang splitting method.

Next we analyze the Strang splitting method for the Liouville equation in terms of the Monge-Kantorovich or Wasserstein distance. With the same notation as in the previous section, we seek to bound

$$\mathrm{dist}_{\mathrm{MK},2}(f^{in}\circ\Phi_{-(n+1)\Delta t},f^{in}\circ(K_{\frac12\Delta t}\circ P_{\Delta t}\circ K_{\frac12\Delta t})^{n+1})^2\,.$$

In order to do so, we seek to bound

$$|(X,\Xi)(-t,x,\xi)-(Z,\Omega)(-t,z,\omega)|^2\,,$$

where the numerical particle trajectory or bi-characteristic flow of the Liouville equation is

$$\begin{aligned}(Z,\Omega)(-t,z,\omega) &= K_{t/2}\circ P_t\circ K_{t/2}(z,\omega)\\ &=(z-t\omega-\tfrac12t^2\nabla V(z-\tfrac12t\omega)),\omega+t\nabla V(z-\tfrac12t\omega))\,.\end{aligned}$$

Writing $Z_t:=Z(t,z,\omega)$ and $\Omega_t:=\Omega(t,z,\omega)$ for simplicity, we first observe that

$$Z_t-\tfrac12t\Omega_t=z+\tfrac12t\omega\,,\quad \Omega_t=\omega-t\nabla V(Z_t-\tfrac12\Omega_t)\,.$$

Differentiating both sides of each equality in t, and eliminating ω from the leading order terms in $t\ll1$, we obtain the numerical bi-characteristic field for the Strang splitting method in the form

$$\begin{aligned}\dot Z_t &=\Omega_t-\tfrac14t^2\nabla^2V(Z_t-\tfrac12t\Omega_t)\omega\\ &=\Omega_t+s(t)\\ \dot\Omega_t &=-\nabla V(Z_t)-\tfrac12t(\nabla^2V(Z_t-\tfrac12t\Omega_t)-\nabla^2V(Z_t))\Omega_t\\ &\quad-\tfrac12t^2\nabla^2V(Z_t-\tfrac12t\Omega_t)\nabla V(Z_t-\tfrac12t\Omega_t)\\ &\quad-\tfrac18t^2\nabla^3V(Z_t-\tfrac12\theta t\Omega_t):\Omega_t^{\otimes2}\\ &=-\nabla V(Z_t)+\sigma(t)\end{aligned}$$

where

$$\begin{aligned}s(t) &:=-\tfrac14t^2\nabla^2V(z+\tfrac12t\omega)\omega\\ \sigma(t) &:=-\tfrac12t(\nabla^2V(z+\tfrac12t\omega)-\nabla^2V(z+\tfrac12t\omega+\tfrac12t\Omega_t))\Omega_t\\ &\quad-\tfrac12t^2\nabla^2V(z+\tfrac12t\omega)\nabla V(z+\tfrac12t\omega)\\ &\quad-\tfrac18t^2\nabla^3V(Z_t-\tfrac12\theta t\Omega_t):\Omega_t^{\otimes2}\end{aligned}$$

Here again, we seek to compare the solution (Z_t,Ω_t) to the Strang splitting differential equation with the solution (X_t,Ξ_t) of the Newton system of motion equations, i.e. we apply the modified equation approach in chapter IX.4 of [13]. Arguing as in the case of the simple splitting method, we observe that

$$\begin{cases}\dot X-\dot Z=(\Xi-\Omega)-s\,,\\ \dot\Xi-\dot\Omega=-(\nabla V(X)-\nabla V(Z))-\sigma(t)\,,\end{cases}$$

so that

$$\begin{aligned}\frac{d}{dt}|X-Z|^2 =&2(X-Z)\cdot(\Xi-\Omega)-2(X-Z)\cdot s\\ \leq&|X-Z|^2+|\Xi-\Omega|^2+|X-Z|^2+|s|^2\,,\\ \frac{d}{dt}|\Xi-\Omega|^2 =&-2(\Xi-\Omega)\cdot(\nabla V(X)-\nabla V(Z))-2(\Xi-\Omega)\cdot\sigma\\ \leq&\operatorname{Lip}(\nabla V)(|\Xi-\Omega|^2+|X-Z|^2)+|\Xi-\Omega|^2+|\sigma|^2\,.\end{aligned}$$

Setting

$$M:=\max(1,\|\nabla V\|^2_{L^\infty},\|\nabla^2 V\|^2_{L^\infty},\|\nabla^3 V\|^2_{L^\infty})\,,$$

we see that

$$\begin{aligned}|s(t)|^2+|\sigma(t)|^2\leq&t^4(\tfrac16 M|\omega|^2+\tfrac12 M(|\omega|^4+t^4M^2)+\tfrac14 M^2+\tfrac1{32}M(|\omega|^2+t^2M))\\ \leq&\tfrac12 M^3t^4(1+t^2+t^4+|\omega|^2+|\omega|^4)\,.\end{aligned}$$

Choosing an optimal coupling q^n of $f(n\Delta t,\cdot,\cdot)$ and f^n, one has

$$\begin{aligned}\operatorname{dist}_{\mathrm{MK},2}(f((n+1)\Delta t,\cdot,\cdot),f^{n+1})^2\leq\int(|X-Z|^2+|\Xi-\Omega|^2)q^{n+1}(dXd\Xi dZd\Omega)\\ =\int(|X(-\Delta t;x,\xi)-Z(-\Delta t;z,\omega)|^2+|\Xi(-\Delta t;x,\xi)-\Omega(-\Delta t;z,\omega)|^2)q^n(dxd\xi dzd\omega)\\ \leq e^{(2+\Lambda)\Delta t}\operatorname{dist}_{\mathrm{MK},2}(f(n\Delta t,\cdot,\cdot),f^n)^2\\ +\frac{e^{(2+\Lambda)\Delta t}-1}{2+\Lambda}\tfrac12 M^3\Delta t^4\left(1+\Delta t^2+\Delta t^4+\int(|\omega|^2+|\omega|^4)f^n(dzd\omega)\right).\end{aligned}$$

Arguing as in the case of the simple splitting algorithm, one has

$$\begin{aligned}\nu_n:=\int(|\omega|^2+|\omega|^4)f^n(dzd\omega)=\int(|\Omega(-\Delta t;z,\omega)|^2+|\Omega(-\Delta t;z,\omega)|^4)f^{n-1}(dzd\omega)\\ \leq\int((|\omega|+\sqrt{M}\Delta t)^2+(|\omega|+\sqrt{M}\Delta t)^4)f^{n-1}(dzd\omega)\end{aligned}$$

by substitution in the integral on the left hand side, since $f^n(y,\eta)dyd\eta$ is the image of the measure $f^{n-1}(y,\eta)dyd\eta$ by the transformation $K_{\frac12\Delta t}\circ P_{\Delta t}\circ K_{\frac12\Delta t}$. Since

$$(|\omega|+\sqrt{M}\Delta t)^2\leq|\omega|^2+\Delta t(M+|\omega|^2)+M\Delta t^2\leq(1+\Delta t)(|\omega|^2+M\Delta t)$$

and

$$(|\omega|+\sqrt{M}\Delta t)^4\leq(1+\Delta t)^2(|\omega|^2+M\Delta t)^2\leq(1+\Delta t)^3(|\omega|^4+M^2\Delta t)\,,$$

one has

$$\nu_n\leq(1+\Delta t)^3(\nu_{n-1}+M(1+M)\Delta t)\leq e^{3\Delta t}(\nu_{n-1}+M(1+M)\Delta t)\,,$$

so that

$$\begin{aligned}\nu_n\leq&e^{3n\Delta t}\nu_0+M(1+M)\Delta te^{3\Delta t}\frac{e^{3n\Delta t}-1}{e^{3\Delta t}-1}\\ \leq&e^{3n\Delta t}\nu_0+M(1+M)(1+\Delta t)(e^{3n\Delta t}-1)\,.\end{aligned}$$

Hence

$$\begin{aligned}\operatorname{dist}_{\mathrm{MK},2}(f((n+1)\Delta t,\cdot,\cdot),f^{n+1})^2\leq e^{(2+\Lambda)\Delta t}\operatorname{dist}_{\mathrm{MK},2}(f(n\Delta t,\cdot,\cdot),f^n)^2\\ +\frac{e^{(2+\Lambda)\Delta t}-1}{2+\Lambda}\tfrac12 M^3\Delta t^4\left(1+\Delta t^2+\Delta t^4+e^{3n\Delta t}\nu_0+M(1+M)(1+\Delta t)(e^{3n\Delta t}-1)\right)\end{aligned}$$

so that, iterating in n,

$$\begin{aligned}&\mathrm{dist}_{\mathrm{MK},2}(f(n\Delta t,\cdot,\cdot),f^n)^2\\ &\le \frac{e^{(2+\Lambda)n\Delta t}-1}{2+\Lambda}\tfrac{1}{2}M^3\Delta t^4\left(1+\Delta t^2+\Delta t^4+e^{3n\Delta t}\nu_0+M(1+M)(1+\Delta t)(e^{3n\Delta t}-1)\right)\\ &\le \frac{e^{(2+\Lambda)T}-1}{2+\Lambda}M^3\Delta t^4\left(1+e^{3T}(\nu_0+2M^2)\right)\end{aligned}$$

for $n=0,1,\ldots,[T/\Delta t]$ with $0<\Delta t\le\frac{1}{2}$. In other words

$$\mathrm{dist}_{\mathrm{MK},2}(f(n\Delta t,\cdot,\cdot),f^n)\le D_T\Delta t^2 \tag{16}$$

for $n=0,1,\ldots,[T/\Delta t]$ with $0<\Delta t\le\frac{1}{2}$, with

$$D_T^2=\frac{e^{(2+\Lambda)T}-1}{2+\Lambda}M^3\left(1+e^{3T}(\nu_0+2M^2)\right)\,. \tag{17}$$

Putting together (11), (16) and (15) shows that

$$\begin{aligned}&E_\hbar(f^n,R^n)+\mathrm{dist}_{\mathrm{MK},2}(f(n\Delta t,\cdot,\cdot),f^n)+E_\hbar(f(n\Delta t,\cdot,\cdot),R(n\Delta t))\\ &\qquad\le 2E_\hbar(f^{in},R^{in})\exp\left(\tfrac{1}{2}T(1+\max(1,\mathrm{Lip}(\nabla V)^2))\right)+D_T\Delta t^2\,.\end{aligned}$$

By Proposition 2.6 (b) and the triangle inequality for $\mathrm{dist}_{\mathrm{MK},2}$,

$$\begin{aligned}&\mathrm{dist}_{\mathrm{MK},2}(\tilde W_\hbar(R^n),\tilde W_\hbar(R(n\Delta t)))\\ &\le 2E_\hbar(f^{in},R^{in})\exp\left(\tfrac{1}{2}T(1+\max(1,\mathrm{Lip}(\nabla V)^2))\right)+D_T\Delta t^2+2\sqrt{d\hbar}\end{aligned}$$

for $n=0,1,\ldots,[T/\Delta t]$ with $0<\Delta t\le\frac{1}{2}$. If R^{in} is the Töplitz operator with symbol $(2\pi\hbar)^d f^{in}$, this bound and Proposition 2.6 (c) imply the desired inequality in Theorem 3.2.

6. Uniform in $\hbar$ Error Estimates

Proof of Corollary 3.4. Throughout this section, we denote

$$\mathcal{U}(t):=\exp(-it(-\tfrac{1}{2}\hbar^2\Delta+V(x))/\hbar)\,,$$

and

$$\mathcal{U}_K(t):=\exp(\tfrac{1}{2}it\hbar\Delta)\,,\qquad \mathcal{U}_V(t):=\exp(-itV(x)/\hbar)\,.$$

For the first order time splitting, one has

$$\begin{aligned}&R_\hbar^n-R_\hbar(n\Delta t)\\ &=(\mathcal{U}_V(\Delta t)\mathcal{U}_K(\Delta t))^nR_\hbar^{in}(\mathcal{U}_K(\Delta t)^*\mathcal{U}_V(\Delta t)^*)^n-\mathcal{U}(n\Delta t)R_\hbar^{in}\mathcal{U}(n\Delta t)^*\\ &=\int_{\mathbf{R}^d\times\mathbf{R}^d}((\mathcal{U}_V(\Delta t)\mathcal{U}_K(\Delta t))^n-\mathcal{U}(n\Delta t))\,|q,p\rangle\langle q,p|(\mathcal{U}_K(\Delta t)^*\mathcal{U}_V(\Delta t)^*)^n\mu^{in}(dqdp)\\ &\quad+\int_{\mathbf{R}^d\times\mathbf{R}^d}\mathcal{U}(n\Delta t)|q,p\rangle\langle q,p|\,((\mathcal{U}_K(\Delta t)^*\mathcal{U}_V(\Delta t)^*)^n-\mathcal{U}(n\Delta t)^*)\,\mu^{in}(dqdp)\,.\end{aligned}$$

Hence

$$\|R_\hbar^n-R_\hbar(n\Delta t)\|_1\le 2\int_{\mathbf{R}^d\times\mathbf{R}^d}\|(\mathcal{U}_V(\Delta t)\mathcal{U}_K(\Delta t))^n-\mathcal{U}(n\Delta t))\,|q,p\rangle\|_{L^2(\mathbf{R}^d)}\,\mu^{in}(dqdp)\,.$$

At this point, we apply Theorem 2 from [5] for the error of the simple splitting scheme:

$$\begin{aligned}&\|(\mathcal{U}_V(\Delta t)\mathcal{U}_K(\Delta t))^n-\mathcal{U}(n\Delta t))\,|q,p\rangle\|_{L^2(\mathbf{R}^d)}\\ &\quad\le 2\frac{\Delta t}{\hbar}M(V)\left(M(V)t^2+\hbar\|\,|q,p\rangle\|_{H^1(\mathbf{R}^d)}\right),\end{aligned}$$

where

$$M(V) := \max(2\|\nabla V\|_{L^\infty(\mathbf{R}^d)}, \|\nabla^2 V\|_{L^\infty(\mathbf{R}^d)})\,.$$

One has

$$\hbar^2\left(\|\,|q,p\rangle\|^2_{L^2(\mathbf{R}^d)} + \|\,\nabla|q,p\rangle\|^2_{L^2(\mathbf{R}^d)}\right) = \hbar^2 + |p|^2 + \tfrac{d}{2}\hbar \le 2\hbar^2 + |p|^2 + d^2$$

so that

$$\|R^n_\hbar - R_\hbar(n\Delta t)\|_1 \le 4\frac{\Delta t}{\hbar}M(V)\left(M(V)t^2 + \sqrt{2}\hbar + d + \int_{\mathbf{R}^{2d}} |p|\mu^{in}(dqdp)\right). \tag{18}$$

Next we apply Lemmas 8.2 and 8.1 in [12]:

$$\begin{aligned}(19)\qquad &\mathrm{dist}_1(\tilde W_\hbar(R^n_\hbar), \tilde W_\hbar(R_\hbar(n\Delta t)))\\ &\le \min(\|\tilde W_\hbar(R^n_\hbar) - \tilde W_\hbar(R_\hbar(n\Delta t))\|_{L^1(\mathbf{R}^{2d})}, \mathrm{dist}_{\mathrm{MK},2}(\tilde W_\hbar(R^n_\hbar), \tilde W_\hbar(R_\hbar(n\Delta t))))\\ &\le \min(\|R^n_\hbar - R_\hbar(n\Delta t)\|_1, \mathrm{dist}_{\mathrm{MK},2}(\tilde W_\hbar(R^n_\hbar), \tilde W_\hbar(R_\hbar(n\Delta t))))\,.\end{aligned}$$

Using (18) and Theorem 3.1 to bound the right hand side of (19) shows that

$$\begin{aligned}&\mathrm{dist}_1(\tilde W_\hbar(R^n_\hbar),\tilde W_\hbar(R_\hbar(n\Delta t)))\\ &\quad\le \min\Bigg(4\frac{\Delta t}{\hbar}M(V)\left(M(V)t^2 + \sqrt{2}\hbar + d + \int_{\mathbf{R}^{2d}} |p|\mu^{in}(dqdp)\right),\\ &\qquad C_T\Delta t + 2\sqrt{d\hbar}\left(1 + \exp\left(\tfrac12 t(1+\max(1,\mathrm{Lip}(\nabla V)^2))\right)\right)\Bigg)\end{aligned} \tag{20}$$

so that

$$\begin{aligned}\mathrm{dist}_1(\tilde W_\hbar(R^n_\hbar), \tilde W_\hbar(R_\hbar(n\Delta t))) &\le C[T,V,\mu^{in}]\left(\Delta t + \min\left(\frac{\Delta t}{\hbar}, \sqrt{\hbar}\right)\right)\\ &= C[T,V,\mu^{in}]\left(\Delta t + \Delta t^{1/3}\right)\end{aligned}$$

with

$$\begin{aligned}(21)\qquad C[T,V,\mu^{in}] := \max\Bigg(&4\sqrt{2}M(V), C_T, 4M(V)\left(M(V)T^2 + d + \int_{\mathbf{R}^{2d}} |p|\mu^{in}(dqdp)\right)\\ &2\sqrt{d}\left(1 + \exp\left(\tfrac12 T(1+\max(1,\mathrm{Lip}(\nabla V)^2))\right)\right)\Bigg).\end{aligned}$$

□

Proof of Corollary 3.5. Arguing as in the proof of Corollary 3.4 for the Strang splitting, we write

$$\mathcal{S}(\Delta t) := \mathcal{U}_K(\tfrac{\Delta t}{2})\mathcal{U}_V(\Delta t)\mathcal{U}_K(\tfrac{\Delta t}{2})$$

and

$$\begin{aligned}R^n_\hbar - R_\hbar(n\Delta t) =& \mathcal{S}(\Delta t)^n R^{in}_\hbar(\mathcal{S}(\Delta t)^*)^n - \mathcal{U}(n\Delta t)R^{in}_\hbar\mathcal{U}(n\Delta t)^*\\ =& \int_{\mathbf{R}^d\times\mathbf{R}^d}(\mathcal{S}(\Delta t)^n - \mathcal{U}(n\Delta t))|q,p\rangle\langle q,p|(\mathcal{S}(\Delta t)^*)^n\mu^{in}(dqdp)\\ &+ \int_{\mathbf{R}^d\times\mathbf{R}^d}\mathcal{U}(n\Delta t)|q,p\rangle\langle q,p|(\mathcal{S}(\Delta t)^*)^n - \mathcal{U}(n\Delta t)^*)\mu^{in}(dqdp)\,,\end{aligned}$$

so that

$$\|R_\hbar^n - R_\hbar(n\Delta t)\|_1 \le 2\int_{\mathbf{R}^d\times\mathbf{R}^d} \|(\mathcal{S}(\Delta t)^n - \mathcal{U}(n\Delta t))|q,p\rangle\|_{L^2(\mathbf{R}^d)}\,\mu^{in}(dqdp)\,.$$

By Theorem 3 from [5]:

$$\|(\mathcal{S}(\Delta t)^n - \mathcal{U}(n\Delta t))|q,p\rangle\|_{L^2(\mathbf{R}^d)} \le M'[T,V,\mu^{in}]\frac{\Delta t^2}{\hbar}$$

where the constant M' depends on the final time T, on $\|V\|_{W^{4,\infty}(\mathbf{R}^d)}$, and on

$$\int_{\mathbf{R}^{2d}} |p|^2\mu^{in}(dqdp) < \infty\,,$$

since

$$\hbar\||q,p\rangle\|_{H^1(\mathbf{R}^d)} = O(|p|) \quad\text{ while }\quad \hbar^2\||q,p\rangle\|_{H^2(\mathbf{R}^d)} = O(|p|^2)\,.$$

Thus

(22)

$$\begin{aligned}&\operatorname{dist}_1(\tilde W_\hbar(R_\hbar^n), \tilde W_\hbar(R_\hbar(n\Delta t)))\\ &\le \min\left(M'[T,V,\mu^{in}]\frac{\Delta t^2}{\hbar}, D_T\Delta t^2 + 2\sqrt{d\hbar}\left(1+\exp\left(\tfrac12 t(1+\max(1,\operatorname{Lip}(\nabla V)^2))\right)\right)\right)\\ &\le D[T,V,\mu^{in}]\left(\Delta t^2 + \min\left(\frac{\Delta t^2}{\hbar},\sqrt{\hbar}\right)\right),\end{aligned}$$

where

(23)

$$D[T,V,\mu^{in}] := \max\left(D_T, M'[T,V,\mu^{in}], 2\sqrt{d}\left(1+\exp\left(\tfrac12 T(1+\max(1,\operatorname{Lip}(\nabla V)^2))\right)\right)\right)\,.$$

Optimizing in $\hbar$ leads to

$$\operatorname{dist}_1(\tilde W_\hbar(R_\hbar^n), \tilde W_\hbar(R_\hbar(n\Delta t))) \le D[T,V,\mu^{in}](\Delta t^2 + \Delta t^{2/3})$$

corresponding to the choice $\hbar = \Delta t^{4/3}$. □

Appendix A. Proof of Theorem 2.7

Let $Q^{in} \in \mathcal{C}(f^{in}, R^{in})$. Set

$$Q(t,X,\Xi) := U(t)^* Q^{in}\circ\Phi_{-t}(X,\Xi)U(t)$$

for all $t\in\mathbf{R}$ and a.e. $(x,\xi)\in\mathbf{R}^d\times\mathbf{R}^d$, and

$$\mathcal{E}(t) := \iint_{\mathbf{R}^{2d}} \operatorname{trace}_{\mathfrak{H}}(Q(t,X,\Xi)^{1/2}c(X,\Xi,y,\hbar D_y)Q(t,X,\Xi)^{1/2})dXd\Xi\,.$$

Since Φ_t leaves the phase space volume element $dxd\xi$ invariant

$$\mathcal{E}(t) = \iint_{\mathbf{R}^{2d}} \operatorname{trace}_{\mathfrak{H}}(\sqrt{Q^{in}(x,\xi)}U(t)c(\Phi_t(x,\xi),y,\hbar D_y)U(t)^*\sqrt{Q^{in}(x,\xi)})dx\xi\,.$$

By construction, $Q(t,\cdot,\cdot)\in\mathcal{C}(f(t,\cdot,\cdot),R(t))$. Indeed, for a.e. $(X,\Xi)\in\mathbf{R}^d$,

$$0 \le Q^{in}(\Phi_{-t}(X,\Xi)) = Q^{in}(\Phi_{-t}(X,\Xi))^* \in \mathcal{L}(\mathfrak{H})$$

so that $Q(t,X,\Xi)\in\mathcal{L}(\mathfrak{H})$ satisfies

$$\begin{aligned}Q(t,X,\Xi) =& U(t)Q^{in}(\Phi_{-t}(X,\Xi))U(t)^*\\ =& U(t)Q^{in}(\Phi_{-t}(X,\Xi))U(t)^* = Q(t,X,\Xi)^* \ge 0\,.\end{aligned}$$

Besides

$$\operatorname{trace}_{\mathfrak{H}}(Q(t,X,\Xi)) = \operatorname{trace}_{\mathfrak{H}}(Q^{in}(\Phi_{-t}(X,\Xi))) = f^{in}(\Phi_{-t}(X,\Xi)) = f(t,X,\Xi)$$

while

$$\begin{aligned}\iint_{\mathbf{R}^d\times\mathbf{R}^d} Q(t,X,\Xi)dXd\Xi &= U(t)\left(\iint_{\mathbf{R}^d\times\mathbf{R}^d} Q^{in}(\Phi_{-t}(X,\Xi))dXd\Xi\right)U(t)^* \\ &= U(t)\left(\iint_{\mathbf{R}^d\times\mathbf{R}^d} Q^{in}(x,\xi)dxd\xi\right)U(t)^* = U(t)R^{in}U(t)^* = R(t)\,.\end{aligned}$$

In particular

$$\mathcal{E}(t) \geq E_\hbar(f(t),R(t))\,, \qquad \text{for each } t\geq 0\,.$$

Let $e_j(x,\xi,\cdot)$ for $j\in\mathbf{N}$ be a $\mathfrak{H}$-complete orthonormal system of eigenvectors of $Q^{in}(x,\xi)$ for a.e. $x,\xi\in\mathbf{R}^d$. Hence

$$\begin{aligned}&\operatorname{trace}_{\mathfrak{H}}(\sqrt{Q^{in}(x,\xi)}U(t)c(\Phi_t(x,\xi),y,\hbar D_y)U(t)^*\sqrt{Q^{in}(x,\xi)}) \\ &= \sum_{j\in\mathbf{N}}\rho_j(x,\xi)\langle U(t)e_j(x,\xi)|c(\Phi_t(x,\xi),y,\hbar D_y)|U(t)e_j(x,\xi)\rangle\end{aligned}$$

where $\rho_j(x,\xi)$ is the eigenvalue of $Q^{in}(x,\xi)$ defined by

$$Q^{in}(x,\xi)e_j(x,\xi) = \rho_j(x,\xi)e_j(x,\xi)\,, \quad \text{for a.e. } (x,\xi)\in\mathbf{R}^d\times\mathbf{R}^d\,.$$

If $\phi\equiv\phi(y)\in C_c^\infty(\mathbf{R}^d)$, the map

$$t\mapsto\langle U(t)\phi|c(\Phi_t(x,\xi),y,\hbar D_y)|U(t)\phi\rangle$$

is of class C^1 on $\mathbf{R}$, and one has

$$\begin{aligned}&\frac{d}{dt}\langle U(t)\phi|c(\Phi_t(x,\xi),y,\hbar D_y)|U(t)\phi\rangle \\ &= \left\langle\frac{i}{\hbar}\mathcal{H}U(t)\phi\middle|c(\Phi_t(x,\xi),y,\hbar D_y)\middle|U(t)\phi\right\rangle \\ &+\left\langle U(t)\phi\middle|c(\Phi_t(x,\xi),y,\hbar D_y)\middle|\frac{i}{\hbar}\mathcal{H}U(t)\phi\right\rangle \\ &+\langle U(t)\phi|\{H(\Phi_t(x,\xi)),c(\Phi_t(x,\xi),y,\hbar D_y)\}|U(t)\phi\rangle\,.\end{aligned}$$

In other words

$$\begin{aligned}&\frac{d}{dt}\langle U(t)\phi|c(\Phi_t(x,\xi),y,\hbar D_y)|U(t)\phi\rangle \\ &= \left\langle U(t)\phi\middle|\frac{i}{\hbar}[\mathcal{H},c(\Phi_t(x,\xi),y,\hbar D_y)]\middle|U(t)\phi\right\rangle \\ &+\langle U(t)\phi|\{H(\Phi_t(x,\xi)),c(\Phi_t(x,\xi),y,\hbar D_y)\}|U(t)\phi\rangle\,.\end{aligned}$$

A straightforward computation shows that

$$\begin{aligned}
\{H_\lambda(\Phi_t(x,\xi)), c(\Phi_t(x,\xi),y,\hbar D_y)\} + \frac{i}{\hbar}[\mathcal{H}_\lambda, c_\lambda(\Phi_t(x,\xi),y,\hbar D_y)]\\
= \lambda\sum_{k=1}^d ((X_k-y_k)(\Xi_k-\hbar D_{y_k})+(\Xi_k-\hbar D_{y_k})(X_k-y_k))\\
-\sum_{k=1}^d ((\partial_k V(X)-\partial_k V(y))(\Xi_k-\hbar D_{y_k})+(\Xi_k-\hbar D_{y_k})(\partial_k V(X)-\partial_k V(y)))\\
\le \lambda\sum_{k=1}^d (|X_k-y_k|^2+|\Xi_k-\hbar D_{y_k}|^2)+\sum_{k=1}^d \left(|\partial_k V(X)-\partial_k V(y)|^2+|\Xi_k-\hbar D_{y_k}|^2\right)\\
\le \lambda\sum_{k=1}^d (|X_k-y_k|^2+|\Xi_k-\hbar D_{y_k}|^2)+\max(1,\operatorname{Lip}(\nabla V)^2)\sum_{k=1}^d \left(|X_k-y|^2+|\Xi_k-\hbar D_{y_k}|^2\right)\\
\le \left(\lambda+\max(1,\operatorname{Lip}(\nabla V)^2)\right)c(X,\Xi,y,\hbar D_y)\,.
\end{aligned}$$

Hence

$$\begin{aligned}
\langle U(t)\phi|c(\Phi_t(x,\xi),y,\hbar D_y)|U(t)\phi\rangle \le \langle\phi|c(x,\xi,y,\hbar D_y)|\phi\rangle\\
+\left(\lambda+\max(1,\operatorname{Lip}(\nabla V)^2)\right)\int_0^t \langle U(s)\phi|c(\Phi_s(x,\xi),y,\hbar D_y)|U(s)\phi\rangle ds
\end{aligned}$$

so that

$$\begin{aligned}
\langle U(t)\phi|c(\Phi_t(x,\xi),y,\hbar D_y)|U(t)\phi\rangle\\
\le \langle\phi|c(x,\xi,y,\hbar D_y)|\phi\rangle \exp\left(\left(\lambda+\max(1,\operatorname{Lip}(\nabla V)^2)\right)t\right)
\end{aligned}$$

for each $\phi\in C_c^\infty(\mathbf{R}^d)$. By density of $C_c^\infty(\mathbf{R}^d)$ in the form domain of $c(x,\xi,y,\hbar D_y)$

$$\begin{aligned}
0\le \langle U(t)e_j(x,\xi)|c(\Phi_t(x,\xi),y,\hbar D_y)|U(t)e_j(x,\xi)\rangle\\
\le \langle e_j(x,\xi)|c_\lambda(x,\xi,y,\hbar D_y)|e_j(x,\xi)\rangle \exp\left(\left(\lambda+\max(1,\operatorname{Lip}(\nabla V)^2)\right)t\right)
\end{aligned}$$

for a.e. $(x,\xi)\in\mathbf{R}^d\times\mathbf{R}^d$, so that

$$\begin{aligned}
\operatorname{trace}_{\mathfrak{H}}(\sqrt{Q^{in}(x,\xi)}U(t)c(\Phi_t(x,\xi),y,\hbar D_y)U(t)^*\sqrt{Q^{in}(x,\xi)})\\
=\sum_{j\in\mathbf{N}}\rho_j(x,\xi)\langle U(t)e_j(x,\xi)|c(\Phi_t(x,\xi),y,\hbar D_y)|U(t)e_j(x,\xi)\rangle\\
\le \exp\left(\left(\lambda+\max(1,\operatorname{Lip}(\nabla V)^2)\right)t\right)\sum_{j\in\mathbf{N}}\rho_j(x,\xi)\langle e_j(x,\xi)|c(x,\xi,y,\hbar D_y)|e_j(x,\xi)\rangle\\
=\exp\left(\left(\lambda+\max(1,\operatorname{Lip}(\nabla V)^2)\right)t\right)\operatorname{trace}_{\mathfrak{H}}(\sqrt{Q^{in}(x,\xi)}c(x,\xi,y,\hbar D_y)\sqrt{Q^{in}(x,\xi)})\,.
\end{aligned}$$

Integrating both side of this inequality over $\mathbf{R}^d\times\mathbf{R}^d$ shows that

$$\mathcal{E}(t)\le\mathcal{E}(0)\exp\left(\left(\lambda+\max(1,\operatorname{Lip}(\nabla V)^2)\right)t\right)\,.$$

Hence, for each $t\ge 0$ and each $Q^{in}\in\mathcal{C}(f,R)$, one has

$$E_\hbar(f(t),R(t))^2\le\mathcal{E}(0)\exp\left(\left(\lambda+\max(1,\operatorname{Lip}(\nabla V)^2)\right)t\right)\,.$$

Minimizing the right hand side of this inequality as Q^{in} runs through $\mathcal{C}(f^{in},R^{in})$ leads to the desired inequality.

Appendix B. Expressing Theorems 3.1, 3.2 in Terms of Density Operators

In this appendix, we express our main results, Theorems 3.1, 3.2 with their Corollaries 3.4 and 3.5, as upper bounds on some appropriate distance between the exact solution of the von Neumann equation and its time-splitting approximation.

Definition B.1. *For all $R,S\in\mathcal{D}(\mathfrak{H})$ and each integer $M\ge 0$, we set*

$$d_M(R,S):=\sup_{\max_{|\alpha|,|\beta|\le M}\|\mathcal{D}^\alpha_{-i\hbar\nabla}\mathcal{D}^\beta_x F\|_1\le 1}|\operatorname{trace}(F(R-S))|\,,$$

where $\mathcal{D}_A=\frac{1}{i\hbar}[A,\cdot]$ for each (possibly unbounded) self-adjoint operator A on $\mathfrak{H}$.

One might worry that the definition of d_M involves $\hbar$ through the operator $-i\hbar\nabla$ and in the definition of $\mathcal{D}_A$. However, the correspondence principle in quantum mechanics stipulates that $\frac{i}{\hbar}[\cdot,\cdot]$ is the quantum analogue of the usual Poisson bracket $\{\cdot,\cdot\}$, while $-i\hbar\nabla$ is the momentum operator, that is the quantum analogue of the momentum variable in the Hamiltonian formulation of classical mechanics. Therefore, both expressions $\frac{i}{\hbar}[\cdot,\cdot]$ and $-i\hbar\nabla$ should be thought of as being "of order $\hbar^0$" in the semiclassical regime.

First we check that d_M metrizes $\mathcal{D}(\mathfrak{H})$. The (uninteresting) case $M=0$ corresponds to the distance associated to the operator norm: $d_0(R,S)=\|R-S\|$.

Lemma B.2. *The function $d_M:\mathcal{D}(\mathfrak{H})\times\mathcal{D}(\mathfrak{H})\to[0,+\infty[$ is a distance.*

Proof. That d_M is symmetric and satisfies the triangle inequality is obvious by construction. The only thing to check is the separation property.

Let $f\equiv f(q,p)\in\mathcal{S}(\mathbf{R}^d\times\mathbf{R}^d)$ and set $F:=\operatorname{OP}^T_\hbar(f)$. Elementary computations show that

$$[x_j,\operatorname{OP}^T_\hbar(f)]=\operatorname{OP}^T_\hbar(-i\hbar\partial_p f)\,,\qquad[-i\hbar\partial_{x_j},\operatorname{OP}^T_\hbar(f)]=\operatorname{OP}^T_\hbar(i\hbar\partial_q f)\,.$$

Moreover, for each bounded Borel measure μ on $\mathbf{R}^d\times\mathbf{R}^d$, one has

$$\|\operatorname{OP}^T_\hbar(\mu)\|_1\le\frac{1}{(2\pi\hbar)^d}\iint_{\mathbf{R}^d\times\mathbf{R}^d}|\mu|(dqdp)\,.$$

(To see this, split μ into its positive and negative parts as $\mu^+-\mu^-$, and observe that

$$\|\operatorname{OP}^T_\hbar(\mu^\pm)\|_1=\operatorname{trace}_{\mathfrak{H}}(\operatorname{OP}^T_\hbar(\mu^\pm))=\frac{1}{(2\pi\hbar)^d}\iint_{\mathbf{R}^d\times\mathbf{R}^d}\mu^\pm(dqdp)\,,$$

together with the fact that $\mu^\pm\ge 0$ implies that $\operatorname{OP}^T_\hbar(\mu^\pm)\ge 0$, while $|\mu|=\mu^++\mu^-$.) Therefore

$$\begin{aligned}d_M(R,S)&\ge\sup_{\substack{f\in\mathcal{S}(\mathbf{R}^d\times\mathbf{R}^d)\\ \max_{|\alpha|,|\beta|\le M}\|\partial^\alpha_\xi\partial^\beta_x f\|_{L^\infty}\le 1}}|\operatorname{trace}_{\mathfrak{H}}(\operatorname{OP}^T_\hbar(f)(R-S))|\\&=\sup_{\substack{f\in\mathcal{S}(\mathbf{R}^d\times\mathbf{R}^d)\\ \max_{|\alpha|,|\beta|\le M}\|\partial^\alpha_\xi\partial^\beta_x f\|_{L^\infty}\le 1}}\iint_{\mathbf{R}^d\times\mathbf{R}^d}f(q,p)(\tilde W_\hbar(R)-\tilde W_\hbar(S))(q,p)dqdp\,.\end{aligned}\tag{24}$$

Therefore $d_M(R,S)=0$ implies that $\tilde W_\hbar(R)=\tilde W_\hbar(S)$ in $\mathcal{S}'(\mathbf{R}^d\times\mathbf{R}^d)$ and therefore pointwise on $\mathbf{R}^d\times\mathbf{R}^d$ (since $\tilde W_\hbar(R),\tilde W_\hbar(S)$ are analytic functions on phase space). Since any density operator on $\mathfrak{H}$ is uniquely determined by its Husimi transform (see Remark 2.3 on p. 64 in [10]), this implies in turn that $R=S$. ∎

Next we formulate our main results, i.e. Theorems 3.1, 3.2 with their Corollaries 3.4 and 3.5 in terms of the distance d_M between the exact solution of the von Neumann equation and its time-splitting approximation. Here is the result for the simple splitting method.

Theorem B.3 (Simple splitting)**.** *Under the same assumptions and with the same constants as in Theorem 3.1, one has*

$$d_{[d/2]+2}(R^n, R(n\Delta t)) \le C_T\Delta t + 2\sqrt{d\hbar}\left(D_d + \exp\left(\tfrac{1}{2}T(1+\max(1,\operatorname{Lip}(\nabla V)^2))\right)\right),$$

where the constant $D_d > 0$ depends only on the dimension d and is defined in (25)*.*

Under the same assumptions and with the same constants as in Corollary 3.4,

$$d_{[d/2]+2}(R^n, R(n\Delta t)) \le C'[T, V, \mu^{in}]\Delta t^{1/3},$$

where $C'[T, V, \mu^{in}]$ is defined in (27)*.*

As for the Strang splitting method, one has the following convergence estimate.

Theorem B.4 (Strang splitting)**.** *Under the same assumptions and with the same constants as in Theorem 3.2, one has*

$$d_{[d/2]+2}(R^n, R(n\Delta t)) \le D_T\Delta t^2 + 2\sqrt{d\hbar}\left(D_d + \exp\left(\tfrac{1}{2}T(1+\max(1,\operatorname{Lip}(\nabla V)^2))\right)\right),$$

where the constant $D_d > 0$ depends only on the dimension d and is defined in (25)*.*

Under the same assumptions and with the same constants as in Corollary 3.5,

$$d_{[d/2]+2}(R^n, R(n\Delta t)) \le D'[T, V, \mu^{in}]\Delta t^{2/3},$$

where $D'[T, V, \mu^{in}]$ is defined in (28)*.*

These four results are obvious or straightforward corollaries of Theorems 3.1 and 3.2, and of Corollaries 3.4 and 3.5, and of the following proposition.

Proposition B.5. *Let $R, S \in \mathcal{D}^2(\mathfrak{H})$, with Wigner transforms $W_\hbar(R), W_\hbar(S)$ and Husimi transforms $\tilde{W}_\hbar(R), \tilde{W}_\hbar(S)$. For each integer $M \ge 0$, define*

$$\delta_M(W_\hbar(R), W_\hbar(S)) := \sup_{\substack{f\in L^2(\mathbf{R}^{2d})\\ \max_{|\alpha|,|\beta|\le M}\|\partial_x^\alpha\partial_\xi^\beta f\|_{L^\infty}\le 1}} \left|\int (W_\hbar(R)(x,\xi) - W_\hbar(S)(x,\xi))f(x,\xi)dxd\xi\right|.$$

Then

$$d_{[d/2]+2}(R, S) \le \delta_{[d/2]+2}(W_\hbar(R), W_\hbar(S)) \le \operatorname{dist}_{\mathrm{MK},2}(\widetilde{W}_\hbar(R), \widetilde{W}_\hbar(S)) + C_d\sqrt{\hbar}$$

where $C_d > 0$ depends only on the dimension d and is given by (29)*. Moreover*

$$\delta_{[d/2]+1}(W_\hbar(R), W_\hbar(S)) \le \|R - S\|_1.$$

Indeed, the first inequality in Proposition B.5 together with Theorem 3.1 (resp. Theorem 3.2) immediately implies the first inequality in Theorem B.3 (resp. Theorem B.4), with

$$D_d := 1 + \frac{C_d}{2\sqrt{d}}. \tag{25}$$

For the uniform bounds in Theorems B.3 and B.4, we proceed as follows: first, Proposition B.5 implies that

$$\begin{aligned} &d_{[d/2]+2}(R_\hbar^n, R_\hbar(n\Delta t)) \\ &\le \min(\|R_\hbar^n - R_\hbar(n\Delta t)\|_1, \mathrm{dist}_{\mathrm{MK},2}(\tilde W_\hbar(R_\hbar^n), \tilde W_\hbar(R_\hbar(n\Delta t))) + C_d\sqrt{\hbar})\,. \end{aligned} \tag{26}$$

Now, in the case of the simple splitting method, we bound $\|R_\hbar^n - R_\hbar(n\Delta t)\|_1$ as in (18), and $\mathrm{dist}_{\mathrm{MK},2}(\tilde W_\hbar(R_\hbar^n), \tilde W_\hbar(R_\hbar(n\Delta t)))$ as in Theorem 3.1. This gives the inequality

$$\begin{aligned} &d_{[d/2]+2}(R_\hbar^n, R_\hbar(n\Delta t)) \\ &\le \min\Bigg(4\frac{\Delta t}{\hbar}M(V)\left(M(V)t^2 + \sqrt{2}\hbar + d + \int_{\mathbf{R}^{2d}} |p|\mu^{in}(dqdp)\right), \\ &\quad C_T\Delta t + 2\sqrt{d\hbar}\left(D_d + \exp\left(\tfrac12 T\left(1 + \max\left(1, \mathrm{Lip}(\nabla V)^2\right)\right)\right)\right)\Bigg). \end{aligned}$$

This implies the second inequality in Theorem B.3 by the same argument as in the proof of Corollary 3.4, with

$$\begin{aligned} C'[T,V,\mu^{in}] := \max\Bigg(&4\sqrt{2}M(V), C_T, 4M(V)\left(M(V)T^2 + d + \int_{\mathbf{R}^{2d}} |p|\mu^{in}(dqdp)\right) \\ &2\sqrt{d}\left(D_d + \exp\left(\tfrac12 T(1 + \max(1, \mathrm{Lip}(\nabla V)^2))\right)\right)\Bigg). \end{aligned} \tag{27}$$

The case of the Strang splitting method is treated similarly: in the right hand side of (26), the first argument in the max, i.e. $\|R_\hbar^n - R_\hbar(n\Delta t)\|_1$ is bounded by $M'[T,V,\mu^{in}]\Delta t^2/\hbar$ as in the proof of Corollary 3.5, while the second argument in the max, i.e. $\mathrm{dist}_{\mathrm{MK},2}(\tilde W_\hbar(R_\hbar^n), \tilde W_\hbar(R_\hbar(n\Delta t)))$ is bounded as in Theorem 3.2. Proceeding in this way, one arrives at

$$\begin{aligned} &d_{[d/2]+2}(R_\hbar^n, R_\hbar(n\Delta t)) \\ &\le \min\left(M'[T,V,\mu^{in}]\frac{\Delta t^2}{\hbar}, D_T\Delta t^2 + 2\sqrt{d\hbar}\left(D_d + \exp\left(\tfrac12 t(1 + \max(1, \mathrm{Lip}(\nabla V)^2))\right)\right)\right) \end{aligned}$$

This implies the second inequality in Theorem B.4 by the same argument as in the proof of Corollary 3.5, with

$$\begin{aligned} D'[T,V,\mu^{in}] := \max\Big(&D_T, M'[T,V,\mu^{in}], \\ &2\sqrt{d}\left(D_d + \exp\left(\tfrac12 T(1 + \max(1, \mathrm{Lip}(\nabla V)^2))\right)\right)\Big). \end{aligned} \tag{28}$$

Proof of Proposition B.5. The proof is split in several steps.
(a) Proof of the first right inequality. For each $f \in \mathcal{S}(\mathbf{R}^d \times \mathbf{R}^d)$, write

$$\begin{aligned} \iint_{\mathbf{R}^d\times\mathbf{R}^d} f(x,\xi)(W_\hbar(R-S))(x,\xi)dxd\xi &= \iint_{\mathbf{R}^d\times\mathbf{R}^d} f(x,\xi)(\tilde W_\hbar(R-S))(x,\xi)dxd\xi \\ &\quad - \iint_{\mathbf{R}^d\times\mathbf{R}^d} g(x,\xi)(W_\hbar(R-S))(x,\xi)dxd\xi\,, \end{aligned}$$

where $g := e^{\hbar\Delta_{x,\xi}/4}f - f$. Since $R, S \in \mathcal{L}^1(\mathfrak{H}) \subset \mathcal{L}^2(\mathfrak{H})$, and the Plancherel theorem implies that

$$\|W_\hbar(T)\|^2_{L^2(\mathbf{R}^d\times\mathbf{R}^d)} = \frac{1}{(2\pi\hbar)^d}\|T\|_2^2$$

for each Hilbert-Schmidt operator T, by using the formula expressing $\|T\|_2$ in terms of the integral kernel of T, all the integrals above are well defined. First

$$\left|\iint_{\mathbf{R}^d\times\mathbf{R}^d} f(x,\xi)(\tilde{W}_\hbar(R-S))(x,\xi)dxd\xi\right| \le \operatorname{Lip}(f)\operatorname{dist}_{\mathrm{MK},2}(\tilde{W}_\hbar(R),\tilde{W}_\hbar(S))$$

by using successively formulas (7.1) and formula (7.3) in chapter 7 of [20]. On the other hand

$$\iint_{\mathbf{R}^d\times\mathbf{R}^d} g(x,\xi)(W_\hbar(R-S))(x,\xi)dxd\xi = \operatorname{trace}_{\mathfrak{H}}(\mathrm{OP}^W_\hbar(g)(R-S))$$

where $\mathrm{OP}^W_\hbar(a)$ is the Weyl operator of symbol $a \equiv a(x,\xi) \in \mathcal{S}(\mathbf{R}^d\times\mathbf{R}^d)$, whose integral kernel is the function

$$(x,y) \mapsto \tfrac{1}{(2\pi\hbar)^d}\int_{\mathbf{R}^d} a\left(\tfrac{1}{2}(x+y),\zeta\right)e^{i\zeta\cdot(x-y)/\hbar}d\zeta\,.$$

According to the Calderon-Vaillancourt theorem (see [3])

$$\|\,\mathrm{OP}^W_\hbar(g)\| \le \gamma_d \max_{|\alpha|,|\beta|\le d/2+1}\|\partial_x^\alpha\partial_\xi^\beta g\|_{L^\infty(\mathbf{R}^d\times\mathbf{R}^d)}\,.$$

On the other hand

$$\begin{aligned}\partial_x^\alpha\partial_\xi^\beta g(x,\xi) &= \left((e^{\hbar\Delta_{x,\xi}/4}-I)\partial_x^\alpha\partial_\xi^\beta f\right)(x,\xi)\\ &= \tfrac{1}{\pi^d}\iint_{\mathbf{R}^d\times\mathbf{R}^d}(\partial_x^\alpha\partial_\xi^\beta f(x+\hbar^{1/2}z,\xi+\hbar^{1/2}\zeta)-\partial_x^\alpha\partial_\xi^\beta f(x,\xi))e^{-|z|^2-|\zeta|^2}dzd\zeta\,,\end{aligned}$$

so that

$$\begin{aligned}&\max_{|\alpha|,|\beta|\le d/2+1}\|\partial_x^\alpha\partial_\xi^\beta g\|_{L^\infty(\mathbf{R}^d\times\mathbf{R}^d)}\\ &\le\sqrt{\hbar}\max_{|\alpha|,|\beta|\le d/2+2}\|\partial_x^\alpha\partial_\xi^\beta f\|_{L^\infty(\mathbf{R}^d\times\mathbf{R}^d)}\tfrac{1}{\pi^d}\iint_{\mathbf{R}^d\times\mathbf{R}^d}(|z|+|\zeta|)e^{-|z|^2-|\zeta|^2}dzd\zeta\\ &\le d\pi^{-1/2}\sqrt{\hbar}\max_{|\alpha|,|\beta|\le d/2+2}\|\partial_x^\alpha\partial_\xi^\beta f\|_{L^\infty(\mathbf{R}^d\times\mathbf{R}^d)}\,.\end{aligned}$$

Therefore

$$\begin{aligned}\left|\iint_{\mathbf{R}^d\times\mathbf{R}^d} f(x,\xi)(W_\hbar(R-S))(x,\xi)dxd\xi\right| &\le \operatorname{Lip}(f)\operatorname{dist}_{\mathrm{MK},2}(\tilde{W}_\hbar(R),\tilde{W}_\hbar(S))\\ &\quad+\tfrac{d}{\sqrt{\pi}}\gamma_d\sqrt{\hbar}\max_{|\alpha|,|\beta|\le d/2+2}\|\partial_x^\alpha\partial_\xi^\beta f\|_{L^\infty(\mathbf{R}^d\times\mathbf{R}^d)}(\|R\|_1+\|S\|_1)\\ &\le \operatorname{dist}_{\mathrm{MK},2}(\tilde{W}_\hbar(R),\tilde{W}_\hbar(S))+\tfrac{2d}{\sqrt{\pi}}\gamma_d\sqrt{\hbar}\end{aligned}$$

for all $f \in \mathcal{S}(\mathbf{R}^d\times\mathbf{R}^d)$ such that

$$\max_{|\alpha|,|\beta|\le d/2+2}\|\partial_x^\alpha\partial_\xi^\beta f\|_{L^\infty(\mathbf{R}^d\times\mathbf{R}^d)} \le 1\,.$$

By density of $\mathcal{S}(\mathbf{R}^d\times\mathbf{R}^d)$ in $L^2(\mathbf{R}^d\times\mathbf{R}^d)$, this implies the first right inequality with

$$C_d := \tfrac{2d}{\sqrt{\pi}}\gamma_d \tag{29}$$

where γ_d is the constant that appears in the Calderon-Vaillancourt theorem (as stated in [3]).

(b) Proof of the first left inequality. Elementary computations show that

$$W_\hbar(T)(x,\xi) = \operatorname{trace}_{\mathfrak{H}}(T\mathcal{N}(x,\xi))\,,$$

where $\mathcal{N}(x,\xi)$ is the operator defined, for each $\phi \in \mathfrak{H}$, by the formula

$$(\mathcal{N}(x,\xi)\phi)(Y) = \frac{1}{(\pi\hbar)^d}\phi(2x-Y)e^{-2i\xi\cdot(x-Y)/\hbar}\,.$$

Moreover

$$\mathcal{N}(x,\xi) = \frac{1}{(\pi\hbar)^d}e^{\frac{i}{\hbar}\xi\cdot Y}e^{-\frac{i}{\hbar}(-i\hbar x\cdot\nabla_Y)}Je^{\frac{i}{\hbar}(-i\hbar x\cdot\nabla_Y)}e^{-\frac{i}{\hbar}\xi\cdot Y}$$

where $J\phi(Y) := \phi(-Y)$. Hence

$$\partial_{\xi_j}\mathcal{N}(x,\xi) = -\frac{1}{i\hbar}[Y_j,\mathcal{N}(x,\xi)]\,,\quad \partial_{x_j}\mathcal{N}(x,\xi) = \frac{1}{i\hbar}[-i\hbar\partial_{Y_j},\mathcal{N}(x,\xi)]\,,\quad j=1,\dots,d\,.$$

Since $\mathcal{D}_{Y_j}$ and $\mathcal{D}_{-i\hbar\partial_{Y_k}}$ commute for all $j,k=1,\dots,d$ by the canonical commutation relations,

$$\partial_x^\alpha\partial_\xi^\beta\mathcal{N}(x,\xi) = (-1)^{|\beta|}\mathcal{D}_Y^\beta\mathcal{D}_{-i\hbar\partial_Y}^\alpha\mathcal{N}(x,\xi)\,,$$

and therefore

$$\begin{aligned}\partial_x^\alpha\partial_\xi^\beta W_\hbar(T)(x,\xi) =& (-1)^{|\beta|}\operatorname{trace}_{\mathfrak{H}}(T\mathcal{D}_Y^\beta\mathcal{D}_{-i\hbar\partial_Y}^\alpha\mathcal{N}(x,\xi))\\ =& (-1)^{|\alpha|}\operatorname{trace}_{\mathfrak{H}}(\mathcal{N}(x,\xi)\mathcal{D}_Y^\beta\mathcal{D}_{-i\hbar\partial_Y}^\alpha T)\\ =& (-1)^{|\alpha|}W_\hbar(\mathcal{D}_Y^\beta\mathcal{D}_{-i\hbar\partial_Y}^\alpha T)(x,\xi)\\ =& (-1)^{|\alpha|}\operatorname{trace}_{\mathfrak{H}}(\mathcal{N}(x,\xi)\mathcal{D}_Y^\beta\mathcal{D}_{-i\hbar\partial_Y}^\alpha T)\end{aligned}$$

for all $\alpha,\beta\in\mathbf{N}^d$ and each T such that $\mathcal{D}_Y^\beta\mathcal{D}_{-i\hbar\partial_Y}^\alpha T\in\mathcal{L}^1(\mathfrak{H})$. Hence

$$\|\partial_x^\alpha\partial_\xi^\beta W_\hbar(T)\|_{L^\infty(\mathbf{R}^d\times\mathbf{R}^d)} \le \frac{1}{(\pi\hbar)^d}\|\mathcal{D}_Y^\beta\mathcal{D}_{-i\hbar\partial_Y}^\alpha T\|_1$$

for all $\alpha,\beta\in\mathbf{N}^d$ and each T such that $\mathcal{D}_Y^\beta\mathcal{D}_{-i\hbar\partial_Y}^\alpha T\in\mathcal{L}^1(\mathfrak{H})$.

Now, for each $R,S\in\mathcal{D}(\mathfrak{H})$ and each $F\in\mathcal{L}^1(\mathfrak{H})$, one has

$$\operatorname{trace}_{\mathfrak{H}}(F^*(R-S)) = (2\pi\hbar)^d\iint_{\mathbf{R}^d\times\mathbf{R}^d}\overline{W_\hbar(F)(x,\xi)}W_\hbar(R-S)(x,\xi)dxd\xi\,.$$

Thus

$$\begin{aligned}d_M(R,S) \le& \sup_{\max_{|\alpha|,|\beta|\le M}\|\mathcal{D}_Y^\beta\mathcal{D}_{-i\hbar\partial_Y}^\alpha F\|_1\le1}|\operatorname{trace}_{\mathfrak{H}}(F(R-S))|\\ \le& \sup_{\max_{|\alpha|,|\beta|\le M}\|(\pi\hbar)^d\partial_x^\alpha\partial_\xi^\beta W_\hbar(F)\|_{L^\infty}\le1}(2\pi\hbar)^d\iint_{\mathbf{R}^d\times\mathbf{R}^d}W_\hbar(F)W_\hbar(R-S)(x,\xi)dxd\xi\\ \le& \sup_{\substack{f\in L^2(\mathbf{R}^d\times\mathbf{R}^d)\\(\pi\hbar)^d\max_{|\alpha|,|\beta|\le M}\|\partial_x^\alpha\partial_\xi^\beta f\|_{L^\infty}\le1}}\left|\iint_{\mathbf{R}^d\times\mathbf{R}^d}(2\pi\hbar)^d fW_\hbar(R-S)(x,\xi)dxd\xi\right|\\ \le& \sup_{\substack{g\in L^2(\mathbf{R}^d\times\mathbf{R}^d)\\\max_{|\alpha|,|\beta|\le M}\|\partial_x^\alpha\partial_\xi^\beta g\|_{L^\infty}\le1}}2^d\left|\iint_{\mathbf{R}^d\times\mathbf{R}^d}gW_\hbar(R-S)(x,\xi)dxd\xi\right|\\ \le& 2^d\delta_M(W_\hbar(R),W_\hbar(S))\,,\end{aligned}$$

which implies the first left inequality.

(c) Proof of the second inequality. Proceeding as in step (a) above, one has, for each $g \in \mathcal{S}(\mathbf{R}^d \times \mathbf{R}^d)$,

$$\begin{aligned}\left|\iint_{\mathbf{R}^d\times\mathbf{R}^d} gW_\hbar(R-S)(x,\xi)dxd\xi\right| &= |\operatorname{trace}_{\mathfrak{H}}(\mathrm{OP}^W_\hbar(g)(R-S))| \\ &\le \|\mathrm{OP}^W_\hbar(g)\|\|R-S\|_1 \\ &\le \gamma_d \max_{|\alpha|,|\beta|\le[d/2]+1} \|\partial_x^\alpha\partial_\xi^\beta g\|_{L^\infty(\mathbf{R}^d\times\mathbf{R}^d)}\|R-S\|_1\end{aligned}$$

by the Calderon-Vaillancourt theorem (see [3]). This implies the second inequality by density of $\mathcal{S}(\mathbf{R}^d \times \mathbf{R}^d)$ in $L^2(\mathbf{R}^d \times \mathbf{R}^d)$. □

Remark B.6. *Two remarks are in order after this proof.*
(1) The same argument as in step (a) of the proof of Proposition B.5 implies that, for each probability density ρ on $\mathbf{R}^d \times \mathbf{R}^d$ such that

$$\iint_{\mathbf{R}^d\times\mathbf{R}^d} (|x|^2 + |\xi|^2)\rho(x,\xi)dxd\xi < \infty$$

one has

$$\begin{aligned}\delta_{[d/2]+2}(\rho, W_\hbar(S)) &\le \operatorname{dist}_{\mathrm{MK},2}(\rho, \tilde{W}_\hbar(S)) + \tfrac{1}{2}C_d\sqrt{\hbar} \\ &\le \sqrt{E_\hbar(\rho,S)^2 + d\hbar} + \tfrac{1}{2}C_d\sqrt{\hbar} \le E_\hbar(\rho,S)) + \left(\tfrac{1}{2}C_d + \sqrt{d}\right)\sqrt{\hbar}\,.\end{aligned}$$

(The second inequality follows from Proposition 2.6 (b), the third being obvious.) While we do not use this bound here, it may be of independent interest.
(2) Of course, one can also use the first right inequality in Proposition B.5 to express Theorems B.3 and B.4 in terms of $\delta_{[d/2]+2}(W_\hbar(R^n_\hbar), W_\hbar(R_\hbar(n\Delta t)))$ instead of $d_{[d/2]+2}(R^n_\hbar, R_\hbar(n\Delta t))$. We have chosen not to add these bounds in the statements of Theorems B.3 and B.4 for the sake of simplicity.

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