A NEW PHASE SPACE DENSITY FOR QUANTUM EXPECTATIONS

JOHANNES KELLER, CAROLINE LASSER, AND TOMOKI OHSAWA

Abstract. We introduce a new density for the representation of quantum states on phase space. It is constructed as a weighted difference of two smooth probability densities using the Husimi function and first-order Hermite spectrograms. In contrast to the Wigner function, it is accessible by sampling strategies for positive densities. In the semiclassical regime, the new density allows to approximate expectation values to second order with respect to the high frequency parameter and is thus more accurate than the uncorrected Husimi function. As an application, we combine the new phase space density with Egorov's theorem for the numerical simulation of time-evolved quantum expectations by an ensemble of classical trajectories. We present supporting numerical experiments in different settings and dimensions.

1. INTRODUCTION

The wave functions describing the nuclear part of a molecular quantum system are square integrable functions on $\mathbb{R}^d$ with specific properties. They are smooth functions, but highly oscillatory and the dimension $d$ is large. The frequencies of oscillations are typically related to a small semiclassical parameter $\varepsilon > 0$, which can be thought of as the square root of the ratio of the electronic versus the average nuclear mass for the molecular system of interest. One expects

$$\int_{\mathbb{R}^d} \bar{\psi}(x) (-i \varepsilon \nabla_x) \psi(x) \, dx = O(1)$$

as $\varepsilon \to 0$ for most nuclear wave functions $\psi \in L^2(\mathbb{R}^d)$. Often the semiclassical analysis of a molecular quantum system requires a phase space representation of the nuclear wave function, the most popular being the Wigner function

$$W_\psi(z) := (2\pi \varepsilon)^{-d} \int_{\mathbb{R}^d} \bar{\psi}(q + \frac{y}{\varepsilon}) \psi(q - \frac{y}{\varepsilon}) e^{iy \cdot p / \varepsilon} \, dy, \quad z = (q, p) \in \mathbb{R}^{2d}.$$
The Wigner function is a square integrable real-valued function on the phase space $T^*\mathbb{R}^d \cong \mathbb{R}^{2d}$ with many striking properties as for example

$$\int_{\mathbb{R}^d} x|\psi(x)|^2 \, dx = \int_{\mathbb{R}^{2d}} q \, W_\psi(z) \, dz,$$

$$\int_{\mathbb{R}^d} \overline{\psi}(x)(-i\varepsilon \nabla_x)\psi(x) \, dx = \int_{\mathbb{R}^{2d}} p \, W_\psi(z) \, dz.$$

However, in most cases the Wigner function is not a probability density on phase space, since it may attain negative values.

A guiding example is provided by the superposition of Gaussian wave packets. The semiclassically scaled Gaussian wave packet $g_{z_0}$ with phase space center $z_0 = (q_0, p_0) \in \mathbb{R}^{2d}$ is defined as

$$g_{z_0}(x) := (\pi \varepsilon)^{-d/4} \exp \left( -\frac{1}{\varepsilon} |x - q_0|^2 + \frac{i}{\varepsilon} p_0 \cdot (x - \frac{1}{2} q_0) \right), \quad x \in \mathbb{R}^d.$$

It satisfies

$$\int_{\mathbb{R}^d} x|g_{z_0}(x)|^2 \, dx = q_0 \quad \text{and} \quad \int_{\mathbb{R}^d} \overline{g_{z_0}(x)}(-i\varepsilon \nabla_x)g_{z_0}(x) \, dx = p_0.$$

Its Wigner function is a nonnegative Gaussian function centered at the point $z_0$. However, the Wigner function of the superposition

$$\psi = g_{z_1} + g_{z_2}, \quad z_1, z_2 \in \mathbb{R}^{2d},$$

has three regions of localization as seen in the left panel of Figure 1. There are two regions around the points $z_1$ and $z_2$, respectively, where the Wigner function has nonnegative Gaussian shape, whereas in between around the midpoint of $z_1$ and $z_2$ there is an oscillatory region with pronounced negative values.

Figure 1. Contour plots of the Wigner function (left), the Husimi function (middle), and the density $\mu_\psi$ (right) for a Gaussian superposition $\psi = g_{z_1} + g_{z_2}$. We chose the phase space centers $z_1 = (0, 1)$, $z_2 = (1, -\frac{3}{2})$, and the semiclassical parameter $\varepsilon = 0.14$. Negative values are indicated by blue color.
One way of obtaining a nonnegative phase space representation of a wave function is to convolve its Wigner function with another Wigner function. One then calls the nonnegative function
\[ W_\psi \ast W_\phi, \quad \phi \in \mathcal{S}(\mathbb{R}^d), \]
a \textit{spectrogram} of \( \psi \). A widely used spectrogram is the Husimi function of \( \psi \),
\[ \mathcal{H}_\psi := W_\psi \ast W_{g_0}, \]
which is the spectrogram of \( \psi \) with \( \phi \) being the Gaussian wave packet \( g_0 \) centered at the phase space origin. For the superposition example, the smoothing of the convolution removes the oscillations and widens the Gaussian profiles around the centers \( z_1 \) and \( z_2 \); see the middle panel of Figure 1. However, the smoothing also destroys important exact relations satisfied by the Wigner function. Let \( a : \mathbb{R}^d \to \mathbb{R} \) be a smooth function with an appropriate decay property. Then,
\[
\int_{\mathbb{R}^d} a(x)|\psi(x)|^2 \, dx = \int_{\mathbb{R}^2d} a(q) W_\psi(z) \, dz,
\]
while
\[
\int_{\mathbb{R}^d} a(x)|\psi(x)|^2 \, dx = \int_{\mathbb{R}^2d} a(q) \mathcal{H}_\psi(z) \, dz + O(\varepsilon)
\]
as \( \varepsilon \to 0 \), where the error term depends on second and higher order derivatives of the function \( a \). Hence only the first moment of the position density \( x \mapsto |\psi(x)|^2 \) is exactly recovered by the Husimi function.

Our aim is now to systematically construct a new phase space density that maintains some of the key properties of the Wigner function, while being amenable to sampling strategies for positive densities. We propose a proper reweighting of the Husimi function and the spectrograms obtained from the first order Hermite functions
\[ \varphi_{e_j}(x) := (\pi \varepsilon)^{-d/4} \frac{x_j}{\varepsilon} \exp\left(-\frac{1}{2\varepsilon}|x|^2\right), \quad x \in \mathbb{R}^d, \quad j = 1, \ldots, d. \]
We define a real-valued function \( \mu_\psi : \mathbb{R}^{2d} \to \mathbb{R} \) by
\[ \mu_\psi := (1 + \frac{d}{2}) W_\psi \ast W_{g_0} - \frac{d}{2} \sum_{j=1}^d W_\psi \ast W_{\varphi_{e_j}}. \]
By construction, \( \mu_\psi \) is the difference of two nonnegative functions, a scalar multiple of the Husimi function \( W_\psi \ast W_{g_0} \) on the one side, and half the sum of the Hermite spectrograms \( W_\psi \ast W_{\varphi_{e_1}}, \ldots, W_\psi \ast W_{\varphi_{e_d}} \) on the other side. For example, a single Gaussian wave packet \( \psi = g_{z_0} \) centered at the point \( z_0 \in \mathbb{R}^{2d} \) results in
\[ \mu_{g_{z_0}}(z) = (1 + \frac{d}{2}) (2\pi \varepsilon)^{-d} \exp\left(-\frac{1}{2\varepsilon}|z - z_0|^2\right) \]
\[ - \frac{1}{2\varepsilon} |z - z_0|^2 (2\pi \varepsilon)^{-d} \exp\left(-\frac{1}{2\varepsilon}|z - z_0|^2\right), \]
which is the difference of two well-localized positive densities. For the superposition of two Gaussian wave packets \( \psi = g_{z_1} + g_{z_2} \), we obtain a density \( \mu_\psi \) characterized by two islands of positive values around the centers \( z_1 \) and \( z_2 \), which are surrounded by a sea of negative values; see the contour plot in the right panel of Figure 1 and the explicit formula in §5.2.
The new phase space function $\mu_\psi$ allows for the exact representation of the moments of $\psi$ up to order three in the following sense. If $a : \mathbb{R}^d \rightarrow \mathbb{R}$ is a polynomial of degree less than or equal to three, then

$$
\int_{\mathbb{R}^d} a(x)|\psi(x)|^2 \, dx = \int_{\mathbb{R}^{2d}} a(q)\mu_\psi(z) \, dz,
$$

and for arbitrary smooth functions $a : \mathbb{R}^{2d} \rightarrow \mathbb{R}$ and the associated Weyl quantized operator $\text{op}(a)$, the expectation value is approximated as

$$
\int_{\mathbb{R}^d} \overline{\psi}(x) \, \text{op}(a) \psi(x) \, dx = \int_{\mathbb{R}^{2d}} a(z)\mu_\psi(z) \, dz + O(\varepsilon^2)
$$

for $\varepsilon \rightarrow 0$, where the error term depends on fourth and higher order derivatives of the function $a$; see Theorem 3.2 later on. The idea of combining different spectrograms can also be found in the time-frequency literature; see e.g. [16]. However, their goal lies in entropy optimization not quantum expectations.

The second order accuracy with respect to $\varepsilon$ in the expectation value approximation suggests to use the new density in the context of molecular quantum dynamics. We consider the time-dependent Schrödinger equation

$$
i\varepsilon \partial_t \psi(t) = \left(-\frac{\varepsilon^2}{2} \Delta + V\right) \psi(t), \quad \psi(0) = \psi_0,$$

with a smooth potential function $V : \mathbb{R}^d \rightarrow \mathbb{R}$ as provided by the time-dependent Born–Oppenheimer approximation. Let us denote by $\Phi_t : \mathbb{R}^{2d} \rightarrow \mathbb{R}^{2d}$ the flow of the corresponding classical equations of motion

$$\dot{q} = p, \quad \dot{p} = -\nabla V(q).$$

Then, by Egorov’s theorem, we have

$$\langle \psi(t), \text{op}(a) \psi(t) \rangle_{L^2} = \int_{\mathbb{R}^{2d}} (a \circ \Phi_t)(z) W_{\psi_0}(z) \, dz + O(\varepsilon^2)$$

as $\varepsilon \rightarrow 0$, where the error depends on third and higher order derivatives of the functions $a \circ \Phi_t$ and $V$ as well as the $L^2$-norm of the initial wave function $\psi_0$. The Egorov approximation is computationally advantageous, in particular in high dimensions, since it allows to simulate the time-evolution of quantum expectations by an ensemble of classical trajectories. Over decades, it has been widely used in the physical chemistry literature under the name linearized semiclassical initial value representation (LSC-IVR) or Wigner phase space method.

Our new phase space density comes into play here, since the combination of the approximations in (1.2) and (1.3) provides

$$\langle \psi(t), \text{op}(a) \psi(t) \rangle_{L^2} = \int_{\mathbb{R}^{2d}} (a \circ \Phi_t)(z) \mu_{\psi_0}(z) \, dz + O(\varepsilon^2),$$

which can be read as a new method for the computation of time-evolved quantum expectations by initial sampling from a difference of nonnegative phase space distributions; see Theorem 4.1 and the numerical experiments in §6.
1.1. Outline. Our investigation proceeds along the following lines. In §2 we briefly review phase space distributions as the Wigner function, spectrograms, and the Husimi function. §3 derives the new phase space density \( \mu_\psi \) and proves our main result, that is, the second order approximation of expectation values by the phase space integration with respect to the new density function. §4 applies this result to the quantum propagation of expectation values. Then, several explicit formulas for the density \( \mu_\psi \) are derived in §5. The numerical experiments in §6 illustrate the applicability of the new approach for the dynamics of molecular quantum systems in dimensions \( d = 1, d = 2, \) and \( d = 32. \) Appendix A presents a sampling strategy for the density \( \mu_\psi \) via the Gamma distribution used for the numerical experiments, while Appendix B provides further computational details.

2. Phase space distributions

In this section we review different possibilities for representing a square integrable function \( \psi \in L^2(\mathbb{R}^d) \) via real-valued distributions on the classical phase space \( T^*\mathbb{R}^d \approx \mathbb{R}^{2d}. \) Considering functions with frequencies of the order \( 1/\varepsilon \) for a small parameter \( 0 < \varepsilon \ll 1, \) we work with the \( \varepsilon \)-rescaled Fourier transform

\[
F_\varepsilon \psi(p) := (2\pi \varepsilon)^{-d/2} \int_{\mathbb{R}^d} \psi(q) e^{-i p \cdot q / \varepsilon} dq, \quad p \in \mathbb{R}^d.
\]

We also use the Heisenberg–Weyl operator in \( \varepsilon \)-scaling:

Definition 2.1. The Heisenberg–Weyl operator associated with a phase space point \( z = (q, p) \in \mathbb{R}^{2d} \) is defined as

\[
T_z \psi := e^{i p \cdot (\bullet - q / 2) / \varepsilon} \psi(\bullet - q), \quad \psi \in L^2(\mathbb{R}^d).
\]

Among its many striking properties, the following two will be important for us later on. We have

\[
T_z^\dagger = T_{-z}, \quad z \in \mathbb{R}^{2d},
\]

and

\[
T_{z_1} T_{z_2} = \exp \left( -\frac{i}{2\varepsilon} \Omega(z_1, z_2) \right) T_{z_1 + z_2}, \quad z_1, z_2 \in \mathbb{R}^{2d},
\]

where \( \Omega : \mathbb{R}^{2d} \times \mathbb{R}^{2d} \to \mathbb{R} \) denotes the standard symplectic form on \( \mathbb{R}^{2d}, \) i.e.,

\[
\Omega(z_1, z_2) := z_1^T J z_2 = q_1^T p_2 - p_1^T q_2 \quad \text{with} \quad J = \begin{bmatrix} 0 & \text{Id} \\ -\text{Id} & 0 \end{bmatrix}.
\]

All phase space distributions considered here turn the action of the Heisenberg–Weyl operator \( T_z \) on a wave function into a phase space translation by \( z, \) which is often referred to as a covariance property; see, e.g., (2.6) below.

Remark 2.2. The Gaussian wave packet (1.1) with its phase space center at \( z_0 \in \mathbb{R}^{2d} \) is obtained by applying the Heisenberg–Weyl operator \( T_{z_0} \) to the Gaussian

\[
g_0(x) := (\pi \varepsilon)^{-d/4} \exp \left( -\frac{1}{\varepsilon} |x|^2 \right)
\]

centered at the origin, i.e., \( g_{z_0} = T_{z_0} g_0. \)
2.1. **Wigner functions.** We start our discussion with the celebrated Wigner function and recapitulate some basic relations.

**Definition 2.3.** The Wigner function of a function $\psi \in L^2(\mathbb{R}^d)$ is defined as

$$W_\psi(z) := (2\pi \varepsilon)^{-d} \int_{\mathbb{R}^d} \overline{\psi(q + \frac{y}{2})} \psi(q - \frac{y}{2}) e^{iy \cdot p/\varepsilon} dy,$$  

where $z = (q, p) \in \mathbb{R}^{2d}$.

Wigner functions are continuous square-integrable functions on phase space; however, they need not be integrable. The marginals are the position and momentum density of the state, respectively. With a proper interpretation of the possibly not absolutely convergent integrals this means

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

and in particular

$$\int_{\mathbb{R}^{2d}} W_\psi(z) dz = \|\psi\|^2.$$

Wigner transformation preserves orthogonality in the sense that

$$\int_{\mathbb{R}^{2d}} W_\psi(z) W_\phi(z) dz = (2\pi \varepsilon)^{-d} |\langle \psi, \phi \rangle|, \quad \psi, \phi \in L^2(\mathbb{R}^d),$$

and it turns the action of the Heisenberg–Weyl operator into a phase space translation, i.e.,

$$W_{T_z} \psi = W_\psi(\bullet - z), \quad z \in \mathbb{R}^{2d},$$

which is an example of the covariance property alluded above.

Moreover, given a Schwartz function $a : \mathbb{R}^{2d} \to \mathbb{R}$, one can use Wigner functions to express expectation values of Weyl quantized linear operators

$$\langle \psi, \text{op}(a) \psi \rangle(q) = (2\pi \varepsilon)^{-d} \int_{\mathbb{R}^{2d}} a(q + \frac{y}{2}, p) \overline{\psi(q + \frac{y}{2})} \psi(q - \frac{y}{2}) e^{iy \cdot p/\varepsilon} dy dp$$

via the weighted phase space integral

$$\langle \psi, \text{op}(a) \psi \rangle = \int_{\mathbb{R}^{2d}} a(z) W_\psi(z) dz.$$

We note that the oscillatory integral formula (2.2) can be extended to more general classes of symbols $a : \mathbb{R}^{2d} \to \mathbb{R}$ with controlled growth properties at infinity; see for example [24, §4], [17, §2] or [9, §2].

2.2. **Spectrograms.** Except for Gaussian states, Wigner functions attain negative values (see [22]), and thus cannot be treated as probability densities. For example, any odd function $\psi \in L^2(\mathbb{R}^d)$ satisfies

$$W_\psi(0) = -(2\pi \varepsilon)^{-d} \int_{\mathbb{R}^d} |\psi(y)|^2 dy \leq 0.$$  

One way to obtain nonnegative phase space representations of a quantum state is to convolve its Wigner function with another Wigner function.

**Definition 2.4.** Let $\psi \in L^2(\mathbb{R}^d)$ and $\phi \in \mathcal{S}(\mathbb{R}^d)$. Then, $W_\psi * W_\phi$ is called a spectrogram of $\psi$.  

In time-frequency analysis, spectrograms are typically introduced as the modulus squared of a short-time Fourier transform (see, e.g., the introduction in [8]) so that the representation via the convolution of two Wigner transforms is derived subsequently. Spectrograms also form a sub-class of Cohen’s class of phase space distributions [6, §3.2.1.]. They satisfy
\begin{equation}
(W_\psi \ast W_\phi)(z) = (2\pi\epsilon)^{-d} |\langle T_z \phi, \psi \rangle|^2, \quad z \in \mathbb{R}^{2d},
\end{equation}
where $\phi_-(x) := \phi(-x)$ for $x \in \mathbb{R}^d$; see also [9, Proposition 1.99]. Thus, spectrograms are nonnegative and smooth by construction. Young’s inequality implies integrability, and normalization is preserved according to
\begin{equation}
\int_{\mathbb{R}^{2d}} (W_\psi \ast W_\phi)(z) dz = \|\psi\|^2 \cdot \|\phi\|^2.
\end{equation}
Spectrograms also inherit the covariance property from the Wigner function, i.e.,
\begin{equation}
(W_{T_z \psi} \ast W_\phi)(z) = (W_\psi \ast W_\phi)(• - z), \quad z \in \mathbb{R}^{2d}.
\end{equation}
A particular spectrogram is obtained by convolving with the Wigner function of a Gaussian wave packet, which we will discuss next.

### 2.3. Husimi functions
The most commonly used nonnegative phase space distribution is the Husimi function; see e.g. [2, §4.1]. We consider the Wigner function
\begin{equation}
W_{g_0}(z) = (\pi\epsilon)^{-d/2} e^{-|z|^2/\epsilon}, \quad z \in \mathbb{R}^{2d},
\end{equation}
of the Gaussian wave packet $g_0$ centered at the phase space origin and define:

**Definition 2.5.** The Husimi function of $\psi \in L^2(\mathbb{R}^d)$ is defined as the spectrogram
\[
H_\psi(z) := (W_\psi \ast W_{g_0})(z) = \int_{\mathbb{R}^{2d}} W_\psi(w) (\pi\epsilon)^{-d/2} e^{-|z-w|^2/\epsilon} dw.
\]

The Husimi function of $\psi$ is the spectrogram (2.4) with $\phi$ being the Gaussian wave packet $g_0$, and since $g_0$ is even, we have
\[
H_\psi(z) = (2\pi\epsilon)^{-d} |\langle T_z g_0, \psi \rangle|^2, \quad z \in \mathbb{R}^{2d}.
\]
Also, since $g_0$ is normalized, i.e., $\|g_0\| = 1$, (2.5) gives
\[
\int_{\mathbb{R}^{2d}} H_\psi(z) dz = \|\psi\|^2.
\]
That is, for $\psi \in L^2(\mathbb{R}^d)$ with $\|\psi\| = 1$, the Husimi function is a smooth probability density on phase space.

**Remark 2.6.** The Husimi function of $\psi \in L^2(\mathbb{R}^d)$ is the modulus squared of the so-called Fourier–Bros–Iagolnitzer (FBI) transform, which associates with $\psi$ the mapping
\[
\mathbb{R}^{2d} \to \mathbb{C}, \quad z \mapsto (2\pi\epsilon)^{-d/2} \langle T_z g_0, \psi \rangle.
\]
In contrast to the Wigner function and the spectrograms, the FBI transform is a linear, albeit complex-valued phase space representation; see [17, Chapter 3].

Integrating a Schwartz function $a : \mathbb{R}^{2d} \to \mathbb{R}$ against the Husimi function, we obtain
\[
\int_{\mathbb{R}^{2d}} a(z) H_\psi(z) dz = \int_{\mathbb{R}^{2d}} a(z) (W_\psi \ast W_{g_0})(z) dz = \int_{\mathbb{R}^{2d}} (a \ast W_{g_0})(z) W_\psi(z) dz = \langle \psi, \text{op}(a \ast W_{g_0}) \psi \rangle,
\]
where the last equation uses the duality relation (2.3) between Weyl quantized operators and the Wigner transform. Therefore,
\[
\int_{\mathbb{R}^d} a(z) \mathcal{H}_\psi(z) \, dz = \langle \psi, \text{op}_{\text{aw}}(a) \psi \rangle,
\]
where
\[
\text{op}_{\text{aw}}(a) := \text{op}(a \ast W_{g_0}), \quad a \in \mathcal{S}(\mathbb{R}^d),
\]
denotes the anti-Wick quantized operator of the function \(a\); see for example [9, §2.7] and [4, §11.4]. Weyl and anti-Wick quantization are \(\varepsilon\)-close in the following sense:

**Lemma 2.7.** Let \(a : \mathbb{R}^d \to \mathbb{R}\) be a Schwartz function and \(\varepsilon > 0\). Then, there are two families of Schwartz functions \(r_{\varepsilon}^1, r_{\varepsilon}^2 : \mathbb{R}^d \to \mathbb{R}\) that depend on fourth and higher order derivatives of \(a\), so that

\[
\text{op}_{\text{aw}}(a) = \text{op}(a + \frac{\varepsilon}{4} \Delta a) + \varepsilon^2 \text{op}(r_{\varepsilon}^1),
\]

\[
\text{op}_{\text{aw}}(a - \frac{\varepsilon}{4} \Delta a) = \text{op}(a) + \varepsilon^2 \text{op}(r_{\varepsilon}^2),
\]

where \(\sup_{\varepsilon > 0} \| \text{op}(r_{\varepsilon}^j) \|_{L^2 \to L^2} < \infty\) for both \(j = 1, 2\).

**Proof.** The lemma is essentially proven in [15, Proposition 2.4.3] or [11, Lemma 1], and hence we only sketch the proof for the second of the two equivalent identities. We write out the definition

\[
\text{op}_{\text{aw}}(a - \frac{\varepsilon}{4} \Delta a) = \text{op}(W_{g_0} \ast (a - \frac{\varepsilon}{4} \Delta a))
\]

and Taylor expand \(a - \frac{\varepsilon}{4} \Delta a\) around \(z\) in the integral

\[
W_{g_0} \ast (a - \frac{\varepsilon}{4} \Delta a) = (\pi \varepsilon)^{-d} \int_{\mathbb{R}^d} (a - \frac{\varepsilon}{4} \Delta a)(\zeta) e^{-|z - \zeta|^2 / \varepsilon} d\zeta.
\]

Due to the symmetry of the Gaussian, all Taylor expansion terms with odd derivatives of \((a - \frac{\varepsilon}{4} \Delta a)\) vanish. The computation

\[
(\pi \varepsilon)^{-d} \sum_{|\alpha| = 1} \int_{\mathbb{R}^d} \frac{1}{(2\alpha)!} (\partial^{2\alpha}(a - \frac{\varepsilon}{4} \Delta a)) (\zeta - z)^{2\alpha} e^{-|z - \zeta|^2 / \varepsilon} d\zeta = \frac{\varepsilon}{4} \Delta (a - \frac{\varepsilon}{4} \Delta a)
\]

implies the second order approximation

\[
W_{g_0} \ast (a - \frac{\varepsilon}{4} \Delta a) = (a - \frac{\varepsilon}{4} \Delta a) + \frac{\varepsilon}{4} \Delta (a - \frac{\varepsilon}{4} \Delta a) + O(\varepsilon^2)
\]

\[
= a + O(\varepsilon^2),
\]

where the \(O(\varepsilon^2)\) term is of Schwartz class. Applying the Calderón–Vaillancourt Theorem (see, e.g., [9, §2.5]) concludes the proof. \(\square\)

**Remark 2.8.** The result of Lemma 2.7 can formally be read in terms of the heat semigroup \(\{\exp(t \Delta)\}_{t \geq 0}\) as

\[
a \ast W_{g_0} = \exp(\frac{\varepsilon}{4} \Delta) a = a + \frac{\varepsilon}{4} \Delta a + O(\varepsilon^2),
\]

where \(a : \mathbb{R}^d \to \mathbb{R}\) is a Schwartz function.
3. The new phase space density

We learn from the preceding discussion of phase space distributions, in particular from Lemma 2.7, that the Husimi function allows to approximate an expectation value according to

\[ \langle \psi, \text{op}(a) \psi \rangle = \int_{\mathbb{R}^2} (a - \frac{\xi}{4} \Delta a)(z) H_\psi(z) dz + O(\varepsilon^2) \]

as \( \varepsilon \to 0 \), where the error depends on the fourth and higher order derivatives of \( a \) and the \( L^2 \)-norm of \( \psi \). An integration by parts provides

\[ \langle \psi, \text{op}(a) \psi \rangle = \int_{\mathbb{R}^2} a(z) \left( H_\psi - \frac{\xi}{4} \Delta H_\psi \right)(z) dz + O(\varepsilon^2), \]

and motivates us to define the following new phase space density.

**Definition 3.1.** For \( \psi \in L^2(\mathbb{R}^d) \) we define the phase space density \( \mu_\psi : \mathbb{R}^2 \to \mathbb{R} \),

\[ \mu_\psi := H_\psi - \frac{\xi}{4} \Delta H_\psi. \]

We summarize the key property of the new density as follows:

**Theorem 3.2.** Let \( a : \mathbb{R}^d \to \mathbb{R} \) be a Schwartz function. Then, there exists a constant \( C > 0 \) depending on fourth and higher order derivatives of \( a \) such that for all \( \psi \in L^2(\mathbb{R}^d) \)

\[ \left| \langle \psi, \text{op}(a) \psi \rangle - \int_{\mathbb{R}^2} a(z) \mu_\psi(z) dz \right| \leq C \varepsilon^2 \| \psi \|^2, \]

where the density \( \mu_\psi : \mathbb{R}^2 \to \mathbb{R} \) was defined in Definition 3.1.

**Proof.** By Lemma 2.7, we have

\[ \langle \psi, \text{op}(a) \psi \rangle = \int_{\mathbb{R}^2} (a - \frac{\xi}{4} \Delta a)(z) H_\psi(z) dz + \varepsilon^2 \langle \psi, \text{op}(r^\varepsilon) \psi \rangle \]

with

\[ |\langle \psi, \text{op}(r^\varepsilon) \psi \rangle| \leq C \| \psi \|^2, \]

where the constant \( C > 0 \) depends on the fourth and higher order derivatives of \( a \). The Husimi function \( H_\psi \) is smooth and bounded since

\[ H_\psi(z) = (2\pi \varepsilon)^{-d} |\langle g_z, \psi \rangle|^2 \leq (2\pi \varepsilon)^{-d} \| g_z \|^2 \| \psi \|^2 = (2\pi \varepsilon)^{-d} \| \psi \|^2. \]

Hence, integration by parts implies

\[ \int_{\mathbb{R}^2} (a - \frac{\xi}{4} \Delta a)(z) H_\psi(z) dz = \int_{\mathbb{R}^2} a(z)(H_\psi - \frac{\xi}{4} \Delta H_\psi)(z) dz = \int_{\mathbb{R}^2} a(z) \mu_\psi(z) dz. \]

Therefore,

\[ \left| \langle \psi, \text{op}(a) \psi \rangle - \int_{\mathbb{R}^2} a(z) \mu_\psi(z) dz \right| = \varepsilon^2 \langle \psi, \text{op}(r^\varepsilon) \psi \rangle \leq C \varepsilon^2 \| \psi \|^2, \]

which concludes the proof. \( \Box \)

Our next aim is to derive an alternative expression for the new density showing that it is a linear combination of spectrograms.
3.1. The new density in terms of Hermite functions. The Laplacian of the Husimi function can be related to the Wigner function of the $\varepsilon$-rescaled first order Hermite functions as follows:

**Proposition 3.3.** Let $\varepsilon > 0$, $j \in \{1, \ldots, d\}$, and

$$\varphi_{\varepsilon j}(x) := (\pi \varepsilon)^{-d/4} \sqrt{\frac{2}{\varepsilon^2}} x_j \exp\left(-\frac{1}{\varepsilon^2} |x|^2\right), \quad x \in \mathbb{R}^d,$$

be the first order Hermite functions. Then, for all $\psi \in L^2(\mathbb{R}^d)$,

$$\Delta \mathcal{H}_\psi = \frac{\varepsilon}{2} \sum_{j=1}^d \mathcal{W}_\psi \ast \mathcal{W}_{\varphi_{\varepsilon j}} - \frac{2d}{\varepsilon} \mathcal{H}_\psi$$

and consequently

$$\mu_\psi = \mathcal{H}_\psi - \frac{\varepsilon}{4} \Delta \mathcal{H}_\psi = (1 + \frac{d}{2}) \mathcal{H}_\psi - \frac{1}{2} \sum_{j=1}^d \mathcal{W}_\psi \ast \mathcal{W}_{\varphi_{\varepsilon j}}.$$

**Proof.** Let $z \in \mathbb{R}^{2d}$. We compute

$$\Delta \mathcal{W}_{g_0}(z) = (\pi \varepsilon)^{-d} \Delta e^{-|z|^2/\varepsilon} = (\pi \varepsilon)^{-d} \nabla \cdot \left(\frac{2}{\varepsilon} z e^{-|z|^2/\varepsilon}\right)$$

$$= (\pi \varepsilon)^{-d} \left(-\frac{4d}{\varepsilon} + \frac{4}{\varepsilon^2} |z|^2\right) e^{-|z|^2/\varepsilon}.$$ 

Moreover, by direct computation or [14, Theorem 1],

$$\mathcal{W}_{\varphi_{\varepsilon j}}(z) = -(\pi \varepsilon)^{-d} \left(1 - \frac{2}{\varepsilon} |z_j|^2\right) e^{-|z|^2/\varepsilon},$$

such that

$$\sum_{j=1}^d \mathcal{W}_{\varphi_{\varepsilon j}}(z) = -(\pi \varepsilon)^{-d} \left(2d - d - \frac{2}{\varepsilon} |z_j|^2\right) e^{-|z|^2/\varepsilon}$$

$$= -(\pi \varepsilon)^{-d} \left(2d - \frac{2}{\varepsilon} |z_j|^2\right) e^{-|z|^2/\varepsilon} + d \cdot \mathcal{W}_{g_0}(z)$$

and

$$\Delta \mathcal{W}_{g_0}(z) = -\frac{2}{\varepsilon} (\pi \varepsilon)^{-d} \left(2d - \frac{2}{\varepsilon} |z_j|^2\right) e^{-|z|^2/\varepsilon} = \frac{2}{\varepsilon} \sum_{j=1}^d \mathcal{W}_{\varphi_{\varepsilon j}}(z) - \frac{2d}{\varepsilon} \mathcal{W}_{g_0}(z).$$

To conclude the proof we note that $\Delta \mathcal{H}_\psi = \Delta (\mathcal{W}_\psi \ast \mathcal{W}_{g_0}) = \mathcal{W}_\psi \ast \Delta \mathcal{W}_{g_0}$. \hfill \box

**Remark 3.4.** For any $\psi \in L^2(\mathbb{R}^d)$, the real-valued density $\mu_\psi$ is a weighted sum of spectrograms and therefore smooth and integrable. It satisfies the normalization condition

$$\int_{\mathbb{R}^{2d}} \mu_\psi(z) dz = ||\psi||^2$$

and the covariance property

$$\mu_{T_z \psi} = \mu_\psi(\bullet - z), \quad z \in \mathbb{R}^{2d}.$$ 

Next, we add a further characterization of the new density that does not explicitly require a convolution.
3.2. The new density in terms of ladder operators. The Gaussian wave packet \( g_0 \) centered at the origin and the first order Hermite functions \( \varphi_{e_1}, \ldots, \varphi_{e_d} \) can be characterized by the raising and lowering operators

\[
A^\dagger = \frac{1}{\sqrt{2\pi}} (x - \varepsilon \nabla_x) \quad \text{and} \quad A = \frac{1}{\sqrt{2\pi}} (x + \varepsilon \nabla_x),
\]

respectively. On the one hand, we have

\[
\text{span}\{g_0\} = \{\psi \in L^2(\mathbb{R}^d) \mid A_j \psi = 0 \text{ for all } j = 1, \ldots, d\},
\]

for the kernel of the lowering operator \( A = (A_1, \ldots, A_d) \). On the other hand, the components of the raising operator applied to the Gaussian wave packet \( g_0 \) generate the first order Hermite functions in the sense that

\[
\varphi_{e_j} = A_j^\dagger g_0, \quad j = 1, \ldots, d.
\]

**Proposition 3.5.** For all \( \psi \in L^2(\mathbb{R}^d), \, j = 1, \ldots, d, \) and \( z = (q, p) \in \mathbb{R}^{2d} \), we have

\[
(W_\psi * W_{\varphi_{e_j}})(z) = (2\pi \varepsilon)^{-d} |\langle T_z A_j^\dagger g_0, \psi \rangle|^2
\]

\[
= (2\pi \varepsilon)^{-d} \left| \langle g_z, \left( A_j - \frac{1}{\sqrt{2\pi}} z^c \right) \psi \rangle \right|^2,
\]

where \( z^c := q + ip \in \mathbb{C}^d \) and \( g_z \) is the Gaussian wave packet defined in (1.1).

Consequently,

\[
\mu_\psi(z) = (2\pi \varepsilon)^{-d} \left( (1 + \frac{d}{2}) |\langle T_z g_0, \psi \rangle|^2 - \frac{1}{2} \sum_{j=1}^d |\langle T_z A_j^\dagger g_0, \psi \rangle|^2 \right)
\]

\[
= (2\pi \varepsilon)^{-d} \left( (1 + \frac{d}{2}) |\langle g_z, \psi \rangle|^2 - \frac{1}{2} \sum_{j=1}^d \left| \langle g_z, \left( A_j - \frac{1}{\sqrt{2\pi}} z^c \right) \psi \rangle \right|^2 \right).
\]

**Proof.** The relation (2.4) implies

\[
(W_\psi * W_{\varphi_{e_j}})(z) = (2\pi \varepsilon)^{-d} |\langle T_z (\varphi_{e_j})_-, \psi \rangle|^2
\]

\[
= (2\pi \varepsilon)^{-d} |\langle T_z A_j^\dagger g_0, \psi \rangle|^2,
\]

since \( (\varphi_{e_j})_-(x) = \varphi_{e_j}(-x) = -\varphi_{e_j}(x) \) for \( x \in \mathbb{R}^d \). For the second representation of the Hermite spectrogram we compute

\[
\varepsilon \partial_j \circ T_z = ip_j T_z + T_z \circ \varepsilon \partial_j
\]

and deduce

\[
T_z \circ A_j^\dagger = \frac{1}{\sqrt{2\pi}} ((x_j - q_j)T_z - T_z \circ \varepsilon \partial_j)
\]

\[
= \frac{1}{\sqrt{2\pi}} ((x_j - q_j)T_z + ip_j T_z - \varepsilon \partial_j \circ T_z)
\]

\[
= \left( A_j^\dagger - \frac{1}{\sqrt{2\pi}} (q_j - ip_j) \right) \circ T_z
\]

so that

\[
\langle T_z A_j^\dagger g_0, \psi \rangle = \langle A_j^\dagger g_z, \psi \rangle - \frac{1}{\sqrt{2\pi}} (q_j + ip_j)(g_z, \psi).
\]

\[\square\]

Proposition 3.5 will be used for explicit expressions of \( \mu_\psi \) later on in §5, when \( \psi \) is a superposition of Gaussian wave packets or a higher order Hermite function.
4. Quantum Dynamics

As an application of the new density we consider the approximation of expectation values for the solution of the time-dependent semiclassical Schrödinger equation
\[ i\varepsilon \partial_t \psi(t) = H\psi(t), \quad \psi(0) = \psi_0, \]
where the Schrödinger operator \( H = \text{op}(h) \) is the Weyl quantization of a smooth function \( h : \mathbb{R}^{2d} \to \mathbb{R} \) of subquadratic growth, that is, all derivatives of the function \( h \) of order two and higher are bounded. Then, \( H \) is essentially self-adjoint (see [21, Exercise IV.12]) so that for all square integrable initial data \( \psi_0 \in L^2(\mathbb{R}^d) \) there is a unique global solution
\[ \psi(t) = e^{-iHt/\varepsilon} \psi_0, \quad t \in \mathbb{R}. \]
The classical counterpart to the Schrödinger equation is the Hamiltonian ordinary differential equation
\[ \dot{z}(t) = J\nabla h(z(t)) \quad \text{with} \quad J = \begin{bmatrix} 0 & \text{Id} \\ -\text{Id} & 0 \end{bmatrix} \in \mathbb{R}^{2d}\times2d. \]
The associated Hamiltonian flow \( \Phi_t : \mathbb{R}^{2d} \to \mathbb{R}^{2d} \) is globally defined and smooth for all times \( t \in \mathbb{R} \), since \( h \) is smooth and subquadratic.

In this setup we obtain the following quasiclassical approximation of time evolved quantum expectations using the new phase space density.

**Corollary 4.1.** Suppose \( h : \mathbb{R}^{2d} \to \mathbb{R} \) is a smooth function of subquadratic growth and \( H = \text{op}(h) \). Let \( \psi \in L^2(\mathbb{R}^d) \) with \( \|\psi\|_{L^2} = 1 \). Then, for all Schwartz functions \( a : \mathbb{R}^{2d} \to \mathbb{R} \), and \( t \in \mathbb{R} \), there exists a constant \( C = C(a, h, t) > 0 \) such that
\[
\left| \left\langle e^{-iHt/\varepsilon} \psi, \text{op}(a)e^{-iHt/\varepsilon} \psi \right\rangle - \int_{\mathbb{R}^{2d}} (a \circ \Phi_t)(z)\mu_\psi(z)dz \right| \leq C\varepsilon^2
\]
with the density \( \mu_\psi \) from Definition 3.1, where \( \Phi_t : \mathbb{R}^{2d} \to \mathbb{R}^{2d} \) is the Hamiltonian flow associated with \( h \).

**Proof.** The crucial element of our argument is Egorov’s theorem [3, Theorem 1.2], which provides
\[
e^{iHt/\varepsilon} \text{op}(a)e^{-iHt/\varepsilon} = \text{op}(a \circ \Phi_t) + O(\varepsilon^2),
\]
where the error depends on third and higher order derivatives of \( a \circ \Phi_t \) and \( h \), respectively. This means for the expectation value
\[
\left\langle e^{-iHt/\varepsilon} \psi, \text{op}(a)e^{-iHt/\varepsilon} \psi \right\rangle = \left\langle \psi, \text{op}(a \circ \Phi_t)\psi \right\rangle + O(\varepsilon^2).
\]
Now it remains to apply Theorem 3.2 to obtain
\[
\left\langle e^{-iHt/\varepsilon} \psi, \text{op}(a)e^{-iHt/\varepsilon} \psi \right\rangle = \int_{\mathbb{R}^{2d}} (a \circ \Phi_t)(z)\mu_\psi(z)dz + O(\varepsilon^2).
\]

**Remark 4.2.** Replacing the new density by the Husimi function in Corollary 4.1 deteriorates the approximation in the sense that
\[
\left\langle e^{-iHt/\varepsilon} \psi, \text{op}(a)e^{-iHt/\varepsilon} \psi \right\rangle = \int_{\mathbb{R}^{2d}} (a \circ \Phi_t)(z)\mathcal{H}_\psi(z)dz + O(\varepsilon)
\]
as $\varepsilon \to 0$. It requires an additional system of coupled ODEs involving higher order derivatives of the Hamilton function $h$ to retain second order accuracy with respect to $\varepsilon$; see [11, Theorem 3].

5. Examples of Phase Space Densities

In this section we explicitly compute the new density $\mu_\psi$ from Definition 3.1 in three different cases, namely when $\psi$ is a Gaussian wave packet, a Gaussian superposition, or a multivariate Hermite function.

5.1. Gaussian wave packets. The Gaussian wave packet

\[ g_z(x) = (\pi \varepsilon)^{-d/4} \exp\left(-\frac{1}{\varepsilon} |x-q|^2 + \frac{i}{\varepsilon} p \cdot (x - \frac{1}{2} q)\right), \quad x \in \mathbb{R}^d. \]

centered at $z = (q, p) \in \mathbb{R}^{2d}$ has the Wigner function

\[ \mathcal{W}_{g_z}(w) = (\pi \varepsilon)^{-d} \exp\left(-\frac{1}{\varepsilon} |w-z|^2\right), \quad w \in \mathbb{R}^{2d}. \]

Its Husimi function is a Gaussian function, too, but broader, that is,

\[ \mathcal{H}_{g_z}(w) = (2\pi \varepsilon)^{-d} \exp\left(-\frac{1}{2\varepsilon} |w-z|^2\right), \quad w \in \mathbb{R}^{2d}. \]

The Hermite spectrograms of $g_z$ can be related to another Husimi function. Indeed, by the covariance property of the spectrograms,

\[ (\mathcal{W}_{g_z} \ast \mathcal{W}_{\psi_j})(w) = (\mathcal{W}_{g_0} \ast \mathcal{W}_{\psi_j})(w-z) = \mathcal{H}_{\psi_j}(w-z) = (2\pi \varepsilon)^{-d} \frac{1}{2\varepsilon} |w_j - z_j|^2 \exp\left(-\frac{1}{2\varepsilon} |w-z|^2\right) \]

for all $w = (w_1, \ldots, w_d) \in \mathbb{R}^{2d}$ with $w_1, \ldots, w_d \in \mathbb{R}^2$ and all $j = 1, \ldots, d$. Summing all the Hermite spectrograms then yields

\[ \mu_{g_z}(w) = (2\pi \varepsilon)^{-d} \left(1 + \frac{d}{2} - \frac{1}{2\varepsilon} |w-z|^2\right) \exp\left(-\frac{1}{2\varepsilon} |w-z|^2\right), \quad w \in \mathbb{R}^{2d}. \]

Figure 2 plots the new density $\mu_{g_z}(w)$ together with the corresponding Wigner and Husimi function in terms of the distance $|w-z|$. Its polynomial prefactor puts the density $\mu_{g_z}$ in between the Wigner and the Husimi Gaussian.

5.2. Gaussian superposition. Next we compute the new density $\mu_\psi$ for a Gaussian superposition, that is, for

\[ \psi = g_{z_1} + g_{z_2}, \quad z_1, z_2 \in \mathbb{R}^{2d}. \]

Writing the value of the Husimi function at a point $z \in \mathbb{R}^{2d}$ as

\[ \mathcal{H}_\psi(z) = (2\pi \varepsilon)^{-d} \left|\langle g_z, g_{z_1} \rangle + \langle g_z, g_{z_2} \rangle\right|^2 \]

\[ = (2\pi \varepsilon)^{-d} \left(|\langle g_z, g_{z_1} \rangle|^2 + |\langle g_z, g_{z_2} \rangle|^2 + 2 \text{Re} \langle g_{z_1}, g_z \rangle \langle g_z, g_{z_2} \rangle\right) \]

motivates us to derive an explicit formula for the inner product of two Gaussian wave packets.

Lemma 5.1. For any $z_1, z_2 \in \mathbb{R}^{2d}$, we have

\[ \langle g_{z_1}, g_{z_2} \rangle = \exp\left(-\frac{|z_1-z_2|^2}{4\varepsilon} + \frac{i}{\varepsilon} \Omega(z_1, z_2)\right), \]

where $\Omega$ is the standard symplectic form on $T^*\mathbb{R}^d \cong \mathbb{R}^{2d}$ as defined in (2.1).
Figure 2. Plots of the Wigner function (black dashed), the Husimi function (blue dashed), and the new density \( \mu_\psi \) (red solid) for Gaussian wave packet \( \psi = g_z \) in dimension \( d = 1 \) with semiclassical parameter \( \varepsilon = 0.14 \). We plot the three functions in terms of the distance \(|w - z|\).

**Proof.** By a direct calculation one can show
\[
\langle g_0, g_z \rangle = \langle g_0, T_z g_0 \rangle = \exp \left( -\frac{|z|^2}{4\varepsilon} \right), \quad z \in \mathbb{R}^2.
\]
For the general case we then have
\[
\langle g_{z_1}, g_{z_2} \rangle = \langle T_{z_1} g_0, T_{z_2} g_0 \rangle = \langle g_0, T_{-z_1} T_{z_2} g_0 \rangle
\]
\[
= \exp \left( \frac{i}{2\varepsilon} \Omega(z_1, z_2) \right) \langle g_0, T_{z_2 - z_1} g_0 \rangle = \exp \left( \frac{i}{2\varepsilon} \Omega(z_1, z_2) - \frac{|z_2 - z_1|^2}{4\varepsilon} \right).
\]

By Lemma 5.1 we have
\[
\langle g_{z_1}, g_z \rangle \langle g_z, g_{z_2} \rangle = \exp \left( -\frac{|z - z_1|^2 + |z - z_2|^2}{4\varepsilon} \right) \exp \left( \frac{i}{2\varepsilon} \Omega(z_1 - z_2, z) \right)
\]
and obtain for the Husimi function
\[
\mathcal{H}_\psi(z) = (2\pi\varepsilon)^{-d} \left( \exp \left( -\frac{|z - z_1|^2}{2\varepsilon} \right) + \exp \left( -\frac{|z - z_2|^2}{2\varepsilon} \right) \right.
\]
\[
+ 2 \exp \left( -\frac{|z - z_1|^2 + |z - z_2|^2}{4\varepsilon} \right) \cos \left( \frac{1}{2\varepsilon} \Omega(z_1 - z_2, z) \right) \bigg)
\]
For the Hermite spectrograms we first use Lemma 3.5 to obtain
\[
(W_\psi * W_{\Phi_j})(z) = (2\pi\varepsilon)^{-d} \left| \sum_{k=1}^{2^d} \langle g_{z_1}, \left( A_j T_{z_k} - \frac{z^c}{\sqrt{2\varepsilon}} T_{z_k} \right) g_0 \rangle \right|^2.
\]
We notice that, for \( j = 1, \ldots, d \) and \( m = 1, 2 \),
\[
A_j T_{z_m} = \frac{z_m^c}{\sqrt{2\varepsilon}} T_{z_m} + T_{z_m} A_j,
\]
where $z_{m,j}^C := q_{m,j} + ip_{m,j} \in \mathbb{C}$. This implies that
\[
\langle g_z, \left(A_j T_{z_m} - \frac{z_{j}^C}{\sqrt{2\varepsilon}} T_{z_m} \right) g_0 \rangle = \langle g_z, \left(\frac{z_{m,j}^C - z_{j}^C}{\sqrt{2\varepsilon}} T_{z_m} + T_{z_m} A_j \right) g_0 \rangle = \frac{z_{m,j}^C - z_{j}^C}{\sqrt{2\varepsilon}} \langle g_z, g_{z_m} \rangle.
\]
Consequently, since $|z_{m,j}^C - z_{j}^C| = |z_{m,j} - z_j|$ for each $m$ and $j$, we have
\[
(2\pi \varepsilon)^d (\mathcal{W}_\psi \ast \mathcal{W}_{\varphi_{z_j}})(z) = \left| \frac{z_{m,j}^C - z_{j}^C}{\sqrt{2\varepsilon}} \langle g_z, g_{z_1} \rangle + \frac{z_{m,j}^C - z_{j}^C}{\sqrt{2\varepsilon}} \langle g_z, g_{z_2} \rangle \right|^2 = \frac{1}{2\varepsilon} \left| z_{1,j}^C - z_{j}^C \right|^2 (\langle g_z, g_{z_1} \rangle^2 + \langle g_z, g_{z_2} \rangle^2) + \frac{1}{\varepsilon} \Re \left[ \left( \frac{z_{m,j}^C - z_{j}^C}{\sqrt{2\varepsilon}} \right) \langle g_z, g_{z_1} \rangle \langle g_z, g_{z_2} \rangle \right].
\]
Now observe that
\[
\sum_{j=1}^{d} (z_{1,j}^C - z_{j}^C)(z_{2,j}^C - z_{j}^C) = \sum_{j=1}^{d} [(q_{1,j} - q_j) - i(p_{1,j} - p_j)][(q_{2,j} - q_j) + i(p_{2,j} - p_j)] = (z - z_1) \cdot (z - z_2) + i \Omega(z - z_1, z - z_2).
\]
Therefore,
\[
\sum_{j=1}^{d} (\mathcal{W}_\psi \ast \mathcal{W}_{\varphi_{z_j}})(z) = \frac{1}{(2\pi \varepsilon)^d} \left\{ \frac{|z - z_1|^2}{2\varepsilon} \exp \left( -\frac{|z - z_1|^2}{2\varepsilon} \right) + \frac{|z - z_2|^2}{2\varepsilon} \exp \left( -\frac{|z - z_2|^2}{2\varepsilon} \right) + \frac{1}{\varepsilon} \exp \left( -\frac{|z - z_1|^2 + |z - z_2|^2}{4\varepsilon} \right) \left[ (z - z_1) \cdot (z - z_2) \cos \left( \frac{1}{2\varepsilon} \Omega(z_1 - z_2, z) \right) - \Omega(z - z_1, z - z_2) \sin \left( \frac{1}{2\varepsilon} \Omega(z_1 - z_2, z) \right) \right] \right\}.
\]
Combining the Husimi function and the Hermite spectrograms gives the density $\mu_\psi$ as plotted before in Figure 1 in the Introduction.

5.3. **Hermite functions.** Let us consider the higher order Hermite functions
\[
\varphi_k := \frac{1}{\sqrt{k!}} (A^\dagger)^k g_0, \quad k = (k_1, \ldots, k_d) \in \mathbb{N}^d,
\]
which result from the $k$-fold application of the raising operator $A^\dagger$ to the Gaussian wave packet $g_0$ centered at the origin. The FBI transform of a Hermite function is known as
\[
(2\pi \varepsilon)^{-d/2} \langle g_z, \varphi_k \rangle = \frac{1}{\sqrt{(2\pi \varepsilon)^d k!}} \left( \frac{1}{\sqrt{2\varepsilon}} (q - ip) \right)^k \exp \left( -\frac{1}{4\varepsilon} |z|^2 \right)
\]
for $z \in \mathbb{R}^{2d}$; see [7, §2] or [14, Proposition 5]. Hence, the Husimi function satisfies
\[
\mathcal{H}_{\varphi_k}(z) = \frac{1}{(2\pi \varepsilon)^{d/2} k!} \left( \frac{1}{\sqrt{2\pi}} z^k \exp \left( -\frac{1}{4\varepsilon} |z|^2 \right) \right)^k = \prod_{j=1}^{d} h_{k_j}(z_j),
\]
where
\[
h_n(w) := \mathcal{H}_{\varphi_n}(w), \quad w \in \mathbb{R}^2,
\]
denotes the Husimi function of the univariate \( n \)-th Hermite function \( \phi_n \), \( n \in \mathbb{N} \). For the multivariate Hermite spectrograms we obtain the following:

**Lemma 5.2.** For all \( k \in \mathbb{N}^d \) and \( j = 1, \ldots, d \) and \( z \in \mathbb{R}^{2d} \), we have

\[
(W_{\phi_k} \ast W_{\varphi_{e_j}})(z) = (k_j h_{k_j-1}(z_j) - 2k_j h_{k_j}(z_j) + (k_j + 1) h_{k_j+1}(z_j)) \cdot \prod_{n \neq j} h_n(z_n).
\]

**Proof.** Since \( A_j \varphi_k = \sqrt{k_j} \varphi_{k-e_j} \), Proposition 3.5 implies

\[
(W_{\phi_k} \ast W_{\varphi_{e_j}})(z) = (2\pi\varepsilon)^{-d} \left| \langle g_z, A_j \varphi_k \rangle - \frac{1}{\sqrt{2\varepsilon}} z_j^C \langle g_z, \varphi_k \rangle \right|^2.
\]

By the formula (5.2) for the FBI transform, we obtain

\[
(W_{\phi_k} \ast W_{\varphi_{e_j}})(z) = \exp \left( -\frac{1}{2\varepsilon} |z_j|^2 \right) \left| k_j \left( \frac{1}{\sqrt{2\varepsilon}} (q - ip) \right)^{k-e_j} - \frac{1}{\sqrt{2\varepsilon}} z_j^C \left( \frac{1}{\sqrt{2\varepsilon}} (q - ip) \right)^{k} \right|^2.
\]

Then it remains to observe that

\[
\exp \left( -\frac{1}{2\varepsilon} |z_j|^2 \right) \left( k_j - \frac{1}{\varepsilon} |z_j|^2 \right)^{k-e_j} \left( \frac{1}{\sqrt{2\varepsilon}} z_j \right)^{2k-j-2} = k_j h_{k_j-1}(z_j) - 2k_j h_{k_j}(z_j) + (k_j + 1) h_{k_j+1}(z_j).
\]

\[
\]

The combination of the Husimi function (5.3) and the Hermite spectrograms of Lemma 5.2 gives an explicit formula for the density \( \mu_\psi \) when \( \psi = \varphi_k \) for \( k \in \mathbb{N}^d \).

### 6. Numerical Experiments

We present numerical experiments\(^1\) for computing expectation values for the solution of the time-dependent Schrödinger equation

\[
i \varepsilon \partial_t \psi(t) = (-\frac{\varepsilon^2}{2} \Delta + V(t)) \psi(t), \quad \psi(0) = \psi_0,
\]

with three different potentials \( V : \mathbb{R}^d \to \mathbb{R} \). The various setups shall illustrate important aspects of our new algorithm, such as the second order accuracy with respect to \( \varepsilon \), the good applicability in higher dimensions, and the capability of describing fundamental quantum effects.

\(^1\)All experiments have been performed with MATLAB 8.3 on a 3.33 GHz Intel Xeon X5680 processor.
6.1. Discretization. For the algorithmic discretization of Corollary 4.1 we proceed similarly as in [13, 10, 11]. We consider various smooth functions \( a : \mathbb{R}^d \to \mathbb{R} \) and evaluate the phase space integral on the right hand side of the semiclassical approximation

\[
\langle \psi(t), \text{op}(a)\psi(t) \rangle = \int_{\mathbb{R}^d} (a \circ \Phi_t)(z)\mu_{\psi_0}(z)dz + O(\varepsilon^2)
\]

for normalized initial data \( \psi_0 \in L^2(\mathbb{R}^d), \|\psi_0\| = 1 \), via the quadrature formula

\[
\int_{\mathbb{R}^d} (a \circ \Phi_t)(z)\mu_{\psi_0}(z)dz = (1 + \frac{d}{2}) \int_{\mathbb{R}^d} (a \circ \Phi_t)(z)\mathcal{H} \psi_0 (z)dz - \frac{1}{2} \sum_{j=1}^{N} (a \circ \Phi_t)(w_k) - \frac{d}{2N} \sum_{k=1}^{N} (a \circ \Phi_t)(w_k),
\]

where one samples the quadrature points according to the probability measures

\[
z_1, \ldots, z_N \sim \mathcal{H} \psi_0, \quad w_1, \ldots, w_N \sim \frac{1}{d} \sum_{j=1}^{d} \mathcal{W} \psi_0 \ast \mathcal{W} \varphi_{x_j};
\]

see also §A for the sampling strategies used for the Hermite spectrograms. The rate of convergence for the above quadrature rule is proportional to \( N^{-1/2} \) for Monte Carlo samplings. For low discrepancy (Quasi-Monte Carlo) sampling the convergence is faster, that is, of the order \( \log(N)^{2d}/N \). However, the literature on non-uniform Quasi-Monte Carlo sampling is scarce, and it seems to be an open question whether the transformed Halton sequences employed in our numerical experiments form indeed a low discrepancy set or just come very close to being so in practice, see also [1].

For the discretization of the Hamiltonian flow \( \Phi_t \), we apply the eighth-order symplectic splitting method from [23, Table 2.D], which is a suitable composition of the linear flows of

\[
\begin{align*}
\dot{q} &= p \\
\dot{p} &= 0
\end{align*}
\quad \text{and} \quad
\begin{align*}
\dot{q} &= 0 \\
\dot{p} &= -\nabla V(q)
\end{align*}
\]

Since our algorithm evolves an ensemble of classical trajectories, the use of symplectic time integrators is crucial; see also [13, Fig. 4.2].

6.2. Two-dimensional torsional potential. Our first numerical experiments are conducted for the two-dimensional torsional potential

\[
V(q_1, q_2) = 2 - \cos(q_1) - \cos(q_2), \quad q \in \mathbb{R}^2,
\]

and different values of the semiclassical parameter \( \varepsilon \). As the initial state we consider the Gaussian wave packet \( \psi_0 = g_z \) with phase space center \( z = (1, 0, 0, 0) \). This setup has already been considered in [5, 13, 11, 10]. We investigate the dynamics of the following observables \( a : \mathbb{R}^4 \to \mathbb{R} \):

1. Position: \( a(q, p) = q_1 \) and \( a(q, p) = q_2 \),
2. Momentum: \( a(q, p) = p_1 \) and \( a(q, p) = p_2 \),
3. Kinetic and potential energy: \( a(q, p) = \frac{1}{2} |p|^2 \) and \( a(q, p) = V(q) \),
The left and middle panel of Figure 3 confirm the second order accuracy of
the new method for both Monte Carlo and Halton type samplings of the initial
density $\mu_{\psi_0}$. The right panel illustrates that the naive Husimi method is indeed
only of first order in $\varepsilon$. The errors are taken with respect to grid based reference
solutions of the Schrödinger equation; for details see Appendix B.1.

6.3. Henon–Heiles dynamics for $d = 32$. Henon–Heiles type systems have
been used for benchmark simulations with the multiconfiguration time-dependent
Hartree method (MCTDH); see [18]. We follow the presentation in [12, §5.B] by
using the potential

$$V_{32}(q) = \frac{1}{2}|q|^2 + 1.8436 \sum_{j=1}^{31} (q_j^2 q_{j+1} - \frac{1}{3} q_j^4) + 0.4 \sum_{j=1}^{31} (q_j^2 + q_{j+1}^2)^2$$

and the semiclassical parameter $\varepsilon = 0.0029$, which is a model for the dynamics
of a hydrogen atom on a high-dimensional potential energy surface that exhibits
regions of chaotic motion. The quartic confinement guarantees that none of the
classical trajectories escapes to infinity. Moreover, as in [18, 12], the initial state is
a Gaussian wave packet $\psi_0 = g_z$ centered at $z = (q, p)$ with $p = 0$ and $q_j = 0.1215$
for all $j = 1, \ldots, 32$.

Since grid-based reference solutions are not available for this high-dimensional
setting, we compare our method with the results obtained by the second order

(4) Total energy: $a(q, p) = \frac{1}{2}|p|^2 + V(q)$,
and compare the outcome of the new algorithm with the naive, first-order Husimi
approximation

$$\langle \psi(t), \text{op}(a) \psi(t) \rangle = \int_{\mathbb{R}^{2d}} (a \circ \Phi_t)(z) \mathcal{H}_{\psi_0}(z) dz + O(\varepsilon).$$

The left and middle panel of Figure 3 confirm the second order accuracy of
the new method for both Monte Carlo and Halton type samplings of the initial
density $\mu_{\psi_0}$. The right panel illustrates that the naive Husimi method is indeed
only of first order in $\varepsilon$. The errors are taken with respect to grid based reference
solutions of the Schrödinger equation; for details see Appendix B.1.
approximation
\[ \langle \psi(t), \text{op}(a)\psi(t) \rangle = \int_{\mathbb{R}^{2d}} (a \circ \Phi_t)(z) \psi_0(z) \, dz + O(\varepsilon^2). \]

Note that, in this particular case, the initial Wigner function \( \psi_0(z) \) is the Gaussian (5.1), and hence the Wigner algorithm does not pose a difficulty in the initial sampling. Figure 4 shows the good agreement of the results from the Wigner and the spectrogram methods by means of the potential energy, and a considerable discrepancy with respect to the naive Husimi approximation (6.1).

6.4. Escape from a cubic potential well. Finally, we explore whether the new method is capable of describing the evolution of a quantum system that moves out of a potential well. For this purpose we consider the semiclassical Schrödinger operator \( H = -\frac{\varepsilon^2}{2} \Delta + V \) with the one-dimensional barrier potential
\[ V(q) = 2.328 \cdot q^2 + q^3 + 0.025 q^4, \quad q \in \mathbb{R}, \]
and \( \varepsilon = 0.4642 \); see also Figure 5. This Hamiltonian can be derived from the Schrödinger operator
\[ -\frac{1}{2} \hbar^2 \Delta + \frac{1}{2} x^2 + 0.1 x^3 \]
with \( \hbar = 1 \) from [19, 20] by applying the space rescaling \( x \mapsto \sqrt{0.1} x \) and adding the confinement term \( 0.025 \cdot q^4 \). The confinement prevents phase space trajectories from finite time blow up and guarantees that \( H \) is essentially self-adjoint. The global potential energy minimum \( V(x_{\text{glob}}) \approx -4765 \) is attained at \( x_{\text{glob}} \approx -28.4 \), and the confinement is very small in the region of interest close to the origin.

As initial states we consider translated Hermite functions
\[ \psi_0 = T_{z_0} \varphi_k, \quad k \in \{0, 1, 3, 6\} \]
localized around \( z_0 = (0.4642, -1) \), which corresponds to the initial phase space center used in [19]. Since the associated classical energy \( h(z_0) \) lies below the barrier energy \( V_b \approx 2.03 \), the classical particle is trapped in the well for all times. In contrast, the quantum energy of the initial state \( g_{z_0} \) is approximately 2.09, and the energies of the excited states are even higher. Consequently, the expected phase
space center of the quantum particle will escape from the classical trapping region after short time.

Figure 6 displays the trajectories of the expected phase space centers obtained by the purely classical, the full quantum, and the semiclassical spectrogram dynamics for the four different initial states. The results from the spectrogram algorithm show decent qualitative agreement with the behavior of the quantum solution even though the semiclassical parameter \( \varepsilon = 0.4642 \) is rather large. We also note that the results become more accurate for initial states of higher energy.

Appendix A. Sampling by the Gamma distribution

A.1. Using the Gamma distribution. We consider the Hermite functions translated by the Heisenberg–Weyl operator,

\[ \psi = T_z \varphi_k, \quad k \in \mathbb{N}^d, \quad z \in \mathbb{R}^d. \]

Then, by the covariance property (2.6), the Hermite spectrogram takes the form

\[ (\mathcal{W}_{T_z \varphi_k} \ast \mathcal{W}_{\varphi_{j'}})(w) = (\mathcal{W}_{\varphi_k} \ast \mathcal{W}_{\varphi_{j'}})(w - z), \quad w \in \mathbb{R}^d, \]

and by Lemma 5.2, we only have to consider the two-dimensional probability densities

\[ w_j \mapsto h_n(w_j - z_j) = \frac{1}{\sqrt{2\pi} n!} \left| \frac{1}{\sqrt{2\pi}} (w_j - z_j) \right|^{2n} \exp\left(-\frac{1}{2\varepsilon} |w_j - z_j|^2\right) \]

with \( n \in \{k_1, \ldots, k_d\} \). Specifically, we first translate by \(-z_j\) and then use the uniform distribution on \([0, 2\pi]\) for the angular part combined with sampling from

\[ r \mapsto \frac{r^{2n+1}}{2^{n+1} \tau^2} \exp\left(-\frac{1}{2\varepsilon} r^2\right) \]

for the radial part. Since

\[ \int_a^b \frac{r^{2n+1}}{2^{n+1} \tau^2} \exp\left(-\frac{1}{2\varepsilon} r^2\right) \, dr = \int_0^{\frac{\tau}{a}} \frac{\tau^n}{2^{n+1} \tau^2} \exp\left(-\frac{1}{2\varepsilon} \tau^2\right) \, d\tau \]

for all \( a, b > 0 \), we use the Gamma distribution with parameters \( n + 1 \) and \( 2\varepsilon \) for the radial sampling.

In the particular case \( k = 0 \), \( \varphi_0 = g_0 \) and so \( T_z \varphi_0 = g_z \) is a Gaussian wave packet and

\[ \mu_{g_z}(w) = (2\pi \varepsilon)^{-d} \left( 1 + \frac{d}{2} - \frac{1}{4\varepsilon} |w - z|^2 \right) \exp\left(-\frac{1}{2\varepsilon} |w - z|^2\right), \quad w \in \mathbb{R}^d; \]
Figure 6. Trajectories of the expected phase space centers obtained from quantum references and the new spectrogram algorithm for different initial states $\psi_0 = T_z \phi_k$. The dashed black line shows the periodic classical orbit associated with $z_0$, and the solid black line illustrates the border of the trapping region.

see §5.1. One can directly sample this $2d$-dimensional probability density without factorizing its summands. After translation by $-z$, one decomposes into a radial part and an independent angular variable which is uniformly distributed on $S^{2d-1}$. The radial density is given by

$$r \mapsto \frac{r^d}{(2\varepsilon)^{d+1}d!} \exp(-r/2\varepsilon),$$

which corresponds to a Gamma distribution with parameters $d+1$ and $2\varepsilon$.

A.2. Monte Carlo sampling. Pseudorandom numbers uniformly distributed on a multi-dimensional unit sphere are obtained by sampling from multivariate normal distributions and subsequent normalization, while Gamma distributed pseudorandom samples only require the uniform distribution on the unit cube together with the (numerical) inverse of the cumulative Gamma distribution function. Hence a Monte-Carlo sampling of $\mu_{T_z \phi_k}$ is straightforward.

A.3. Quasi-Monte Carlo sampling. For the generation of Quasi-Monte Carlo points we have heuristically mimicked the Monte-Carlo procedure of §A.2 by replacing the pseudorandom samples from the uniform distribution on the unit cube
by a Halton sequence. Whether the resulting points are of low discrepancy with respect to the distribution $\mu_{T,\phi_k}$ seems to be an open question not answered by the current literature, see e.g. [1].

**Appendix B. Numerical data**

**B.1. Two-dimensional torsional system.** Table 1 contains the number of initial sampling points and the computational time for the new spectrogram algorithm. In the case of Monte Carlo integration, the results in Figure 3 are averaged over ten independent runs. For the time propagation we apply the above mentioned eighth-order symplectic integrator with time stepping $10^{-1}$. The parameters of the grid-based reference solver are collected in Table 2.

<table>
<thead>
<tr>
<th>$\varepsilon$</th>
<th>MC points</th>
<th>comp. time</th>
<th>Halton points</th>
<th>comp. time</th>
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<td>$10^{-1}$</td>
<td>$5 \cdot 10^4$</td>
<td>23s</td>
<td>$5 \cdot 10^4$</td>
<td>16s</td>
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<td>$10^5$</td>
<td>33s</td>
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<tr>
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<td>7m16s</td>
<td>$2 \cdot 10^5$</td>
<td>1m59s</td>
</tr>
<tr>
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<td>$1.5 \cdot 10^6$</td>
<td>14m15s</td>
<td>$8 \cdot 10^5$</td>
<td>6m50s</td>
</tr>
<tr>
<td>$10^{-3}$</td>
<td>$10 \cdot 10^6$</td>
<td>68m30s</td>
<td>$2 \cdot 10^6$</td>
<td>18m31s</td>
</tr>
</tbody>
</table>

Table 1. Computational data for the execution of the new spectrogram algorithm for the two dimensional torsional potential and Gaussian initial data on the time interval $[0, 20]$. The computation times are for one run only. They scale linearly with respect to the number of initial sampling points.

<table>
<thead>
<tr>
<th>$\varepsilon$</th>
<th>#timesteps</th>
<th>comp. domain</th>
<th>space grid</th>
</tr>
</thead>
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<tr>
<td>$10^{-1}$</td>
<td>$5 \cdot 10^3$</td>
<td>$[-3,3] \times [-3,3]$</td>
<td>$1536 \times 1536$</td>
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<tr>
<td>$5 \cdot 10^{-2}$</td>
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<td>$10^{-2}$</td>
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<td>$[-2,2] \times [-2,2]$</td>
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</tr>
<tr>
<td>$5 \cdot 10^{-3}$</td>
<td>$10^4$</td>
<td>$[-2,2] \times [-2,2]$</td>
<td>$2048 \times 2048$</td>
</tr>
<tr>
<td>$10^{-3}$</td>
<td>$10^4$</td>
<td>$[-2,2] \times [-2,2]$</td>
<td>$2048 \times 2048$</td>
</tr>
</tbody>
</table>

Table 2. Parameters of the grid-based reference solutions for the two-dimensional torsional potential. The discretization has been done by Fourier collocation in $\mathbb{R}^2$ and Strang splitting in time.

**B.2. Henon–Heiles system for $d = 32$.** For the initial sampling we used $2^{17}$ Halton type points for all three initial densities, that is, the Wigner and the Husimi functions and the new density $\mu_{\psi_0}$. The time stepping of the eighth order time integrator is $2 \cdot 10^{-2}$.

**B.3. One-dimensional cubic well.** For the spectrogram algorithm we employed $2^{14}$ Halton points and the eighth-order integrator with time stepping $10^{-2}$, which results in a computational time of 2 seconds. The quantum references are generated by means of a Strang splitting with $2^{15}$ Fourier modes on the interval $[-40, 4]$. 
# References


ZENTRUM MATHEMATIK, TECHNISCHE UNIVERSITÄT MÜNCHEN, BOLTZMANNSTRASSE 3, 85748
GARCHING BEI MÜNCHEN.
E-mail address: keller@ma.tum.de

ZENTRUM MATHEMATIK, TECHNISCHE UNIVERSITÄT MÜNCHEN, BOLTZMANNSTRASSE 3, 85748
GARCHING BEI MÜNCHEN.
E-mail address: classer@ma.tum.de

DEPARTMENT OF MATHEMATICAL SCIENCES, THE UNIVERSITY OF TEXAS AT DALLAS, 800 WEST
CAMPBELL RD, RICHARDSON, TX 75080-3021.
E-mail address: tomoki@utdallas.edu