PROPAGATION OF QUANTUM EXPECTATIONS WITH HUSIMI FUNCTIONS

JOHANNES KELLER * AND CAROLINE LASSER †

Abstract. We analyse the dynamics of expectation values of quantum observables for the time-dependent semiclassical Schrödinger equation. To benefit from the positivity of Husimi functions, we switch between observables obtained from Weyl and Anti-Wick quantization. We develop and prove a second order Egorov type propagation theorem with Husimi functions by establishing transition and commutator rules for Weyl and Anti-Wick operators. We provide a discretized version of our theorem and present numerical experiments for Schrödinger equations in dimensions two and six that validate our results.

Key words. time-dependent Schrödinger equation, expectation values, Husimi functions

AMS subject classifications. 81S30, 81Q20, 81-08, 65D30, 65Z05

1. Introduction. Our investigation is devoted to the time-dependent Schrödinger equation

$$i\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi + V\psi, \qquad \psi(0) = \psi_0$$
 (1.1)

for general square integrable initial data $\psi_0: \mathbb{R}^d \to \mathbb{C}$ with $\|\psi_0\|_{L^2} = 1$. We assume that the potential $V: \mathbb{R}^d \to \mathbb{R}$ is smooth and satisfies suitable growth conditions at infinity, such that the semi-classical Schrödinger operator

$$H = -\frac{\varepsilon^2}{2}\Delta + V$$

is essentially selfadjoint. Such potentials are met in molecular quantum dynamics for the effective description of nuclear motion after performing the time-dependent Born-Oppenheimer approximation [ST01, Theorem 1]. In this application, the parameter ε is the square root of the ratio of electronic versus average nuclear mass. Hence, $\varepsilon > 0$ is small and typically ranges between ½1000 and ½10. This implies that the solution of (1.1) is highly oscillatory in space and time with frequencies of the order ½ ε . However, the time evolution of expectation values

$$t \mapsto \langle \psi_t, A\psi_t \rangle_{L^2} = \int_{\mathbb{R}^d} \overline{\psi_t(x)} A\psi_t(x) dx$$

is less oscillatory, and the Egorov theorem [BR02, Theorem 1.2] suggests a semiclassical approximation using the Hamiltonian flow $\Phi^t: \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ of the classical equations of motion $\dot{q} = p$, $\dot{p} = -\nabla V(q)$.

For this approximation we adopt the phase space point of view and consider operators $A = \operatorname{op^{We}}(a)$, which are obtained from functions $a : \mathbb{R}^{2d} \to \mathbb{R}$ by the Weyl quantization. Consequently, the Schrödinger operator $H = \operatorname{op}_{\varepsilon}(h)$ is seen as the Weyl quantization of the Hamilton function

$$h: \mathbb{R}^{2d} \to \mathbb{R}, \qquad h(q, p) = \frac{1}{2}|p|^2 + V(q).$$

^{*}Zentrum Mathematik, Technische Universität München, Boltzmannstraße 3, 85748 Garching bei München, Germany (keller@ma.tum.de)

[†]Zentrum Mathematik, Technische Universität München, Boltzmannstraße 3, 85748 Garching bei München, Germany (classer@ma.tum.de).

Expectation values of Weyl quantized operators can be written as phase space integrals

$$\langle \psi_t, \operatorname{op}^{\operatorname{We}}(a) \psi_t \rangle_{L^2} = \int_{\mathbb{R}^{2d}} a(z) \mathcal{W}^{\varepsilon}(\psi_t)(z) dz,$$

where $W^{\varepsilon}(\psi_t): \mathbb{R}^{2d} \to \mathbb{R}$ is the Wigner function of the square integrable function $\psi_t: \mathbb{R}^d \to \mathbb{C}$. The Egorov theorem can be expressed in terms of Wigner functions as

$$\langle \psi_t, \operatorname{op}^{\operatorname{We}}(a)\psi_t \rangle_{L^2} = \int_{\mathbb{R}^{2d}} (a \circ \Phi^t)(z) \, \mathcal{W}^{\varepsilon}(\psi_0)(z) \, dz + O(\varepsilon^2).$$
 (1.2)

In general, Wigner functions attain negative values. However, a proper smoothing by a Gaussian function $G_{\varepsilon/2}$ with mean zero and covariance $\frac{\varepsilon}{2}$ Id results in a nonnegative function

$$\mathcal{H}^{\varepsilon}(\psi_t) = \mathcal{W}^{\varepsilon}(\psi_t) * G_{\varepsilon/2},$$

the so-called Husimi function [GMMP97, Remark 1.4]. Hence, contrary to the Wigner function, the Husimi function can be viewed as a probability distribution on phase space, which entails the straightforward application of Monte Carlo type methods for sampling, especially in high dimensions. However, the gain in positivity is accompanied by a loss in accuracy with respect to time propagation, since replacing the Wigner function $W^{\varepsilon}(\psi_0)$ by the Husimi function $\mathcal{H}^{\varepsilon}(\psi_0)$ in the Egorov theorem (1.2) deteriorates the approximation error from second to first order in ε . This motivates the question, whether an ε -corrected flow can compensate this accuracy loss when propagating Husimi functions.

Our main result answers the question positively. Its basic constituents are the ε -dependent modification

$$a_{\varepsilon} = a - \frac{\varepsilon}{4} \Delta a$$

of a phase space function $a: \mathbb{R}^{2d} \to \mathbb{R}$ by subtracting its phase space Laplacian, the flow $\Phi_{\varepsilon}^t: \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ associated with the Hamilton function $h_{\varepsilon} = h - \frac{\varepsilon}{4}\Delta : \mathbb{R}^{2d} \to \mathbb{R}$,

$$h_{\varepsilon}(q,p) = \frac{1}{2}|p|^2 + V(q) - \frac{\varepsilon}{4} (d + \Delta V(q)),$$

together with the solutions

$$\Lambda_\varepsilon^t \in \mathbb{R}^{2d \times 2d}, \qquad \Gamma_\varepsilon^t \in \mathbb{R}^{2d}$$

of two first order ordinary differential equations, whose right hand side is built from evaluations of D^2h and D^3h along Φ_{ε}^t , respectively. We obtain:

THEOREM 1. There exists a constant C = C(a, V, t) > 0 such that for all square integrable initial data $\psi_0 : \mathbb{R}^d \to \mathbb{C}$ with $\|\psi_0\|_{L^2} = 1$ and all $\varepsilon > 0$ the solution of the Schrödinger equation (1.1) satisfies

$$\left| \langle \psi_t, \operatorname{op^{We}}(a) \psi_t \rangle_{L^2} - \int_{\mathbb{R}^{2d}} F_{\varepsilon}^t(a_{\varepsilon})(z) \, \mathcal{H}^{\varepsilon}(\psi_0)(z) \, dz \right| \leq C \varepsilon^2$$

with

$$F_{\varepsilon}^{t}(a_{\varepsilon}) = a_{\varepsilon} \circ \Phi_{\varepsilon}^{t} - \frac{\varepsilon}{2} \left(\Gamma_{\varepsilon}^{t} \cdot \left(\nabla a \circ \Phi_{\varepsilon}^{t} \right) + \operatorname{tr} \left(\Lambda_{\varepsilon}^{t} \left(D^{2} a \circ \Phi_{\varepsilon}^{t} \right) \right) \right).$$

The method of proof relies on a systematic transition between Weyl and Anti-Wick quantization combined with an ε -expansion of commutators in Weyl quantization. Therefore, the generalization of the approximation to errors of the order ε^k , $k \geq 2$, is possible.

The theorem allows an algorithmic realization in the spirit of the particle method developed in [LR10], which is suitable for the fast computation of expectation values in high dimensions: sample the initial Husimi function $\mathcal{H}^{\varepsilon}(\psi_0)$, discretize the ordinary differential equations for Φ^t_{ε} , Γ^{ε}_t and Λ^{ε}_t , propagate the sample points along the discretized flow, and compute the expectation value at time t by averaging over $F^t_{\varepsilon}(a)$ -evaluations for the sample points. Our numerical experiments for Schrödinger equations in dimensions two and six, one with a torsional potential the other with a Henon-Heiles potential, indicate that both the initial sampling and the flow discretizations can achieve sufficient accuracy to confirm the approximation's asymptotic convergence rate.

1.1. Related research. [LR10] has developed a discrete version of the Egorov theorem by propagating samples drawn from the initial Wigner function along the classical flow Φ^t . The negativity of the Wigner function has been accounted for by stratified sampling as well as sampling from the uniform distribution on the effective support of the Wigner function. The observation, that the approximation order deteriorates from second to first order in ε when merely replacing the Wigner by the Husimi function, has been formulated in [KLW09, Proposition 1] in the context of surface hopping algorithms.

If the aim is not just the approximation of expectation values but of the wave function itself, then semiclassics have been successfully applied as well. The time-splitting algorithm of [FGL09] uses a Galerkin approximation with Hagedorn wave packets, which are products of polynomials with a Gaussian function of time-varying first and second moments. Related approximations are the Gaussian beam methods, whose convergence for the Schrödinger equation, the acoustic wave equation as well as strictly hyperbolic systems has been proven in [LRT10, Theorem 1.1].

A complementary approximation ansatz combines Gaussians of fixed width with time-varying prefactors, whose evolution resembles the one of the width matrices of the Gaussian envelopes of both the Hagedorn wave packets and the Gaussian beams as well as the evolution of our correction term Λ_{ε}^t . The Herman-Kluk propagator [SR09, Theorem 2], [R10, Theorem 1.2] as well as the frozen Gaussian approximation for strictly hyperbolic systems [LY12, Theorem 4.1] have been systematically developed to k-th order in ε .

1.2. Outline. The following Section §2 begins with the comparison of Husimi and Wigner functions and provides asymptotic expansions in ε for the transition from Weyl to Anti-Wick quantization and backwards in Lemma 1 and Lemma 2, respectively. Section §3 develops and proves as Theorem 2 our first result, the second order Egorov approximation for Husimi functions. Our second result, Theorem 3, reformulates the correction term of Theorem 2, which has been derived as a time-integral along the Φ_{ε}^t -flow, with ordinary differential equations. Section §4 proposes a symmetric splitting method for the simultaneous discretization of Φ_{ε}^t , Λ_{ε}^t , and Γ_{ε}^t . The final Section §5 presents our numerical results for two molecular Schrödinger equations in dimension two and six, respectively.

2. Husimi functions and commutators. Let $\psi : \mathbb{R}^d \to \mathbb{C}$ be a square integrable function and $W^{\varepsilon}(\psi) : \mathbb{R}^{2d} \to \mathbb{R}$,

$$\mathcal{W}^{\varepsilon}(\psi)(q,p) = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^d} e^{ip \cdot y/\varepsilon} \psi(q - \frac{1}{2}y) \overline{\psi}(q + \frac{1}{2}y) dy,$$

its Wigner function. The Wigner function is a continuous function on phase space. Its marginals are the position and momentum density of ψ , respectively,

$$\int_{\mathbb{R}^d} \mathcal{W}^{\varepsilon}(\psi)(q,p) dp = |\psi(q)|^2, \qquad \int_{\mathbb{R}^d} \mathcal{W}^{\varepsilon}(\psi)(q,p) dq = |\mathcal{F}^{\varepsilon}(\psi)(p)|^2,$$

where $\mathcal{F}^{\varepsilon}(\psi)(p)=(2\pi\varepsilon)^{-d/2}\int_{\mathbb{R}^d}e^{-iq\cdot p/\varepsilon}\psi(q)dq$ is the ε -scaled Fourier transform. Moreover, associating with a Schwartz function $a:\mathbb{R}^{2d}\to\mathbb{R}$ the Weyl quantized operator

$$(\operatorname{op}^{\operatorname{We}}(a)\psi)(q) = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} a(\frac{q+y}{2}, p) e^{i(q-y)\cdot p/\varepsilon} \psi(y) dp dy,$$

the Wigner function encodes corresponding expectation values via phase space integration,

$$\langle \psi, \operatorname{op}^{\operatorname{We}}(a)\psi \rangle_{L^2} = \int_{\mathbb{R}^{2d}} a(z) \mathcal{W}^{\varepsilon}(\psi)(z) dz.$$

However, despite its positive marginals, the Wigner function may attain negative values. This is easily seen for odd functions, which must satisfy

$$\mathcal{W}^{\varepsilon}(\psi)(0,0) = -(2\pi\varepsilon)^{-d} \|\psi\|_{L^2}^2.$$

2.1. Husimi functions. A proper smoothing of the Wigner function results in a nonnonegative phase space function, the so-called Husimi function:

DEFINITION 1. Let $\psi : \mathbb{R}^d \to \mathbb{C}$ be square integrable and $\mathcal{W}^{\varepsilon}(\psi)$ its Wigner function. Let $a : \mathbb{R}^{2d} \to \mathbb{R}$ be a Schwartz function. We denote by

$$G_{\varepsilon/2}(z) = (\pi \varepsilon)^{-d} e^{-|z|^2/\varepsilon}, \qquad z \in \mathbb{R}^{2d},$$

the centered phase space Gaussian with covariance $\frac{\varepsilon}{2} \mathrm{Id}$. Then,

$$\mathcal{H}^{\varepsilon}(\psi) = \mathcal{W}^{\varepsilon}(\psi) * G_{\varepsilon/2}, \qquad \operatorname{op}^{AW}(a) = \operatorname{op}^{We}(a * G_{\varepsilon/2})$$

are called the Husimi function of ψ and the Anti-Wick operator of a, respectively. By construction the Husimi function is a smooth function satisfying

$$\langle \psi, \operatorname{op}^{\operatorname{AW}}(a)\psi \rangle_{L^2} = \int_{\mathbb{R}^{2d}} a(z) \mathcal{H}^{\varepsilon}(\psi)(z) dz.$$
 (2.1)

Especially, $\|\mathcal{H}^{\varepsilon}(\psi)\|_{L^{1}} = \|\psi\|_{L^{2}}^{2}$. One can prove, that $\mathcal{H}^{\varepsilon}(\psi)$ is the modulus squared of the FBI transform of ψ and therefore nonnegative. Moreover, smoothing the Wigner function with Gaussians of smaller covariance does not yield positivity. In the following Proposition 1, we summarize these observations combining arguments of the proofs of [Z08, Proposition 2.20] and [B67, Theorem 4.2].

PROPOSITION 1. If $\sigma \geq \varepsilon$, then $W^{\varepsilon}(\psi) * G_{\sigma/2} \geq 0$ for all $\psi \in L^{2}(\mathbb{R}^{d})$. If $\sigma < \varepsilon$, then there exists $\psi \in L^{2}(\mathbb{R}^{d})$ such that $W^{\varepsilon}(\psi) * G_{\sigma/2}$ attains negative values.

Proof. We write

$$(\mathcal{W}^{\varepsilon}(\psi) * G_{\sigma/2}) (q, p)$$

$$= (\pi \sigma)^{-d} (2\pi \varepsilon)^{-d} \int_{\mathbb{R}^{3d}} e^{i\xi \cdot y/\varepsilon} \psi(x - \frac{1}{2}y) \overline{\psi}(x + \frac{1}{2}y) e^{-(|x-q|^2 + |\xi-p|^2)/\sigma} dy dx d\xi$$

$$= (\pi \sigma)^{-d/2} (2\pi \varepsilon)^{-d} \int_{\mathbb{R}^{2d}} e^{ip \cdot y/\varepsilon} \psi(x - \frac{1}{2}y) \overline{\psi}(x + \frac{1}{2}y) e^{-|x-q|^2/\sigma} e^{-\frac{\sigma}{4\varepsilon^2}|y|^2} dy dx,$$

since

$$\int_{\mathbb{R}^d} e^{i\xi \cdot y/\varepsilon} e^{-|\xi - p|^2/\sigma} d\xi = (\sigma \pi)^{d/2} e^{ip \cdot y/\varepsilon} e^{-\frac{\sigma}{4\varepsilon^2}|y|^2}.$$

We set $\alpha = \left(\sigma^2/\varepsilon^2 - 1\right)/(4\sigma)$. The change of variables $x - \frac{1}{2}y = v$, $x + \frac{1}{2}y = w$ together with the relation

$$|x-q|^2 + \frac{1}{4}|y|^2 = \frac{1}{2}|v-q|^2 + \frac{1}{2}|w-q|^2$$

and

$$\frac{1}{\sigma}|x-q|^2 + \frac{\sigma}{4\varepsilon^2}|y|^2 = \frac{1}{2\sigma}|v-q|^2 + \frac{1}{2\sigma}|w-q|^2 + \alpha|w-v|^2$$

yields

$$\left(\mathcal{W}^{\varepsilon}(\psi) * G_{\sigma/2}\right)(q,p) = \int_{\mathbb{R}^{2d}} f(v)\overline{f}(w)e^{-\alpha|w-v|^2}dvdw$$

with

$$f(v) = (\pi\sigma)^{-d/4} (2\pi\varepsilon)^{-d/2} \ e^{-ip\cdot v/\varepsilon} \psi(v) e^{-|v-q|^2/(2\sigma)}.$$

The Taylor series of $\alpha \mapsto e^{2\alpha v \cdot w}$ then gives

$$\left(\mathcal{W}^{\varepsilon}(\psi) * G_{\sigma/2}\right)(q,p) = \sum_{k=0}^{\infty} \frac{(2\alpha)^k}{k!} \sum_{i_1,\dots,i_k} \left| \int_{\mathbb{R}^d} v_{i_1} \cdots v_{i_k} f(v) e^{-\alpha|v|^2} dv \right|^2.$$

If $\sigma = \varepsilon$, then $\alpha = 0$ and

$$\forall \psi \in L^2(\mathbb{R}^d): \quad \mathcal{W}^{\varepsilon}(\psi) * G_{\varepsilon/2} = \left| \int_{\mathbb{R}^d} f(v) dv \right|^2 \ge 0.$$

If $\sigma > \varepsilon$, then $G_{\sigma/2} = G_{\varepsilon/2} * G_{(\sigma-\varepsilon)/2}$ and

$$\forall \psi \in L^2(\mathbb{R}^d): \quad \mathcal{W}^{\varepsilon}(\psi) * G_{\sigma/2} = \left(\mathcal{W}^{\varepsilon}(\psi) * G_{\varepsilon/2}\right) * G_{(\sigma-\varepsilon)/2} > 0.$$

If $\sigma < \varepsilon$, then $\alpha < 0$. Therefore, choosing $\psi(v) = v_1 e^{-|v|^2}$, we obtain

$$\left(\mathcal{W}^{\varepsilon}(\psi) * G_{\sigma/2}\right)(0,0) = \sum_{k \text{ odd}}^{\infty} \frac{(2\alpha)^k}{k!} \sum_{i_1,\dots,i_k} \left| \int_{\mathbb{R}^d} v_{i_1} \cdots v_{i_k} f(v) e^{-\alpha|v|^2} dv \right|^2 < 0.$$

2.2. Weyl and Anti-Wick quantization. The nonnegativity of the Husimi function is shared by the Anti-Wick quantization, which satisfies $a \ge 0 \Rightarrow \operatorname{op^{AW}}(a) \ge 0$ by identity (2.1). The following Lemma expresses $\operatorname{op^{AW}}(a)$ as a Weyl quantized operator, whose symbol is obtained from a by adding higher order derivatives. It extends the first order approximation of [L10, Proposition 2.4.3] to higher orders.

LEMMA 1. Let $a: \mathbb{R}^{2d} \to \mathbb{R}$ be a Schwartz function, $n \in \mathbb{N}$, and $\varepsilon > 0$. There exists a family of Schwartz functions $r_n^{\varepsilon}(a): \mathbb{R}^{2d} \to \mathbb{R}$ with $\sup_{\varepsilon > 0} \|\operatorname{op^{We}}(r_n^{\varepsilon}(a))\|_{\mathcal{L}(L^2)} < \infty$ such that

$$\mathrm{op^{AW}}(a) = \mathrm{op^{We}}\left(a + \sum_{k=1}^{n-1} \frac{\varepsilon^k}{4^k k!} \Delta^k a\right) + \varepsilon^n \mathrm{op^{We}}(r_n^{\varepsilon}(a)).$$

Proof. We work with

$$(a*G_{\varepsilon/2})(z) = (\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} a(\zeta)e^{-|\zeta-z|^2/\varepsilon} d\zeta$$

and Taylor expand a around the base point z,

$$a(\zeta) = \sum_{|\alpha|=0}^{2n-1} \frac{1}{\alpha!} (\partial^{\alpha} a)(z)(\zeta - z)^{\alpha}$$
$$+2n \sum_{|\alpha|=2n} \frac{(\zeta - z)^{\alpha}}{\alpha!} \int_{0}^{1} (1 - \theta)^{2n-1} (\partial^{\alpha} a)(z + \theta(\zeta - z)) d\theta$$

with standard multiindex notation. The terms with a-derivatives of odd degree do not contribute, since

$$\int_{\mathbb{R}^{2d}} f(\zeta - z) e^{-|\zeta - z|^2/\varepsilon} d\zeta = 0$$

for odd functions f. For the derivatives of even degree we obtain

$$(\pi \varepsilon)^{-d} \sum_{|\alpha|=m} \int_{\mathbb{R}^{2d}} \frac{1}{(2\alpha)!} (\partial^{2\alpha} a)(z) (\zeta - z)^{2\alpha} e^{-|\zeta - z|^2/\varepsilon} d\zeta$$
$$= \sum_{|\alpha|=m} \varepsilon^m \frac{\pi^{-d}}{(2\alpha)!} (\partial^{2\alpha} a)(z) \int_{\mathbb{R}^{2d}} y_{i_1}^{2\alpha_1} \cdots y_{i_{2k}}^{2\alpha_{2d}} e^{-|y|^2} dy.$$

Since

$$\frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} y^{2m} e^{-y^2} dy = \frac{(2m-1)!!}{2^m} = \frac{(2m)!}{4^m m!}$$

with $(2m-1)!! := (2m-1) \cdot (2m-3) \cdot \cdot \cdot 3 \cdot 1$, we obtain

$$\sum_{|\alpha|=m} \varepsilon^m \frac{\pi^{-d}}{(2\alpha)!} (\partial^{2\alpha} a)(z) \int_{\mathbb{R}^{2d}} y_{i_1}^{2\alpha_1} \cdots y_{i_{2d}}^{2\alpha_{2d}} e^{-|y|^2} dy$$

$$= \frac{\varepsilon^m}{4^m} \sum_{|\alpha|=m} \frac{1}{\alpha!} (\partial^{2\alpha} a)(z) = \frac{\varepsilon^m}{4^m m!} \Delta^m a(z).$$

Consequently,

$$(a * G_{\varepsilon/2})(z) = \sum_{k=0}^{n-1} \frac{\varepsilon^k}{4^k k!} \Delta^k a(z) + \varepsilon^n r_n^{\varepsilon}(a)(z),$$

with

$$r_n^{\varepsilon}(a)(z) = \sum_{|\alpha|=2n} \frac{\pi^{-d} 2n}{\alpha!} \int_{\mathbb{R}^{2d}} \int_0^1 (1-\theta)^{2n-1} (\partial^{\alpha} a)(z + \sqrt{\varepsilon} \theta y) y^{\alpha} e^{-|y|^2} d\theta dy.$$

Moreover,

$$\|\mathrm{op^{We}}(r_n^\varepsilon(a))\|_{\mathcal{L}(L^2)} < C \sup_{|\alpha|, |\beta| \le \lceil d/2 \rceil + 1} \|\partial_q^\alpha \partial_p^\beta a^{(2n)}\|_{\infty}$$

for some constant C=C(d,n)>0 by the Calderon-Vaillan court Theorem. \square

By means of Lemma 1, we can also write $op^{We}(a)$ as an Anti-Wick quantized operator by additively correcting a with its derivatives.

LEMMA 2. Let $a: \mathbb{R}^{2d} \to \mathbb{R}$ be a Schwartz function, $n \in \mathbb{N}$, and $\varepsilon > 0$. There exists a family of Schwartz functions $\rho_n^{\varepsilon}(a): \mathbb{R}^{2d} \to \mathbb{R}$ with $\sup_{\varepsilon > 0} \|\operatorname{op^{We}}(\rho_n^{\varepsilon}(a))\|_{\mathcal{L}(L^2)} < \infty$ such that

$$\mathrm{op^{We}}(a) = \mathrm{op^{AW}}\left(a + \sum_{k=1}^{n-1} \frac{(-\varepsilon)^k}{4^k k!} \Delta^k a\right) + \varepsilon^n \mathrm{op^{We}}(\rho_n^{\varepsilon}(a)).$$

Proof. Applying Lemma 1 yields

$$G_{\varepsilon/2} * \left(a + \sum_{k=1}^{n-1} \frac{(-\varepsilon)^k}{4^k \cdot k!} \Delta^k a \right) = \sum_{j=0}^{n-1} \left(\sum_{k=0}^{n-1-j} \frac{\varepsilon^{k+j} (-1)^j}{4^{k+j} \cdot k! \cdot j!} \Delta^{k+j} a \right) - \varepsilon^n \rho_n^{\varepsilon}(a)$$

$$= \sum_{m=0}^{n-1} \frac{\varepsilon^m}{4^m} \Delta^m a \frac{1}{m!} \sum_{j=0}^m \binom{m}{j} (-1)^j - \varepsilon^n \rho_n^{\varepsilon}(a)$$

$$= a - \varepsilon^n \rho_n^{\varepsilon}(a)$$

where the Schwartz function $\rho_n^{\varepsilon}(a)$ satisfies

$$\|\mathrm{op^{We}}(\rho_n^\varepsilon(a))\|_{\mathcal{L}(L^2)} < C \sup_{|\alpha|, |\beta| \le \lceil d/2 \rceil + 1} \|\partial_q^\alpha \partial_p^\beta a^{(2n)}\|_\infty$$

for some constant C = C(d, n) > 0. \square

For further reference, we summarize the explicit form of the second order approximations of Lemma 1 and Lemma 2:

$$op^{AW}(a) = op^{We}\left(a + \frac{\varepsilon}{4}\Delta a\right) + \varepsilon^{2}op^{We}(r_{2}^{\varepsilon}(a)), \tag{2.2}$$

$$op^{We}(a) = op^{AW} \left(a - \frac{\varepsilon}{4} \Delta a \right) + \varepsilon^2 op^{We} (\rho_2^{\varepsilon}(a)). \tag{2.3}$$

2.3. Commutators. When approximating Husimi functions and expectation values for Anti-Wick quantized operators with respect to the solution of semiclassical Schrödinger equations, we will face commutators of Weyl and Anti-Wick quantized operators. For their asymptotic expansion we need additional notation: Let

 $a, b \in \mathcal{S}(\mathbb{R}^{2d})$ be Schwartz functions. Then, the composition of their Weyl quantized operators is the Weyl quantized operator of the Moyal product $a\sharp b$,

$$\operatorname{op}^{\operatorname{We}}(a)\operatorname{op}^{\operatorname{We}}(b) = \operatorname{op}^{\operatorname{We}}(a\sharp b). \tag{2.4}$$

The commutator $[\operatorname{op^{We}}(a), \operatorname{op^{We}}(b)] = \operatorname{op^{We}}(a)\operatorname{op^{We}}(b) - \operatorname{op^{We}}(b)\operatorname{op^{We}}(a)$ is the Weyl quantization of the Moyal commutator $a\sharp b - b\sharp a$, which has an ε -expansion

$$a\sharp b - b\sharp a = \sum_{k=0}^{n-1} \varepsilon^k \Theta_k(a,b) + \varepsilon^n R_n^{\varepsilon}(a,b), \tag{2.5}$$

where

$$\Theta_k(a,b)(z) = \frac{i^k}{k!} A(D)^k (a(z)b(z') - b(z)a(z')) \big|_{z'=z}$$
 (2.6)

is obtained from the k-fold application of

$$A(D)(a(z)b(z')) = \frac{1}{2}J\nabla a(z)\cdot\nabla b(z'), \qquad J = \begin{pmatrix} 0 & \mathrm{Id} \\ -\mathrm{Id} & 0 \end{pmatrix}$$
 (2.7)

and $\sup_{\varepsilon>0} \|\operatorname{op^{We}}(R_n^{\varepsilon}(a,b))\|_{\mathcal{L}(L^2)} < \infty$, see e.g. [Z12, Section 4.3]. We note, that $\Theta_k(a,b) = 0$ for k even. For commutators of Weyl and Anti-Wick quantized operators we derive the following expansion.

LEMMA 3. Let $a, b : \mathbb{R}^{2d} \to \mathbb{R}$ be a smooth function of subquadratic growth and a Schwartz function, respectively, and let $n \in \mathbb{N}$, and $\varepsilon > 0$. Then, $\frac{i}{\varepsilon} \left[\operatorname{op^{We}}(a), \operatorname{op^{AW}}(b) \right]$ is essentially self-adjoint in $L^2(\mathbb{R}^d)$ with core $\mathcal{S}(\mathbb{R}^d)$, and there exists a family of Schwartz functions $\varrho_n^{\varepsilon}(a,b) : \mathbb{R}^{2d} \to \mathbb{R}$ with $\sup_{\varepsilon>0} \|\operatorname{op^{We}}(\varrho_n^{\varepsilon}(a,b))\|_{\mathcal{L}(L^2)} < \infty$ such that

$$\frac{i}{\varepsilon} \left[\text{op}^{\text{We}}(a), \text{op}^{\text{AW}}(b) \right] = \sum_{k=0}^{n-1} \varepsilon^k \text{op}^{\text{We}}(\theta_k(a, b)) + \varepsilon^n \text{op}^{\text{We}}(\varrho_n^{\varepsilon}(a, b))$$

with

$$\theta_k(a,b) = i \sum_{\ell+m=k+1} \frac{1}{4^{\ell}\ell!} \Theta_m(a,\Delta^{\ell}b),$$

where Θ_m has been defined in (2.6).

Proof. Since b is a Schwartz function, op^{AW}(b) maps $L^2(\mathbb{R}^d)$ into $\mathcal{S}(\mathbb{R}^d)$ and hence the commutator with op^{We}(a) is densely defined and essentially selfadjoint. By Lemma 1,

$$\begin{split} &\frac{i}{\varepsilon} \left[\mathrm{op^{We}}(a), \mathrm{op^{AW}}(b) \right] \\ &= \frac{i}{\varepsilon} \sum_{k=0}^{n} \frac{\varepsilon^{k}}{4^{k} k!} \left[\mathrm{op^{We}}(a), \mathrm{op^{We}}(\Delta^{k} b) \right] + i \, \varepsilon^{n} \left[\mathrm{op^{We}}(a), \mathrm{op^{We}}(r_{n+1}^{\varepsilon}(b)) \right]. \end{split}$$

Using the Moyal expansion (2.5), we then obtain

$$\begin{split} &\frac{i}{\varepsilon} \left[\operatorname{op^{\operatorname{We}}}(a), \operatorname{op^{\operatorname{AW}}}(b) \right] \\ &= \frac{i}{\varepsilon} \sum_{k=0}^{n} \sum_{m=0}^{n-k} \frac{\varepsilon^{k+m}}{4^k k!} \operatorname{op^{\operatorname{We}}} \left(\Theta_m(a, \Delta^k b) \right) \\ &+ i \, \varepsilon^n \left(\sum_{k=0}^{n} \frac{1}{4^k k!} \operatorname{op^{\operatorname{We}}} \left(R_{n-k+1}^{\varepsilon}(a, \Delta^k b) \right) + \operatorname{op^{\operatorname{We}}} \left(a \sharp r_{n+1}^{\varepsilon}(b) - r_{n+1}^{\varepsilon}(b) \sharp a \right) \right) \\ &=: \frac{i}{\varepsilon} \sum_{k=0}^{n} \sum_{m=0}^{n-k} \varepsilon^{k+m} \frac{\varepsilon^{k+m}}{4^k k!} \operatorname{op^{\operatorname{We}}} \left(\Theta_m(a, \Delta^k b) \right) + \varepsilon^n \operatorname{op^{\operatorname{We}}} (\varrho_n^{\varepsilon}(a, b)). \end{split}$$

with some family of Schwartz functions $(\varrho_n^{\varepsilon}(a,b))_{\varepsilon>0}$. Finally, we use the fact that $\Theta_0(a,b)=0$ to rewrite

$$\frac{i}{\varepsilon} \sum_{k=0}^{n} \sum_{m=0}^{n-k} \frac{\varepsilon^{k+m}}{4^k k!} \Theta_m(a, \Delta^k b) = \frac{i}{\varepsilon} \sum_{p=0}^{n} \varepsilon^p \sum_{k+m=p} \frac{1}{4^k k!} \Theta_m(a, \Delta^k b)
= i \sum_{p=0}^{n-1} \varepsilon^p \sum_{k+m=p+1} \frac{1}{4^k k!} \Theta_m(a, \Delta^k b).$$

REMARK 1. We note that $\theta_0(a,b) = \{a,b\}$, where $\{a,b\} = J\nabla a \cdot \nabla b$ denotes the Poisson bracket. Since $\theta_1(a,b) = \frac{1}{4}\{a,\Delta b\}$, we have

$$\frac{i}{\varepsilon} \left[\mathrm{op^{We}}(a), \mathrm{op^{AW}}(b) \right] = \mathrm{op^{We}}(\{a, b + \frac{\varepsilon}{4}\Delta b\}) + \varepsilon^2 \mathrm{op^{We}}(\varrho_2^{\varepsilon}(a, b)).$$

3. Propagation. In this section we apply the systematic transition between Weyl- and Anti-Wick calculus to prove a second order Egorov approximation for Anti-Wick quantized symbols. We can allow for unitary time evolutions $e^{-iHt/\varepsilon}$ whose Hamiltonian $H = \operatorname{op}^{\operatorname{We}}(h)$ is obtained from a smooth symbol $h: \mathbb{R}^{2d} \to \mathbb{R}$ of subquadratic growth. That is, for all $|\gamma| \geq 2$ there exists $C_{\gamma} > 0$ such that

$$\|\partial^{\gamma} h\|_{\infty} < C_{\gamma}.$$

In this situation, H is essentially self-adjoint in $L^2(\mathbb{R}^d)$ with core $\mathcal{S}(\mathbb{R}^d)$, $e^{-iHt/\varepsilon}$ is a well-defined unitary operator on $L^2(\mathbb{R}^d)$, and the Hamiltonian flow $\Phi^t : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ associated with h is a smooth mapping for all $t \in \mathbb{R}$. Schrödinger operators

$$-\tfrac{\varepsilon^2}{2}\Delta + V$$

with smooth subquadratic potential V are one important example.

3.1. A first Egorov type approximation. The proof of the Egorov type approximation is mainly built on the following commutator estimate:

LEMMA 4. Let $\varepsilon > 0$. Let $b, c : \mathbb{R}^{2d} \to \mathbb{R}$ be a smooth function of subquadratic growth and a Schwartz function, respectively. Then, $\frac{i}{\varepsilon} \left[\operatorname{op^{We}}(b), \operatorname{op^{AW}}(c) \right]$ is essentially self-adjoint in $L^2(\mathbb{R}^d)$ with core $\mathcal{S}(\mathbb{R}^d)$, and there exists a family of Schwartz

functions $\chi_2^{\varepsilon}(b,c): \mathbb{R}^{2d} \to \mathbb{R}$ with $\sup_{\varepsilon>0} \|\operatorname{op^{We}}(\chi_2^{\varepsilon}(b,c))\|_{\mathcal{L}(L^2)} < \infty$ such that

$$\begin{split} &\frac{i}{\varepsilon} \left[\mathrm{op^{We}}(b), \mathrm{op^{AW}}(c) \right] \\ &= \mathrm{op^{AW}} \left(\{ b - \frac{\varepsilon}{4} \Delta b, c \} - \frac{\varepsilon}{2} \operatorname{tr}(J \, D^2 b \, D^2 c) \right) + \varepsilon^2 \mathrm{op^{We}}(\chi_2^{\varepsilon}(b, c)). \end{split}$$

Proof. Since c is a Schwartz function, op^{AW}(c) maps $L^2(\mathbb{R}^d)$ into $\mathcal{S}(\mathbb{R}^d)$, and the commutator with op^{We}(b) is well-defined. By Lemma 3,

$$\frac{i}{\varepsilon} \left[\mathrm{op^{We}}(b), \mathrm{op^{AW}}(c) \right] = \mathrm{op^{We}}(\{b, c + \tfrac{\varepsilon}{4}\Delta c\}) + \varepsilon^2 \mathrm{op^{We}}(\varrho_2^\varepsilon(b, c))$$

By Lemma 2,

$$\begin{aligned} \operatorname{op^{We}}(\{b,c+\tfrac{\varepsilon}{4}\Delta c\}) &= \operatorname{op^{AW}}(\{b,c+\tfrac{\varepsilon}{4}\Delta c\} - \tfrac{\varepsilon}{4}\Delta \{b,c\}) \\ &+ \varepsilon^2 \operatorname{op^{We}}\left(\rho_2^\varepsilon(\{b,c+\tfrac{\varepsilon}{4}\Delta c\}) - \tfrac{\varepsilon^2}{16} \operatorname{op^{AW}}(\Delta \{b,\Delta c\}). \end{aligned}$$

By Lemma 1,

$$\operatorname{op^{AW}}(\Delta\{b, \Delta c\}) = \operatorname{op^{We}}(\Delta\{b, \Delta c\}) + \varepsilon \operatorname{op^{We}}(r_1^{\varepsilon}(\Delta\{b, \Delta c\})),$$

and therefore

$$\frac{i}{\varepsilon} \left[\mathrm{op^{We}}(b), \mathrm{op^{AW}}(c) \right] = \mathrm{op^{AW}}(\{b, c + \frac{\varepsilon}{4}\Delta c\} - \frac{\varepsilon}{4}\Delta \{b, c\}) + \varepsilon^2 \mathrm{op^{We}}(\chi_2^\varepsilon(b, c))$$

with

$$\chi_2^{\varepsilon}(b,c) = \varrho_2^{\varepsilon}(b,c) + \rho_2^{\varepsilon}(\{b,c + \frac{\varepsilon}{4}\Delta c\}) - \frac{1}{16}\Delta\{b,\Delta c\} - \frac{\varepsilon}{16}r_1^{\varepsilon}(\Delta\{b,\Delta c\}).$$

a Schwartz function. We write $\Delta\{b,c\}=\{\Delta b,c\}+\{b,\Delta c\}+2\sum_{k=1}^{2d}\{\partial_{z_k}b,\partial_{z_k}c\}$ and compute

$$\begin{split} \sum_{k=1}^{2d} \{\partial_{z_k} b, \partial_{z_k} c\} &= \sum_{k=1}^{2d} J \, D^2 b(:,k) \cdot D^2 c(:,k) = \sum_{k=1}^{2d} D^2 c(k,:) (J \, D^2 b)(:,k) \\ &= \operatorname{tr}(J \, D^2 b \, D^2 c), \end{split}$$

where M(:,k) and M(k,:) denote the kth column and the kth row of a matrix M, respectively. Therefore,

$$\{b, c + \frac{\varepsilon}{4}\Delta c\} - \frac{\varepsilon}{4}\Delta\{b, c\} = \{b - \frac{\varepsilon}{4}\Delta b, c\} - \frac{\varepsilon}{2}\operatorname{tr}(JD^2bD^2c),$$

which concludes the proof. \square

Remark 2. If b is a polynomial of degree one, then the result of Lemma 4 obviously simplifies to

$$\label{eq:equation:equation} \tfrac{i}{\varepsilon} \left[\mathrm{op^{We}}(b), \mathrm{op^{AW}}(c) \right] = \mathrm{op^{AW}} \left(\{b, c\} \right).$$

If b is a polynomial of degree two, then the only simplification is due to $\{b - \frac{\varepsilon}{4}\Delta b, c\} = \{b, c\}$, since $\chi_2^{\varepsilon}(b, c)$ is not identical zero.

Having prepared the necessary estimates, we state and prove our approximation result for the unitary propagation of Anti-Wick operators.

THEOREM 2. Let $h: \mathbb{R}^{2d} \to \mathbb{R}$ be a smooth function of subquadratic growth. Let $a: \mathbb{R}^{2d} \to \mathbb{R}$ be a Schwartz function and $t \in \mathbb{R}$. There exists a constant C = C(a, h, t) > 0 such that all $\varepsilon > 0$

$$\left\| e^{iHt/\varepsilon} \operatorname{op^{AW}}(a) e^{-iHt/\varepsilon} - \operatorname{op^{AW}}(a \circ \Phi_{\varepsilon}^t - \frac{\varepsilon}{2} \Xi_{\varepsilon}^t(a)) \right\|_{\mathcal{L}(L^2)} \le C\varepsilon^2$$

with

$$\Xi_{\varepsilon}^{t}(a) = \int_{0}^{t} \operatorname{tr}\left(J D^{2} h D^{2}(a \circ \Phi_{\varepsilon}^{\tau})\right) \circ \Phi_{\varepsilon}^{t-\tau} d\tau \tag{3.1}$$

and $\Phi_{\varepsilon}^t: \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ the Hamiltonian flow associated with $h_{\varepsilon} = h - \frac{\varepsilon}{4}\Delta h$. Proof. We denote

$$a(t) = a \circ \Phi_{\varepsilon}^t - \frac{\varepsilon}{2} \Xi_{\varepsilon}^t(a)$$

and observe that $a(t): \mathbb{R}^{2d} \to \mathbb{R}$ is a Schwartz function. Since a(0) = a, we have

$$\begin{split} &e^{iHt/\varepsilon} \mathrm{op^{AW}}(a) e^{-iHt/\varepsilon} - \mathrm{op^{AW}}(a(t)) \\ &= \int_0^t \frac{d}{ds} \left(e^{iHs/\varepsilon} \mathrm{op^{AW}}(a(t-s)) e^{-iHs/\varepsilon} \right) ds \\ &= \int_0^t e^{iHs/\varepsilon} \left(\frac{i}{\varepsilon} \left[H, \mathrm{op^{AW}}(a(t-s)) \right] - \mathrm{op^{AW}}(\partial_t a(t-s)) \right) e^{-iHs/\varepsilon} ds. \end{split}$$

The second order commutator expansion of Lemma 4 yields

$$\begin{split} &\frac{i}{\varepsilon} \left[H, \operatorname{op^{AW}}(a(t-s)) \right] = \frac{i}{\varepsilon} \left[\operatorname{op^{We}}(h), \operatorname{op^{AW}}(a(t-s)) \right] = \\ &\operatorname{op^{AW}} \left(\left\{ h_{\varepsilon}, a(t-s) \right\} - \frac{\varepsilon}{2} \operatorname{tr}(J \, D^2 h \, D^2 a(t-s)) \right) + \varepsilon^2 \operatorname{op^{We}}(\rho_2^{\varepsilon}(h, a(t-s))). \end{split}$$

Now, we compute

$$\partial_t(a \circ \Phi_{\varepsilon}^{t-s}) = \{h_{\varepsilon}, a \circ \Phi_{\varepsilon}^{t-s}\}$$

and

$$\partial_t \Xi_{\varepsilon}^{t-s}(a) = \operatorname{tr} \left(J D^2 h D^2 (a \circ \Phi_{\varepsilon}^{t-s}) \right) + \{ h_{\varepsilon}, \Xi_{\varepsilon}^{t-s}(a) \}.$$

Therefore,

$$\partial_t a(t-s) = \{h_{\varepsilon}, a(t-s)\} - \frac{\varepsilon}{2} \operatorname{tr} \left(J D^2 h D^2 (a \circ \Phi_{\varepsilon}^{t-s})\right)$$

and

$$\frac{i}{\varepsilon} \left[H, \operatorname{op^{AW}}(a(t-s)) \right] - \operatorname{op^{AW}}(\partial_t a(t-s)) = \frac{\varepsilon^2}{\varepsilon^2} \operatorname{op^{AW}} \operatorname{tr}(J D^2 h D^2 \Xi_{\varepsilon}^{t-s}(a)) + \varepsilon^2 \operatorname{op^{We}}(\rho_2^{\varepsilon}(h, a(t-s))).$$

The observation that

$$\operatorname{tr}(J D^2 h D^2 \Xi_{\varepsilon}^{t-s}(a)), \ \rho_2^{\varepsilon}(h, a(t-s)) \in \mathcal{S}(\mathbb{R}^{2d})$$

concludes the proof. \square

3.2. Corrections by ordinary differential equations. Our next task is to reformulate the time evolution of the correction term

$$\Xi_{\varepsilon}^{t}(a) = \int_{0}^{t} \operatorname{tr}\left(J D^{2} h D^{2}(a \circ \Phi_{\varepsilon}^{\tau})\right) \circ \Phi_{\varepsilon}^{t-\tau} d\tau$$

using ordinary differential equations which are independent of the observable a.

LEMMA 5. Let $a: \mathbb{R}^{2d} \to \mathbb{R}$ be a Schwartz function and $h: \mathbb{R}^{2d} \to \mathbb{R}$ a smooth function of subquadratic growth. Let $\varepsilon > 0$ and $\Phi_{\varepsilon}^t: \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ the Hamiltonian flow associated with $h_{\varepsilon} = h - \frac{\varepsilon}{4} \Delta h$. Then, for all $t \in \mathbb{R}$,

$$\Xi_{\varepsilon}^{t}(a) = \operatorname{tr}\left(\widetilde{\Lambda}_{\varepsilon}^{t}\left(D^{2}a \circ \Phi_{\varepsilon}^{t}\right)\right) + \widetilde{\Gamma}_{\varepsilon}^{t} \cdot \left(\nabla a \circ \Phi_{\varepsilon}^{t}\right)$$

with $\widetilde{\Lambda}_{\varepsilon}^t : \mathbb{R}^{2d} \to \mathbb{R}^{2d \times 2d}$,

$$\widetilde{\Lambda}_{\varepsilon}^{t} = \int_{0}^{t} \left((D\Phi_{\varepsilon}^{\tau})^{\mathrm{T}} J D^{2} h D\Phi_{\varepsilon}^{\tau} \right) \circ \Phi_{\varepsilon}^{t-\tau} d\tau, \tag{3.2}$$

and $\widetilde{\Gamma}^t_{\varepsilon}: \mathbb{R}^{2d} \to \mathbb{R}^{2d}$

$$\widetilde{\Gamma}_{\varepsilon}^{t} = \int_{0}^{t} \sum_{k,l=1}^{2d} \left((J D^{2} h)_{kl} \, \partial_{z_{k} z_{l}}^{2} \Phi_{\varepsilon}^{\tau} \right) \circ \Phi_{\varepsilon}^{t-\tau} d\tau, \tag{3.3}$$

where the Jacobian of $\Phi_{\varepsilon}^{\tau}$ is denoted as $D\Phi_{\varepsilon}^{\tau} = (\nabla(\Phi_{\varepsilon}^{\tau})_1, \dots, \nabla(\Phi_{\varepsilon}^{\tau})_{2d})$. Proof. We compute

$$\partial^2_{z_k z_l}(a \circ \Phi_\varepsilon^\tau) = (D^2 a \circ \Phi_\varepsilon^\tau)(\partial_{z_l} \Phi_\varepsilon^\tau, \partial_{z_k} \Phi_\varepsilon^\tau) + (\nabla a \circ \Phi_\varepsilon^\tau) \cdot \partial^2_{z_k z_l} \Phi_\varepsilon^\tau.$$

Then,

$$\operatorname{tr}\left(\widetilde{\Lambda}_{\varepsilon}^{t}\left(D^{2}a \circ \Phi_{\varepsilon}^{t}\right)\right) = \int_{0}^{t} \operatorname{tr}\left(\left(D\Phi_{\varepsilon}^{\tau}\right)^{\mathrm{T}} J D^{2}h D\Phi_{\varepsilon}^{\tau}\left(D^{2}a \circ \Phi_{\varepsilon}^{\tau}\right)\right) \circ \Phi_{\varepsilon}^{t-\tau} d\tau$$

$$= \int_{0}^{t} \operatorname{tr}\left(J D^{2}h D\Phi_{\varepsilon}^{\tau}\left(D^{2}a \circ \Phi_{\varepsilon}^{\tau}\right) \left(D\Phi_{\varepsilon}^{\tau}\right)^{\mathrm{T}}\right) \circ \Phi_{\varepsilon}^{t-\tau} d\tau$$

$$= \sum_{k,l=1}^{2d} \int_{0}^{t} \left(\left(J D^{2}h\right)_{kl} \left(D^{2}a \circ \Phi_{\varepsilon}^{\tau}\right) \left(\partial_{z_{l}} \Phi_{\varepsilon}^{\tau}, \partial_{z_{k}} \Phi_{\varepsilon}^{\tau}\right)\right) \circ \Phi_{\varepsilon}^{t-\tau} d\tau$$

and

$$\widetilde{\Gamma}^t_{\varepsilon} \cdot (\nabla a \circ \Phi^t_{\varepsilon}) = \int_0^t \sum_{k:l=1}^{2d} \left((J \, D^2 h)_{kl} \, \partial^2_{z_k z_l} \Phi^{\tau}_{\varepsilon} \cdot (\nabla a \circ \Phi^{\tau}_{\varepsilon}) \right) \circ \Phi^{t-\tau}_{\varepsilon} d\tau.$$

Adding the two terms gives the claimed identity. \square

Having written the correction term $\Xi_{\varepsilon}^{t}(a)$ as the sum of a trace and an inner product, we can derive the desired a-independent ordinary differential equations for the time evolution of $\Xi_{\varepsilon}^{t}(a)$.

THEOREM 3. Let $a: \mathbb{R}^{2d} \to \mathbb{R}$ be a Schwartz function, $h: \mathbb{R}^{2d} \to \mathbb{R}$ a smooth function of subquadratic growth, and $t \in \mathbb{R}$. Then, there exists a constant C = C(a, h, t) > 0 such that for all $\varepsilon > 0$

$$\left\|e^{iHt/\varepsilon}\mathrm{op^{AW}}(a)e^{-iHt/\varepsilon}-\mathrm{op^{AW}}(\Psi_\varepsilon^t(a))\right\|_{\mathcal{L}(L^2)}\leq C\varepsilon^2$$

with

$$\Psi_{\varepsilon}^{t}(a) = a \circ \Phi_{\varepsilon}^{t} - \frac{\varepsilon}{2} \left(\operatorname{tr}(\Lambda_{\varepsilon}^{t} \left(D^{2} a \circ \Phi_{\varepsilon}^{t} \right) \right) + \Gamma_{\varepsilon}^{t} \cdot \left(\nabla a \circ \Phi_{\varepsilon}^{t} \right) \right),$$

where $\Phi_{\varepsilon}^t: \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is the Hamiltonian flow of $h_{\varepsilon} = h - \frac{\varepsilon}{4}\Delta h$,

$$\partial_t \Phi_\varepsilon^t = J \, \nabla h_\varepsilon \circ \Phi_\varepsilon^t, \tag{3.4}$$

and $\Lambda_{\varepsilon}^t: \mathbb{R}^{2d} \to \mathbb{R}^{2d \times 2d}$, $\Gamma_{\varepsilon}^t: \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ solve

$$\partial_t \Lambda_{\varepsilon}^t = M_{\varepsilon}(t) + M_{\varepsilon}(t) \Lambda_{\varepsilon}^t + \Lambda_{\varepsilon}^t M_{\varepsilon}(t)^{\mathrm{T}}, \qquad \Lambda_{\varepsilon}^0 = 0$$
 (3.5)

$$\partial_t \Gamma_{\varepsilon}^t = M_{\varepsilon}(t) \Gamma_{\varepsilon}^t + \operatorname{tr}(C_i(t)^{\mathrm{T}} \Lambda_{\varepsilon}^t)_{i=1}^{2d}, \qquad \Gamma_{\varepsilon}^0 = 0$$
(3.6)

with

$$M_{\varepsilon}(t): \mathbb{R}^{2d} \to \mathbb{R}^{2d \times 2d}, M_{\varepsilon}(t) = J D^{2} h \circ \Phi_{\varepsilon}^{t},$$

$$C_{i}(t): \mathbb{R}^{2d} \to \mathbb{R}^{2d \times 2d}, (C_{i}(t))_{jk} = \partial_{k} (J D^{2} h)_{ij} \circ \Phi_{\varepsilon}^{t}.$$

Proof. We start with the reformulation of $\Xi_{\varepsilon}^{t}(a)$ of Lemma 5 and observe that both relations (3.2) and (3.3) for $\widetilde{\Lambda}_{\varepsilon}^{t}$ and $\widetilde{\Gamma}_{\varepsilon}^{t}$, respectively, involve time integrals of the form

$$\int_0^t (f_1(\tau)gf_2(\tau)) \circ \Phi_{\varepsilon}^{t-\tau} d\tau.$$

We compute

$$\partial_t \int_0^t \left(f_1(\tau) g f_2(\tau) \right) \circ \Phi_\varepsilon^{t-\tau} d\tau = \int_0^t \partial_t \left(\left(f_1(\tau) g f_2(\tau) \right) \circ \Phi_\varepsilon^{t-\tau} \right) d\tau + f_1(t) g f_2(t)$$

and

$$\begin{split} &\partial_t \left(\left(f_1(\tau) g f_2(\tau) \right) \circ \Phi_\varepsilon^{t-\tau} \right) \\ &= -\partial_\tau \left(\left(f_1(\tau) g f_2(\tau) \right) \circ \Phi_\varepsilon^{t-\tau} \right) + \partial_\tau \left(f_1(\tau) g f_2(\tau) \right) \circ \Phi_\varepsilon^{t-\tau}. \end{split}$$

We obtain

$$\partial_t \int_0^t (f_1(\tau)gf_2(\tau)) \circ \Phi_{\varepsilon}^{t-\tau} d\tau$$

$$= (f_1(0)gf_2(0)) \circ \Phi_{\varepsilon}^t + \int_0^t \partial_{\tau} (f_1(\tau)gf_2(\tau)) \circ \Phi_{\varepsilon}^{t-\tau} d\tau. \tag{3.7}$$

This implies for

$$\widetilde{\Lambda}_{\varepsilon}^{t} = \int_{0}^{t} \left((D\Phi_{\varepsilon}^{\tau})^{\mathrm{T}} J D^{2} h D\Phi_{\varepsilon}^{\tau} \right) \circ \Phi_{\varepsilon}^{t-\tau} d\tau$$

that

$$\begin{split} \partial_t \widetilde{\Lambda}^t_\varepsilon &= M_\varepsilon(t) + \int_0^t \left((J\, D^2 h_\varepsilon \circ \Phi_\varepsilon^\tau) (D\Phi_\varepsilon^\tau)^\mathrm{T} \, J \, D^2 h \, D\Phi_\varepsilon^\tau \right) \circ \Phi_\varepsilon^{t-\tau} d\tau \\ &+ \int_0^t \left((D\Phi_\varepsilon^\tau)^\mathrm{T} \, J \, D^2 h \, D\Phi_\varepsilon^\tau (J \, D^2 h_\varepsilon \circ \Phi_\varepsilon^\tau)^\mathrm{T} \right) \circ \Phi_\varepsilon^{t-\tau} d\tau, \\ &= M_\varepsilon(t) + (J \, D^2 h_\varepsilon \circ \Phi_\varepsilon^t) \widetilde{\Lambda}^t_\varepsilon + \widetilde{\Lambda}^t_\varepsilon (J \, D^2 h_\varepsilon \circ \Phi_\varepsilon^t)^\mathrm{T}, \end{split}$$

since the Hamilton equation (3.4) implies $\partial_{\tau}\partial_{z_k}\Phi^{\tau}_{\varepsilon} = (J D^2 h_{\varepsilon} \circ \Phi^{\tau}_{\varepsilon}) \partial_{z_k}\Phi^{\tau}_{\varepsilon}$ and

$$\partial_{\tau} (D\Phi_{\varepsilon}^{\tau})^{\mathrm{T}} = (J D^{2} h_{\varepsilon} \circ \Phi_{\varepsilon}^{\tau}) (D\Phi_{\varepsilon}^{\tau})^{\mathrm{T}}, \partial_{\tau} D\Phi_{\varepsilon}^{\tau} = D\Phi_{\varepsilon}^{\tau} (J D^{2} h_{\varepsilon} \circ \Phi_{\varepsilon}^{\tau})^{\mathrm{T}}.$$

Since $J D^2 h_{\varepsilon} \circ \Phi_{\varepsilon}^t = M_{\varepsilon}(t) + O(\varepsilon)$, the solution Λ_{ε}^t of equation (3.5) satisfies $\Lambda_{\varepsilon}^t = \widetilde{\Lambda}_{\varepsilon}^t + O(\varepsilon)$, and we obtain

$$a \circ \Phi_{\varepsilon}^{t} - \frac{\varepsilon}{2} \Xi_{\varepsilon}^{t}(a) = a \circ \Phi_{\varepsilon}^{t} - \frac{\varepsilon}{2} \left(\operatorname{tr}(\Lambda_{\varepsilon}^{t} (D^{2}a \circ \Phi_{\varepsilon}^{t})) + \widetilde{\Gamma}_{\varepsilon}^{t} \cdot (\nabla a \circ \Phi_{\varepsilon}^{t}) \right) + O(\varepsilon^{2}).$$

For the time derivative of

$$\widetilde{\Gamma}_{\varepsilon}^{t} = \int_{0}^{t} \sum_{k,l=1}^{2d} \left((J D^{2} h)_{kl} \, \partial_{z_{k} z_{l}}^{2} \Phi_{\varepsilon}^{\tau} \right) \circ \Phi_{\varepsilon}^{t-\tau} d\tau$$

equation (3.7) implies

$$\partial_t \widetilde{\Gamma}_{\varepsilon}^t = \int_0^t \sum_{k,l=1}^{2d} \left((J D^2 h)_{kl} \, \partial_{\tau} \partial_{z_k z_l}^2 \Phi_{\varepsilon}^{\tau} \right) \circ \Phi_{\varepsilon}^{t-\tau} d\tau.$$

We consider $\partial_{z_k}(\Phi_{\varepsilon}^{\tau})_i = \left(\left(J\,D^2h_{\varepsilon}\circ\Phi_{\varepsilon}^{\tau}\right)\partial_{z_k}\Phi_{\varepsilon}^{\tau}\right)_i$ and compute

$$\begin{split} &\partial_{\tau}\partial_{z_kz_l}^2(\Phi_{\varepsilon}^{\tau})_i\\ &=\sum_{j,n=1}^{2d}\left(\partial_n(J\,D^2h_{\varepsilon})_{ij}\circ\Phi_{\varepsilon}^{\tau}\right)\,\partial_{z_l}(\Phi_{\varepsilon}^{\tau})_n\,\partial_{z_k}(\Phi_{\varepsilon}^{\tau})_j+\left((J\,D^2h_{\varepsilon}\circ\Phi_{\varepsilon}^{\tau})\partial_{z_kz_l}^2\Phi_{\varepsilon}^{\tau}\right)_i\\ &=:\sum_{j,n=1}^{2d}\left(\widetilde{C}_i(\tau)\right)_{jn}(D\Phi_{\varepsilon}^{\tau})_{ln}\,(D\Phi_{\varepsilon}^{\tau})_{kj}+\left((J\,D^2h_{\varepsilon}\circ\Phi_{\varepsilon}^{\tau})\partial_{z_kz_l}^2\Phi_{\varepsilon}^{\tau}\right)_i\,. \end{split}$$

Therefore,

$$\begin{split} \partial_t (\widetilde{\Gamma}_\varepsilon^t)_i &= ((J\,D^2 h_\varepsilon \circ \Phi_\varepsilon^t)\,\widetilde{\Gamma}_\varepsilon^t)_i \\ &+ \sum_{j,k,l,n=1}^{2d} (\widetilde{C}_i(t))_{jn} \int_0^t \left((J\,D^2 h)_{kl} \, (D\Phi_\varepsilon^\tau)_{ln} \, (D\Phi_\varepsilon^\tau)_{kj} \right) \circ \Phi_\varepsilon^{t-\tau} d\tau \\ &= ((J\,D^2 h_\varepsilon \circ \Phi_\varepsilon^t)\,\widetilde{\Gamma}_\varepsilon^t)_i + \sum_{j,n=1}^{2d} (\widetilde{C}_i(t))_{jn} (\widetilde{\Lambda}_\varepsilon^t)_{jn} \\ &= ((J\,D^2 h_\varepsilon \circ \Phi_\varepsilon^t)\,\widetilde{\Gamma}_\varepsilon^t)_i + \mathrm{tr}(\widetilde{C}_i(t)^{\mathrm{T}}\,\widetilde{\Lambda}_\varepsilon^t). \end{split}$$

Since $J D^2 h_{\varepsilon} \circ \Phi_{\varepsilon}^t = M^{\varepsilon}(t) + O(\varepsilon)$, $C_i(t) = \widetilde{C}_i(t) + O(\varepsilon)$, and $\Lambda_{\varepsilon}^t = \widetilde{\Lambda}_{\varepsilon}^t + O(\varepsilon)$, the solution Γ_{ε}^t of equation (3.6) satisfies $\Gamma_{\varepsilon}^t = \widetilde{\Gamma}_{\varepsilon}^t + O(\varepsilon)$, and we conclude

$$a\circ\Phi_\varepsilon^t-\tfrac{\varepsilon}{2}\,\Xi_\varepsilon^t(a)=a\circ\Phi_\varepsilon^t-\tfrac{\varepsilon}{2}\left(\mathrm{tr}(\Lambda_\varepsilon^t\,(D^2a\circ\Phi_\varepsilon^t))+\Gamma_\varepsilon^t\cdot(\nabla a\circ\Phi_\varepsilon^t)\right)+O(\varepsilon^2).$$

Corollary 1. Under the assumptions of Theorem 3, there exists a constant C = C(a, h, t) > 0 such that $\psi_t = e^{-iHt/\varepsilon}\psi_0$ satisfies

$$\left| \langle \psi_t, \operatorname{op}^{\operatorname{We}}(a) \psi_t \rangle_{L^2} - \int_{\mathbb{R}^{2d}} F_{\varepsilon}^t(a_{\varepsilon})(z) \,\mathcal{H}^{\varepsilon}(\psi_0)(z) \,dz \right| \le C\varepsilon^2 \tag{3.8}$$

for all $\psi_0 \in L^2(\mathbb{R}^d)$ with $\|\psi_0\|_{L^2} = 1$, where

$$F_{\varepsilon}^t(a) = a_{\varepsilon} \circ \Phi_{\varepsilon}^t - \frac{\varepsilon}{2} \left(\operatorname{tr}(\Lambda_{\varepsilon}^t \left(D^2 a \circ \Phi_{\varepsilon}^t \right)) + \Gamma_{\varepsilon}^t \cdot \left(\nabla a \circ \Phi_{\varepsilon}^t \right) \right).$$

Proof. We have

$$\langle \psi_t, \operatorname{op}^{\operatorname{We}}(a)\psi_t \rangle_{L^2} = \langle \psi_t, \operatorname{op}^{\operatorname{AW}}(a_{\varepsilon})\psi_t \rangle_{L^2} + O(\varepsilon^2)$$

$$= \langle \psi_0, \operatorname{op}^{\operatorname{AW}}(\Psi_{\varepsilon}^t(a_{\varepsilon}))\psi_0 \rangle_{L^2} + O(\varepsilon^2) = \int_{\mathbb{R}^{2d}} \Psi_{\varepsilon}^t(a_{\varepsilon})(z) \,\mathcal{H}^{\varepsilon}(\psi_0)(z) \,dz + O(\varepsilon^2)$$

and
$$\Psi_{\varepsilon}^t(a_{\varepsilon}) = F_{\varepsilon}^t(a) + O(\varepsilon^2)$$
. \square

- **4. Discretization.** For a numerical realization of the semiclassical approximation (3.8), we proceed in two steps. First, we discretize the phase space integral by equiweighted quadrature with nodes $z_1, \ldots, z_N \in \mathbb{R}^{2d}$ distributed according to the Husimi function $\mathcal{H}^{\varepsilon}(\psi_0)$. Then, we discretize the time evolution of Φ^t_{ε} , Λ^t_{ε} , and Γ^t_{ε} initialized with the sampling points z_1, \ldots, z_N . For both discretization steps, we compute the ε -correction with lower accuracy.
 - **4.1.** Numerical quadrature. To discretize the phase space integral

$$\int_{\mathbb{R}^{2d}} F_{\varepsilon}^{t}(a_{\varepsilon})(z) \mathcal{H}^{\varepsilon}(\psi_{0})(z) dz$$

$$= \int_{\mathbb{R}^{2d}} (a_{\varepsilon} \circ \Phi_{\varepsilon}^{t})(z) \mathcal{H}^{\varepsilon}(\psi_{0})(z) dz - \frac{\varepsilon}{2} \int_{\mathbb{R}^{2d}} \Xi_{\varepsilon}^{t}(a)(z) \mathcal{H}^{\varepsilon}(\psi_{0})(z) dz$$

$$=: I(a_{\varepsilon} \circ \Phi_{\varepsilon}^{t}) - \frac{\varepsilon}{2} I(\Xi_{\varepsilon}^{t}(a))$$

we use the fact, that the Husimi function of a normalized wave function ψ_0 is a probability density, and work either with Markov chain Monte Carlo quadrature or with Quasi-Monte Carlo quadrature. That is, we approximate

$$I(f) \approx \frac{1}{N} \sum_{j=1}^{N} f(z_j) =: Q_N(f)$$

with quadrature nodes $z_1, \ldots, z_N \in \mathbb{R}^{2d}$ distributed according to $\mathcal{H}^{\varepsilon}(\psi_0)$. Thanks to the small ε -prefactor, the correction integral $I(\Xi_{\varepsilon}^t(a))$ can be computed with less quadrature nodes than the leading order $I(a_{\varepsilon} \circ \Phi_{\varepsilon}^t)$.

4.1.1. Markov chain Monte Carlo quadrature. We use Metropolis Monte Carlo and generate sample points z_1, \ldots, z_N , which form a Markov chain with stationary distribution $\mathcal{H}^{\varepsilon}(\psi_0)$, see e.g. [KLW09, §4.1]. If the chain is uniformly ergodic, then a central limit theorem holds, and there exists a constant $\gamma = \gamma(f) > 0$ such that for all c > 0

$$\lim_{N\to\infty} \mathbb{P}\left(|I(f)-Q_N(f)| \leq \frac{c\gamma}{\sqrt{N}}\right) = \frac{1}{\sqrt{2\pi}} \int_{-c}^{c} e^{-\tau^2/2} d\tau.$$

We note, that for the numerical experiments in Section §5, the constant $\gamma(f)$ shows a beneficial dependence on the semiclassical parameter $\varepsilon > 0$, since the variance of the integrands decreases with decreasing ε .

4.1.2. Quasi-Monte Carlo quadrature. For Gaussian wave packets ψ_0 , the Husimi function $\mathcal{H}^{\varepsilon}(\psi_0)$ is a phase space Gaussian, and we view it as the density of a multivariate normal distribution. For notational simplicity, we focus on the special case of an isotropic Gaussian wave packet g_{z_0} centered in $z_0 = (q_0, p_0) \in \mathbb{R}^{2d}$,

$$g_{z_0}(q) = (\pi \varepsilon)^{-d/4} \exp\left(-\frac{1}{2\varepsilon}|q - q_0|^2 + \frac{i}{\varepsilon}p_0 \cdot (q - q_0)\right). \tag{4.1}$$

In this case, the Husimi function is the isotropic phase space Gaussian

$$\mathcal{H}^{\varepsilon}(g_{z_0})(z) = (2\pi\varepsilon)^{-d} \exp\left(-\frac{1}{2\varepsilon}|z-z_0|^2\right),$$

that is, the density of a normal distribution with mean z_0 and covariance εId . Generating points of low star discrepancy with respect to the uniform distribution on $[0,1]^{2d}$, that is, for example Sobol points, we use the cumulative distributive function of the normal distribution and map them to points z_1, \ldots, z_N such that their star discrepancy with respect to the normal distribution

$$\mathcal{D}^*(z_1,\ldots,z_N) = \sup_{\alpha \in \mathbb{R}^{2d}} \left| \frac{1}{N} \# \{ z_j : z_j \in (-\infty,\alpha), j = 1,\ldots,N \} - \mathcal{H}^{\varepsilon}(\psi_0)((-\infty,\alpha)) \right|$$

is optimal, that is, $\mathcal{D}^*(z_1,\ldots,z_N) = O((\log N)^{2d}/N)$. Then, the Koksma-Hlawka inequality yields a constant $\gamma = \gamma(f) > 0$ such that

$$|I(f) - Q_N(f)| \le \frac{\gamma(\log N)^{c_d}}{N},$$

where $c_d \geq 2d$ dependends on the dimension of phase space, see [LR10, 3.2]. We note, that as for the Monte Carlo quadrature, the numerical experiments of Section §5 show a favourable dependence of the constant $\gamma(f)$ on the semiclassical parameter $\varepsilon > 0$.

4.2. A time splitting scheme. For numerically computing Φ_{ε}^t , Λ_{ε}^t , and Γ_{ε}^t , we discretize the Hamiltonian flow (3.4) with a higher order symplectic scheme for an accurate approximation of the leading order contribution $a_{\varepsilon} \circ \Phi_{\varepsilon}^t$. The correction equations (3.5) and (3.6) are simultaneously discretized after vectorizing the Lyapunov matrix differential equation (3.5). For this purpose we use the Kronecker product

$$A \otimes B = \begin{pmatrix} a_{11}B & \cdots & a_{1n}B \\ \vdots & & \vdots \\ a_{n1}B & \cdots & a_{nn}B \end{pmatrix} \in \mathbb{R}^{n \cdot m \times n \cdot m} .$$

of two matrices $A \in \mathbb{R}^{n \times n}$ and $B \in \mathbb{R}^{m \times m}$ as well as the rowwise vectorization

$$Vec(A) = (a_{11}, a_{12}, \dots, a_{nn})^{T} = \vec{A} \in \mathbb{R}^{n^{2}}.$$

LEMMA 6. The differential equations (3.4), (3.5), and (3.6) are equivalent to the coupled vector differential equation with $4d + 4d^2$ components

$$\partial_t \begin{pmatrix} \Phi_{\varepsilon}^t \\ \vec{\Lambda}_{\varepsilon}^t \\ \Gamma_{\varepsilon}^t \end{pmatrix} = \begin{pmatrix} \operatorname{Id}_{2d} & 0 & 0 \\ 0 & K_{\varepsilon}(t) & 0 \\ 0 & C_{\varepsilon}(t) & M_{\varepsilon}(t) \end{pmatrix} \begin{pmatrix} J \nabla h_{\varepsilon} \circ \Phi_{\varepsilon}^t \\ \vec{\Lambda}_{\varepsilon}^t \\ \Gamma_{\varepsilon}^t \end{pmatrix} + \begin{pmatrix} 0 \\ \vec{M}_{\varepsilon}(t) \\ 0 \end{pmatrix}$$
(4.2)

with

$$K_{\varepsilon}(t) = M_{\varepsilon}(t) \otimes \operatorname{Id}_{2d} + \operatorname{Id}_{2d} \otimes M_{\varepsilon}(t),$$

$$C_{\varepsilon}(t) = \begin{pmatrix} \vec{C}_{1}(t)^{\mathrm{T}} \\ \vdots \\ \vec{C}_{2d}(t)^{\mathrm{T}} \end{pmatrix}.$$

Proof. First we show

$$\operatorname{Vec}(AB) = (A \otimes I_n) \operatorname{Vec}(B)$$

for $A, B \in \mathbb{R}^{n \times n}$. Indeed, for $1 \le cn + i \le n^2$

$$\operatorname{Vec}(AB)_{cn+i} = \sum_{j=1}^{n} a_{cj} b_{ji} = \sum_{j=1}^{n} (A \otimes I_n)_{(cn+i),(jn+i)} \operatorname{Vec}(B)_{jn+i}$$
$$= \sum_{k=1}^{n^2} (A \otimes I_n)_{(cn+i),k} \operatorname{Vec}(B)_k = ((A \otimes I_n) \operatorname{Vec}(B))_{cn+i}.$$

Similarly one can prove that $Vec(BA^T) = (I_n \otimes A) Vec(B)$. Hence,

$$\begin{split} \partial_t \mathrm{Vec}(\Lambda_\varepsilon^t) &= \vec{M}_\varepsilon(t) + \mathrm{Vec}\left(M_\varepsilon(t)\,\Lambda_\varepsilon^t + \Lambda_\varepsilon^t\,M_\varepsilon(t)^\mathrm{T}\right) \\ &= \vec{M}_\varepsilon(t) + \left(M_\varepsilon(t) \otimes \mathrm{Id}_{2d}\right) \vec{\Lambda}_\varepsilon^t + \left(\mathrm{Id}_{2d} \otimes M_\varepsilon(t)\right) \vec{\Lambda}_\varepsilon^t \\ &= \vec{M}_\varepsilon(t) + K_\varepsilon(t)\,\vec{\Lambda}_\varepsilon^t. \end{split}$$

Moreover, $\operatorname{tr}(C_i(t)\Lambda_{\varepsilon}^t) = \vec{C}_i(t)^T \vec{\Lambda}_{\varepsilon}^t$ and

$$\partial_t \Gamma_{\varepsilon}^t = M_{\varepsilon}(t) \Gamma_{\varepsilon}^t + \begin{pmatrix} \vec{C}_1(t)^{\mathrm{T}} \\ \vdots \\ \vec{C}_{2d}(t)^{\mathrm{T}} \end{pmatrix} \vec{\Lambda}_{\varepsilon}^t = M_{\varepsilon}(t) \Gamma_{\varepsilon}^t + C_{\varepsilon}(t) \vec{\Lambda}_{\varepsilon}^t.$$

For Schrödinger Hamiltonians $h(q,p) = \frac{1}{2}|p|^2 + V(q)$ with smooth subquadratic potential $V : \mathbb{R}^d \to \mathbb{R}$, we observe that

$$M_{\varepsilon}(t) = J D^2 h \circ \Phi_{\varepsilon}^t = \begin{pmatrix} 0 & \operatorname{Id}_d \\ -D^2 V((\Phi_{\varepsilon}^t)_q) & 0 \end{pmatrix},$$

while $C_i(t)_{jk} = \partial_k (JD^2h)_{ij} \circ \Phi^t_{\varepsilon}$ satisfies $C_i(t) = 0$ for i = 1, ..., d and depends on third derivatives of V and $(\Phi^t_{\varepsilon})_q$ for i = d+1, ..., 2d. This motivates to split

$$\Upsilon^t := \begin{pmatrix} (\Phi_{\varepsilon}^t)_q \\ (\Phi_{\varepsilon}^t)_p \\ \vec{\Lambda}_{\varepsilon}^t \\ \Gamma_{\varepsilon}^t \end{pmatrix} = \begin{pmatrix} 0 \\ (\Phi_{\varepsilon}^t)_p \\ \vec{\Lambda}_{\varepsilon}^t \\ \Gamma_{\varepsilon}^t \end{pmatrix} + \begin{pmatrix} (\Phi_{\varepsilon}^t)_q \\ 0 \\ 0 \\ 0 \end{pmatrix} =: \Upsilon_1^t + \Upsilon_2^t$$

and to rewrite the differential equation (4.2) as

$$\partial_t \Upsilon^t = A(\Upsilon_2^t) \Upsilon_1^t + N(\Upsilon_2^t) + B \Upsilon_1^t \tag{4.3}$$

with

and

$$N(\Upsilon_2^t) = egin{pmatrix} 0 \ -
abla V((\Phi_arepsilon^t)_q) \ ec{M}_arepsilon(t) \ 0 \end{pmatrix}.$$

Let ϕ_a^t and ϕ_b^t be the flows of the systems

$$\partial_t \Upsilon^t = A(\Upsilon_2^t) \Upsilon_1^t + N(\Upsilon_2^t), \qquad \partial_t \Upsilon^t = B \Upsilon_1^t,$$

respectively, and

$$F^h = \phi_a^{h/2} \phi_b^h \phi_a^{h/2}$$

the Strang splitting for h > 0, which provides a second order time discretization of equation 4.3, see e.g. [HWL06, §III.3.4]. This splitting scheme produces an approximate solution via

$$\begin{split} &\Upsilon_1^{h/2} = \Upsilon_1^0 + \frac{h}{2}(A(\Upsilon_2^0)\Upsilon_1^0 + N(\Upsilon_2^0)), \\ &\Upsilon_2^h = \Upsilon_2^0 + hB\Upsilon_1^{h/2}, \\ &\Upsilon_1^h = \Upsilon_1^{h/2} + \frac{h}{2}(A(\Upsilon_2^h)\Upsilon_1^{h/2} + N(\Upsilon_2^h)). \end{split}$$

and discretizes Φ_{ε}^t by the Störmer-Verlet scheme, while Λ_{ε}^t and Γ_{ε}^t are discretized by the midpoint rule.

Remark 3. The flows ϕ_a^t and ϕ_b^t are numerically easy to evaluate, since they are determined by differential equations with constant coefficient matrices and a constant inhomogeneity.

5. Numerical experiments. Let $\psi_t : \mathbb{R}^d \to \mathbb{C}$ the solution of the Schrödinger equation (1.1) and $a : \mathbb{R}^{2d} \to \mathbb{R}$ a Schwartz function. The preceding algorithmical considerations suggest

$$\langle \psi_t, \operatorname{op^{We}}(a)\psi_t \rangle_{L^2} \approx \frac{1}{N_1} \sum_{j=1}^{N_1} (a_{\varepsilon} \circ \widetilde{\Phi}_{\varepsilon}^t)(w_j) - \frac{\varepsilon}{2 \cdot N_2} \sum_{j=1}^{N_2} \widetilde{\Xi}_{\varepsilon}^t(a)(z_j),$$
 (5.1)

where $w_1, \ldots, w_{N_1} \in \mathbb{R}^{2d}$ and $z_1, \ldots, z_{N_2} \in \mathbb{R}^{2d}$, $N_1 \geq N_2$, are distributed according to $\mathcal{H}^{\varepsilon}(\psi_0)$. $\widetilde{\Xi}^t_{\varepsilon}(a)$ is obtained by $\lfloor t/h_2 \rfloor$ iterates of the Strang splitting scheme F^{h_2} and the application of the resulting vector to a and its derivatives according to Corollary 1. The leading order contribution $\widetilde{\Phi}^t_{\varepsilon}$ comes from a sixth order symplectic Yoshida splitting [Y90, Table 1, Solution B] with time step h_1 . Our numerical experiments validate this approach for different observables a: the position and momentum operators defined by

$$(q, p) \mapsto q_i, \quad (q, p) \mapsto p_i, \quad j = 1, \dots, d,$$

 $^{^1\}mathrm{All}$ experiments have been performed with MATLAB 7.14 on a 3.33 GHz Intel Xeon X5680 processor.

as well as the potential, kinetic, and total energy operators defined by

$$(q,p) \mapsto V(q), \quad (q,p) \mapsto \frac{1}{2}|p|^2, \quad (q,p) \mapsto h(q,p),$$

respectively. The main focus of the experiments is on the positive answer of the following two questions: Is the algorithm feasible in a moderate high dimensional setting? Can the asymptotic $O(\varepsilon^2)$ accuracy be acchieved efficiently, that is, with a reasonable number of sampling points N_1 , N_2 and time stepping h_1 , h_2 ?

5.1. Six dimensions. Our first experiment is concerned with the Henon-Heiles potential in six dimensions,

$$V(q) = \sum_{j=1}^{6} \frac{1}{2}q_j^2 + \sum_{j=1}^{5} \sigma_*(q_j q_{j+1}^2 - \frac{1}{3}q_j^3) + \frac{1}{16}\sigma_*^2(q_j^2 + q_{j+1}^2)^2$$

with $\sigma_* = 1/\sqrt{80}$. As in [FGL09, §5.4] and [LR10, §6], we choose the semiclassical parameter $\varepsilon = 0.01$ and a Gaussian initial state (4.1) centered in $z_0 = (q_0, 0)$ with $q_0 = (2, 2, 2, 2, 2, 2)^{\mathrm{T}}$. Since a grid based reference solution of the six-dimensional Schrödinger equation is not feasible, we compare the following three asymptotic particle methods:

- **A.** The Husimi based method defined in (5.1) using $N_1 = 2^{14}$ and $N_2 = 2^{10}$ transformed Sobol points for the numerical quadratures and the same time stepping $h = 10^{-3}$ for both $\widetilde{\Phi}_{\varepsilon}^t$ and $\widetilde{\Xi}_{\varepsilon}^t(a)$. We note that these numbers of Sobol points provide initial sampling errors smaller than $\varepsilon^2 = 10^{-4}$ for the leading term, and considerably smaller than $\varepsilon = 10^{-2}$ for the correction term, see Table 5.1.
- **B.** The naive Husimi method

$$\langle \psi_t, \operatorname{op}^{\operatorname{We}}(a)\psi_t \rangle_{L^2} \approx \frac{1}{N_1} \sum_{j=1}^{N_1} (a \circ \widetilde{\Phi}^t)(z_j),$$

where $\widetilde{\Phi}^t$ is a sixth order symplectic Yoshida discretization of Hamilton's equation $\dot{q}=p, \ \dot{p}=-\nabla V(q)$ with time stepping h. The quadrature nodes z_1,\ldots,z_N are obtained by transforming Sobol points, such that they are distributed according to $\mathcal{H}^{\varepsilon}(\psi_0)$. This approach is first order accurate with respect to ε .

C. The second order Wigner based method

$$\langle \psi_t, \operatorname{op}^{\operatorname{We}}(a) \psi_t \rangle_{L^2} \approx \frac{1}{N_1} \sum_{j=1}^{N_1} (a \circ \widetilde{\Phi}^t)(w_j)$$

of [LR10, §6], where the quadrature nodes w_1, \ldots, w_N are obtained by transforming Sobol points, such that they are distributed according to the initial Wigner function $\mathcal{W}^{\varepsilon}(\psi_0)$.

Figure 5.1 shows that the difference of the second order algorithms A and C is bounded by $6 \cdot 10^{-4} = 6\varepsilon^2$, while the naive Husimi approach of algorithm B deviates from method C by $0.06 = 6\varepsilon$. The computing time for the algorithms B and C, which use uncorrected classical transport, is 6 minutes, while the corrected Husimi algorithm A requires 17 minutes.

initial error	Husimi N_1	Husimi N_2	Wigner N_1			
kinetic energy	$3.2 \cdot 10^{-5}$	$3.3 \cdot 10^{-4}$	$1.6 \cdot 10^{-5}$			
potential energy	$8.1 \cdot 10^{-5}$	$5.8 \cdot 10^{-4}$	$4.8 \cdot 10^{-5}$			
Table 5.1						

Initial sampling errors of algorithms A (Husimi) and C (Wigner) with respect to the analytically computed expectation values for the initial kinetic and potential energy of the Henon-Heiles system, using $N_1=2^{14}$ and $N_2=2^{10}$ transformed Sobol points.

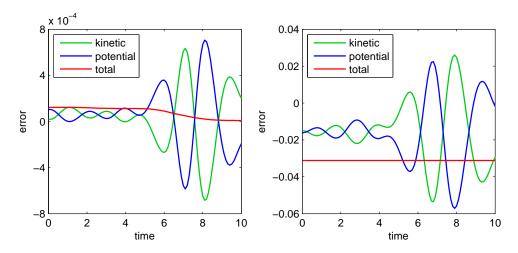


Fig. 5.1. The difference of the expectation values of the kinetic, potential and total energy for the six-dimensional Henon-Heiles system ($\varepsilon=0.01$) computed by the second order algorithms A and C (left) as well as B and C (right) as functions of time. The plots illustrate that the corrected Husimi method A is more accurate than the naive Husimi approach B.

5.2. Different semiclassical parameters. The next set of experiments is performed for the two-dimensional torsional potential,

$$V(q) = 2 - \cos(q_1) - \cos(q_2), \tag{5.2}$$

and different values of the semiclassical parameter ε . As initial data we consider both Gaussian states, and superpositions of Gaussian states.

While the Husimi transform of a single Gaussian wave packet is a phase space Gaussian, for Gaussian superpositions the Husimi function can easily be calculated as

$$\mathcal{H}^{\varepsilon}(g_{z_1} + g_{z_2}) = \mathcal{H}^{\varepsilon}(g_{z_1}) + \mathcal{H}^{\varepsilon}(g_{z_2}) + 2C_{z_1, z_2},$$

where the cross term

$$C_{z_1,z_2}(z) = (2\pi\varepsilon)^{-d} \exp\left(-\frac{1}{8\varepsilon}|z_-|^2\right) \exp\left(-\frac{1}{2\varepsilon}|z_-|^2\right) \cos\left(\frac{1}{2\varepsilon}(c_{1,2} - Jz \cdot z_-)\right)$$

has a Gaussian envelope centered around the mean $z_{+} = \frac{1}{2}(z_{1} + z_{2})$ and oscillates with a frequency proportional to the difference $z_{-} = z_{1} - z_{2}$. The shift is $c_{1,2} = q(z_{1})p(z_{1}) - q(z_{2})p(z_{2})$. The cross term contains a constant damping factor, which is exponentially small in $|z_{-}|^{2}$. This allows the tails of $\mathcal{H}^{\varepsilon}(g_{z_{1}})$ and $\mathcal{H}^{\varepsilon}(g_{z_{2}})$ to absorb the oscillations of the cross term, which turns the Husimi function positive. We perform experiments for the following two different set-ups:

- **D.** We apply the Husimi based method defined in (5.1) for Gaussian initial data g_{z_0} centered in $z_0 = (1,0,0,0)^{\mathrm{T}}$. The considered semiclassical parameters are $\varepsilon \in \{10^{-1}, 5 \cdot 10^{-2}, 10^{-2}, 5 \cdot 10^{-3}, 10^{-3}\}$.
- **E.** We apply the Husimi based method defined in (5.1). The initial states ψ_0 are superpositions $g_{z_1}+g_{z_2}$ with phase space centers $z_1=(0.5,-0.6,0,0)^{\rm T}$ and $z_2=(0,1,0,0)^{\rm T}$, normalized such that $\|\psi_0\|_{L^2}=1$. The considered semiclassical parameters are $\varepsilon\in\{10^{-1},5\cdot10^{-2},10^{-2},5\cdot10^{-3},10^{-3}\}$.

For the experiments in set-up D, we use Quasi-Monte Carlo quadrature with transformed Sobol points for all values of ε . In set-up E, we use two different quadrature methods, depending on the size of the semiclassical parameter ε . For $\varepsilon \in \{10^{-1}, 5 \cdot 10^{-2}\}$ we generate Markov chains of length N_1 and N_2 by a Metropolis algorithm with jumps between sampling regions centered around z_1, z_2 , and z_+ , see [KLW09, §4.1]. The final results are arithmetic means over ten independent runs, which provides unbiased estimates for the phase space integrals. For all $\varepsilon \leq 10^{-2}$, the cross term C_{z_1,z_2} in the Husimi function is smaller than $2 \cdot 10^{-13}$, due to the exponential damping factor $\exp(-\frac{1}{8\varepsilon}|z_-|^2)$. Therefore, the cross term is neglected, and the two Gaussians $\mathcal{H}^{\varepsilon}(g_{z_1})$ and $\mathcal{H}^{\varepsilon}(g_{z_2})$ are each sampled by $\frac{1}{2}N_1$ and $\frac{1}{2}N_2$ Sobol points for the leading term and the correction, respectively.

Table 5.2 summarizes the chosen numbers of sampling points N_1 , N_2 and the time steppings h_1 , h_2 for the discretized flows. We note that the smaller the semi-classical parameter ε , the more accurate the approximation of the corrected Husimi algorithm (5.1), the higher the computational cost in terms of sampling points and time steps for achieving the asymptotic rate $O(\varepsilon^2)$. However, the constants $\gamma(f) > 0$ of the error estimates for Monte Carlo and Quasi-Monte Carlo quadrature decrease with decreasing ε , due to the shrinking variance of the integrands. This observation allows to work with moderate numbers of sampling points, even for small values of the semiclassical parameter.

ε	$N_1(D) / N_1(E)$	$N_2(D) / N_2(E)$	h_1	h_2		
10^{-1}	$10^4 / 10^5$	$10^3 / 10^4$	10^{-2}	10^{-3}		
$5 \cdot 10^{-2}$	$3 \cdot 10^4 / 2 \cdot 10^5$	$3 \cdot 10^3 / 2 \cdot 10^4$	10^{-2}	10^{-3}		
10^{-2}	10^{5}	10^{4}	10^{-3}	10^{-3}		
$5 \cdot 10^{-3}$	$3 \cdot 10^{5}$	$2 \cdot 10^{4}$	10^{-3}	10^{-3}		
10^{-3}	10^{6}	$5 \cdot 10^{4}$	10^{-3}	$2\cdot 10^{-4}$		
Table 5.2						

The number of sampling points N_1 and N_2 as well as the time steps h_1 and h_2 used for the simulations with the second order Husimi algorithm (5.1) in both set-ups D and E. For $\varepsilon > 10^{-2}$, we need more sampling points in set-up E than in set-up D due to the slower convergence of the Metropolis quadrature.

We generate numerically converged reference solutions for the Schrödinger equation (1.1) using a Strang splitting scheme with Fourier collocation for the discretization of the Laplacian. The discretization parameters for the reference solutions, that is, the number of time steps, the computational domain, and the size of the space grid, are summarized in Table 5.3. The comparison of the Husimi algorithm (5.1) with the expectation values inferred from the reference solutions is presented in Figure 5.2. It confirms our expectations and shows second order accuracy with respect to ε . Moreover, the time evolution of the errors for two of the experiments, set-up D with $\varepsilon = 10^{-1}$ and set-up E with $\varepsilon = 10^{-3}$, is presented in Figure 5.3.

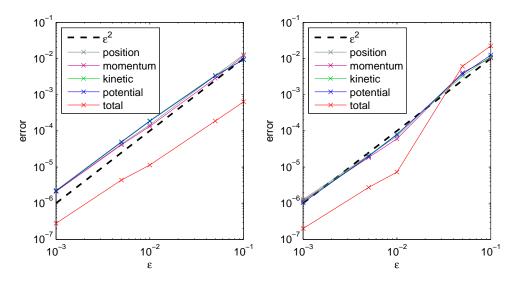


Fig. 5.2. The errors of the expectation values of position, momentum, potential, kinetic, and total energy for the two-dimensional torsional potential computed with the corrected Husimi algorithm (5.1) in the experimental set-ups D (left) and E (right), averaged over the time interval [0,20]. In both cases, the errors are of the order ε^2 .

arepsilon	#timesteps	domain	space grid
10^{-1}	$5 \cdot 10^3$	$[-3,3] \times [-3,3]$	1536×1536
$5 \cdot 10^{-2}$	$5 \cdot 10^3$	$[-3,3] \times [-3,3]$	1536×1536
10^{-2}	$7.5 \cdot 10^{3}$	$[-2,2] \times [-2,2]$	2048×2048
$5 \cdot 10^{-3}$	10^{4}	$[-2,2] \times [-2,2]$	2048×2048
10^{-3}	10^{4}	$[-2,2] \times [-2,2]$	2048×2048
	,	Table 5.3	

The discretization parameters for the grid-based reference solutions computed by a Strang splitting scheme with Fourier collocation.

Appendix A. Composition formula.

The calculus developed in $\S 2$ implies a composition formula for Anti-Wick quantized operators.

LEMMA 7. Let $a,b: \mathbb{R}^{2d} \to \mathbb{R}$ be Schwartz functions, $n \in \mathbb{N}$, and $\varepsilon > 0$. There is a family of Schwartz functions $(\gamma_n^{\varepsilon}(a,b))_{\varepsilon>0}$, $\gamma_n^{\varepsilon}(a,b): \mathbb{R}^{2d} \to \mathbb{R}$, with $\sup_{\varepsilon>0} \|\operatorname{op^{We}}(\gamma_n^{\varepsilon}(a,b))\|_{\mathcal{L}(L^2)} < \infty$, such that

$$\operatorname{op^{AW}}(a)\operatorname{op^{AW}}(b) = \operatorname{op^{AW}}\left(ab + \sum_{m=1}^{n} \varepsilon^{m} \lambda_{m}(a, b)\right) + \varepsilon^{n+1}\operatorname{op^{We}}\left(\gamma_{n}^{\varepsilon}(a, b)\right)$$

with

$$\lambda_m(a,b)(z) = \frac{(-1)^m}{2^m m!} \left[\left(\left(\nabla_z, \nabla_w \right) + i \left(J \nabla_z, \nabla_w \right) \right)^m (a(z) \cdot b(w)) \right]_{w=z} .$$

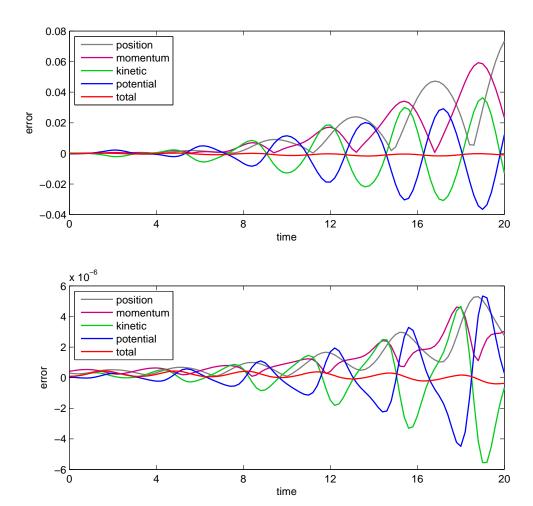


Fig. 5.3. The errors of the expectation values of position, momentum, potential, kinetic, and total energy computed with the corrected Husimi algorithm (5.1) as functions of time for experimen D with $\varepsilon = 10^{-1}$ (top) and experiment E with $\varepsilon = 10^{-3}$ (bottom).

Proof. By means of Lemma 1 we can write

$$\begin{aligned} &\operatorname{op^{\mathrm{AW}}}(a)\operatorname{op^{\mathrm{AW}}}(b) \\ &= \operatorname{op^{\mathrm{We}}}\left(\sum_{k=0}^{n} \frac{\varepsilon^{k}}{4^{k}k!} \, \Delta^{k}a\right) \operatorname{op^{\mathrm{We}}}\left(\sum_{k=0}^{n} \frac{\varepsilon^{k}}{4^{k}k!} \, \Delta^{k}b\right) + \varepsilon^{n+1} \operatorname{op^{\mathrm{We}}}\left(v_{n}^{\varepsilon}(a,b)\right) \end{aligned}$$

for some family of Schwartz functions $(v_n^{\varepsilon}(a,b))_{\varepsilon>0}$. With the expansion of the Moyal

product (2.4) and Lemma 2 we obtain

$$\begin{aligned} &\operatorname{op^{AW}}(a)\operatorname{op^{AW}}(b) \\ &= \operatorname{op^{We}}\left(\sum_{k+m \leq n} \frac{4^{-(k+m)}\varepsilon^{k+m}}{k!m!} (\Delta^k a) \sharp (\Delta^m b)\right) + \varepsilon^{n+1}\operatorname{op^{We}}\left(\widetilde{v}_n^\varepsilon(a,b)\right) \\ &= \sum_{p=0}^n \varepsilon^p \cdot \operatorname{op^{We}}\left(\sum_{k+m+j=p} \frac{4^{-(k+m)}(-i)^j}{k!m!j!} \left[A(D)^j (\Delta^k a \otimes \Delta^m b)\right]_{\operatorname{diag}}\right) \\ &+ \varepsilon^{n+1}\operatorname{op^{We}}\left(w_n^\varepsilon(a,b)\right) \\ &= \sum_{p=0}^n \varepsilon^p \cdot \operatorname{op^{AW}}\left(\sum_{k+m+j+r=p} \frac{4^{-(k+m+r)}(-i)^j}{k!m!j!r!} (-\Delta)^r \left[A(D)^j (\Delta^k a \otimes \Delta^m b)\right]_{\operatorname{diag}}\right) \\ &+ \varepsilon^{n+1}\operatorname{op^{We}}\left(w_n^\varepsilon(a,b)\right) \end{aligned}$$

with some Schwartz class family $(w_n^{\varepsilon}(a,b))_{\varepsilon>0}$ by invoking the operator A(D) defined in (2.7). Observing

$$\Delta_z \left[a(z) \cdot b(w) \right]_{w=z} = \left[\left(\Delta_z + \Delta_w + 2 \left(\nabla_z, \nabla_w \right) \right) \left(a(z) \cdot b(w) \right) \right]_{w=z}$$

yields

$$\sum_{k+m+j+r=p} \binom{p}{k,m,j,r} \frac{(-\Delta)^r}{4^r} \left[(-iA(D))^j \left(\frac{\Delta_z^k}{4^k} a(z) \cdot \frac{\Delta_w^m}{4^m} b(w) \right) \right]_{\text{diag}}$$

$$= 2^{-p} \sum_{k+m+j+r=p} \binom{p}{k,m,j,r} \frac{(-\Delta)^r}{2^r} \left[\left(-i \left(J \nabla_z, \nabla_w \right) \right)^j \frac{\Delta_z^k}{2^k} \frac{\Delta_w^m}{2^m} (a(z) \cdot b(w)) \right]_{\text{diag}}$$

$$= 2^{-p} \left[\left(-(\nabla_z, \nabla_w) - i \left(J \nabla_z, \nabla_w \right) \right)^p (a(z) \cdot b(w)) \right]_{\text{diag}}$$

where we utilized multinomial coefficient notation. \square

A proof of Lemma 7 in classical scaling can be found in [AM02, Theorem 2.5]. The expansion of the composition of two Anti-Wick quantized operators from Lemma 7 immediately implies a commutator expansion for Anti-Wick operators, similarly as the Moyal bracket expansion (2.6) for Weyl quantized operators.

Remark 4. For n = 1, we obtain

$$\mathrm{op^{AW}}(a)\mathrm{op^{AW}}(b) = \mathrm{op^{AW}}\left(ab + i\tfrac{\varepsilon}{2}J\nabla a\cdot\nabla b - \tfrac{\varepsilon}{2}\nabla a\cdot\nabla b\right) + O(\varepsilon^2),$$

whose real part coincides with [L10, Lemma 2.4.6].

Acknowledgements. This research was supported by the German Research Foundation (DFG), Collaborative Research Center SFB-TR 109, and the graduate program TopMath of the Elite Network of Bavaria.

REFERENCES

[AM02] Ando, H.; Morimoto, Y. Wick calculus and the Cauchy problem for some dispersive equations. Osaka J. Math. 39 (2002), no. 1, 123–147.

- [BR02] Bouzouina, A.; Robert, D. Uniform semiclassical estimates for the propagation of quantum observables. Duke Math. J. 111 (2002), no. 2, 223–252.
- [B67] de Bruijn, N. Uncertainty principles in Fourier analysis. Inequalities (Proc. Sympos. Wright-Patterson Air Force Base, Ohio, 1965), pp. 57-71, Academic Press (1967).
- [FGL09] Faou, E.; Gradinaru, V.; Lubich, C. Computing semi-classical quantum dynamics with Hagedorn wavepackets. SIAM J. Sci. Comput. 31 (2009), no. 4, 3027–3041.
- [GMMP97] Gérard, P.; Markowich, P.; Mauser, N.; Poupaud, F. Homogenization Limits and Wigner Transforms. Comm. Pure Appl. Math. 50 (1997), no. 4, 323–379.
- [HWL06] Hairer, E.; Lubich, C.; Wanner, G. Geometric numerical integration. Structure-preserving algorithms for ordinary differential equations. Second edition. Springer Series in Computational Mathematics, 31. Springer-Verlag, Berlin, 2006.
- [KLW09] Kube, S.; Lasser, C.; Weber, M. Monte Carlo sampling of Wigner functions and surface hopping quantum dynamics. J. Comp. Phys. 228 (2009), no. 6, 1947–1962.
- [L10] Lerner, N. Metrics on the phase space and non-selfadjoint pseudo-differential operators. Pseudo-Differential Operators. Theory and Applications, 3. Birkhäuser Verlag, Basel, 2010.
- [LR10] Lasser, C.; Röblitz, S. Computing expectation values for molecular quantum dynamics. SIAM J. Sci. Comput. 32 (2010), no. 3, 1465–1483.
- [LRT10] Liu, H.; Runborg, O.; Tanushev, N. Error estimates for Gaussian beam superpositions. Preprint, 2010. Available at: arXiv:1008.1320.
- [LY12] Lu, J.; Yang, X. Convergence of frozen Gaussian approximation for high-frequency wave propagation. Comm. Pure Appl. Math. 65 (2012), no. 6, 759–789.
- [R10] Robert, D. On the Herman-Kluk semiclassical approximation. Rev. Math. Phys. 22 (2010), no. 10, 1123–1145.
- [ST01] Spohn, H.; Teufel, S. Adiabatic decoupling and time-dependent Born-Oppenheimer theory. Commun. Math. Phys. 224 (2001), no.1, 113–132.
- [SR09] Swart, T.; Rousse, V. A mathematical justification for the Herman-Kluk propagator. Comm. Math. Phys. 286 (2009), no. 2, 725–750.
- [Y90] Yoshida, H. Construction of higher order symplectic integrators. Phys. Lett. A 150 (1990), no. 5-7, 262-268.
- [Z08] Zhang, P. Wigner Measure and Semiclassical Limits of Nonlinear Schrödinger Equations. Courant Lecture Notes in Mathematics 17, AMS, Providence, 2008.
- [Z12] Zworski, M. Semiclassical Analysis. Graduate Studies in Mathematics 138, AMS, Providence, 2012.