

Research Article

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Phase-space description of the coherent state dynamics in a small one-dimensional system

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Abstract: The Wigner-Moyal approach is applied to investigate the dynamics of the Gaussian wave packet moving in a double-well potential in the ‘Mexican hat’ form. Quantum trajectories in the phase space are computed for different kinetic energies of the initial wave packet in the Wigner form. The results are compared with the classical trajectories. Some additional information on the dynamics of the wave packet in the phase space is extracted from the analysis of the cross-correlation of the Wigner distribution function with itself at different points in time.

Keywords: Wigner distribution, wave packet, quantum trajectory

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1 Introduction

Description of the quantum dynamical processes in the phase space can be realized on the Wigner-Moyal algebra which is the non-commutative algebra of observables based on the symplectic symmetry of the phase-space [1]. In this approach, the state of the quantum dynamical system cannot be longer represented by the Dirac measure localized at a point in the phase space, but rather by an appropriate quasi-distribution function [2–4], because the Heisenberg’s uncertainty principle prohibits precise determination of momentum and position at the same time [5]. The uncertainty also tampers with the algebra of observables which are represented by functions of the phase-

space variables. In this case, the product of any functions on the phase space is noncommutative. The classical algebra of observables (commutative) is recovered in the limit of the reduced Planck constant approaching zero ($\hbar \rightarrow 0$). Hence the presented approach is called the phase space quantum mechanics, or sometimes is referred to as the deformation quantization [6–8]. Currently, the deformation theory has found applications in many fields of modern physics, such as quantum gravity, string and M-theory, nuclear physics, quantum optics, condensed matter physics, and quantum field theory.

In the present contribution, we examine the dynamics of the initially coherent state in the double-well potential using the phase space formulation of the quantum mechanics. This autonomous path to quantization of the classical theory is based on the Wigner distribution function (WDF), ϱ_W , which is defined by the Weyl transform of the density operator [4, 9, 10],

$$\varrho_W(x, p; t) = \frac{1}{2\pi\hbar} \int dX \rho\left(x - \frac{1}{2}X, x + \frac{1}{2}X; t\right) e^{-(i/\hbar)pX}. \quad (1)$$

The WDF is normalized and real, but not always positive function of position and momentum over the phase space [11]. The negative values of the WDF in some regions of the space are a consequence of the Heisenberg’s uncertainty principle and they can be regarded as an indicator of the non-classicality of the state [12]. Despite the fact that the WDF can be negative, the expectation value of any dynamical variable can be computed with respect to the WDF in the same way as the average value in the classical statistical mechanics, namely [4, 11]

$$\langle F(t) \rangle = \int dx dp F_W(x, p) \varrho_W(x, p; t), \quad (2)$$

where $F_W(x, p)$ is the Weyl symbol of quantum-mechanical operator $\mathcal{F}$ in the position representation [13],

$$F_W(x, p) = \frac{1}{2\pi\hbar} \int dX \mathcal{F}\left(x - \frac{1}{2}X, x + \frac{1}{2}X\right) e^{-(i/\hbar)pX}. \quad (3)$$

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2 Theory

The unitary time evolution of the WDF is generated by the Moyal equation which exhibits the non-local nature of the quantum dynamics. The equation of motion has a Liouville-like form, i.e.,

$$\frac{\partial}{\partial t} \varrho_W(x, p; t) = \mathcal{L} \varrho_W(x, p; t), \quad (4)$$

where the right hand side of the equation (4) is expressed by the Moyal bracket. Its explicit form is given by the following formula [1, 8]:

$$\begin{aligned} \mathcal{L} \varrho_W(x, p; t) &= \{H_W(x), \varrho_W(x, p; t)\}^* \\ &= \frac{1}{i\hbar} \left\{ H_W(x, p) \exp \left[\frac{\hbar}{2} \left(\overrightarrow{\frac{\partial}{\partial p}} \overleftarrow{\frac{\partial}{\partial x}} - \overrightarrow{\frac{\partial}{\partial x}} \overleftarrow{\frac{\partial}{\partial p}} \right) \right] \right. \\ &\quad \left. \times \varrho_W(x, p; t) \right\} \\ &= H_W(x, p) * \varrho_W(x, p; t), \end{aligned} \quad (5)$$

where $H_W(x, p)$ is the Weyl symbol of the small system Hamiltonian, and the arrows indicate in which direction the derivatives act. We note that the lowest order of the series expansion of the time evolution generator for the Moyal equation with respect to the deformation parameter $\hbar/2$ corresponds to the Poisson bracket, and therefore the Moyal equation is reduced to the exact form of the classical Liouville equation [1]. Alternatively the classical limit of the dynamics generated by the Moyal equation can be deduced on the basis of the Egorov's theorem [14]. Following this theorem, the quantum dynamics is reduced to the classical as the semiclassical parameter ϵ which effectively replaces $\hbar$ determined by the physical scales involved in the system goes to zero corresponding to ϵ^2 [15].

Some general similarities between the propagation of the classical and coherent states in the phase space based on the careful studies of the semiclassical limit [16] allow incorporating the split-operator technique to determine the time evolution of the WDF [17–19]. In the present calculations, the initial condition for the Moyal equation is taken in the coherent state form which is represented by the Wigner form of the Gaussian wave packet centered around some point (x_0, p_0) in the phase space [20],

$$\varrho_W(x, p; 0) = \frac{1}{\pi\hbar} \exp \left\{ -\frac{2\delta_x^2(p - p_0)^2}{\hbar^2} - \frac{(x - x_0)^2}{2\delta_x^2} \right\}, \quad (6)$$

where δ_x is the initial half-width of the wave packet. The form represents the most classical quantum state permitted by the uncertainty principle [21].

We apply this formalism to the description of the coherent state dynamics in the small system which is modeled by the double well potential in the “Mexican hat”

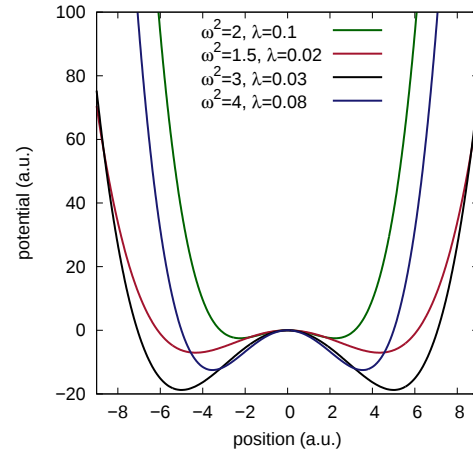


Figure 1: The potential used in the calculations. All values are given in atomic units.

form (presented in Fig. 1). The system may serve as a prototype of an electronic nanosystem exhibiting nonequilibrium dynamics in the presence of the external gradients or fields [22]. The Weyl symbol of the small system Hamiltonian takes the form

$$H_W = \frac{p^2}{2m} - \frac{1}{2} m \omega^2 x^2 + \lambda x^4, \quad (7)$$

where m is the mass of the electron, while ω and λ are the parameters of the potential. For the present calculations their values are taken to be equal $\omega = 2$ a.u. (atomic units of $e = \hbar = m = 1$) and $\lambda = 0.08$ a.u.

3 Results

We have determined the propagation of the WDF in the small system by means of the method presented in Ref. [23]. For the present calculations the following values of the wave packet are assumed: $\delta_x = 1/\sqrt{2}$ a.u., $x_0 = -3.5$ a.u., and three different initial momenta: $p_0 = -10, -3.5$ and 5 a.u., which correspond to different kinetic energies of the coherent state. The phase-space calculations are performed on the computational grid with $N_x = 512$ mesh points for the x -coordinate, and $N_p = 512$ mesh points for the x -component of momentum. The quantum trajectories are determined by simultaneous calculations of the expectation values of the position and momentum variables according to the formula (2) with the WDF being a solution of the Moyal equation (4). On the other hand, the classical trajectories are computed on the basis of the Hamilton's equations [24]. The results of performed computer simulations are presented in Figs. 2, 3, and 4, which

display not only the snapshots of the WDF at different times, but also the quantum and classical trajectories.

A comparison of the both types of the trajectories seems to be extremely informative, because it displays the main differences between the dynamics of the classical and quantum states in the phase space, generated by the Poisson and Moyal brackets, respectively. In the case of the classical dynamics of the particle which moves under the influence of a conservative force (in the present case, the force is $F = m\omega^2x - 4\lambda x^3$), the trajectory does not have intersections and is always closed, although its geometrical center as well as the shape strongly depends on the initial momentum. Due to the knowledge of the classical trajectories, the Liouville formulation of the classical dynamics in the phase space [25] can be simply reconstructed, namely the Dirac measure, $\rho(x, p, t)$,

$$\rho(x, p, t) = \delta(x - x(t))\delta(p - p(t)), \quad (8)$$

which imitates the distribution function for the single particle, moves along the classical trajectory. This picture partly overlaps with the classical limit of the quantum dynamics of the quantum state, where the WDF moves along the classical trajectory [26]. On the other hand, the quantum limit of the WDF dynamics leads to the trajectory in a form of a spiral, i.e., the quantum trajectory is not a closed curve. In general, this is due to a gradual spreading, distortion and the negative values of the WDF during its time evolution. The nature of these deformations is a consequence of the finite size of the initial WDF, and additional complications result from the Heisenberg's uncertainty principle. All of these effects give a contribution to the calculation of the average values of the position and momentum [c.f. Eq. (2)], which define the quantum trajectory in the phase space. The justification for the statement partly can be physical, namely the “Mexican hat” generates the non-local potential in the form

$$U_W(x, p) = \frac{2\pi}{\hbar} \left[(4\lambda x^3 - m\omega^2 x) \frac{d}{dp} \delta(p) - \lambda x \frac{d^3}{dp^3} \delta(p) \right]. \quad (9)$$

Hence the dynamics of the phase-space points covered by the WDF can be represented by the set of the equations in the form

$$\begin{cases} \frac{dx(t)}{dt} = \frac{p}{m} \\ \frac{dp(t)}{dt} = -\frac{1}{2\pi\hbar} \int dp' U_W(x, p - p') \rho_W(x, p', t) \end{cases} \quad (10)$$

which clearly generate the set of trajectories which depend on the the global state of the system. During the time evolution of the WDF according to the Moyal equation the region

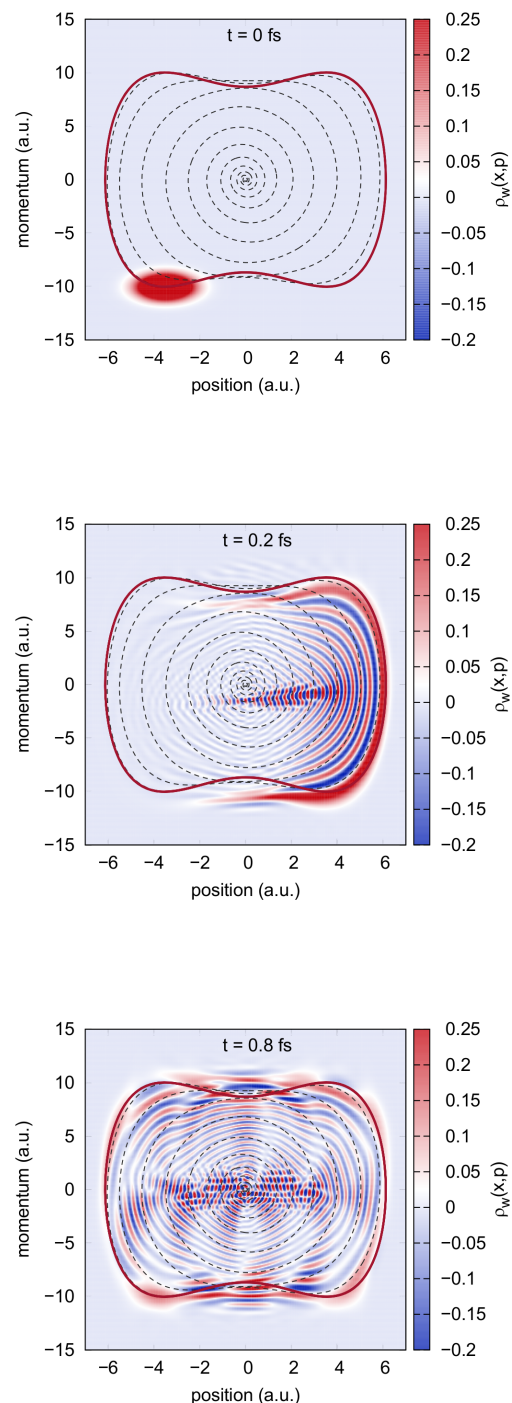


Figure 2: Color maps showing the WDF at $t = 0$, $t = 0.2$ fs, and $t = 0.8$ fs, in case of $p_0 = -10$ a.u. The quantum trajectory (dashed line), the classical trajectory (red solid line).

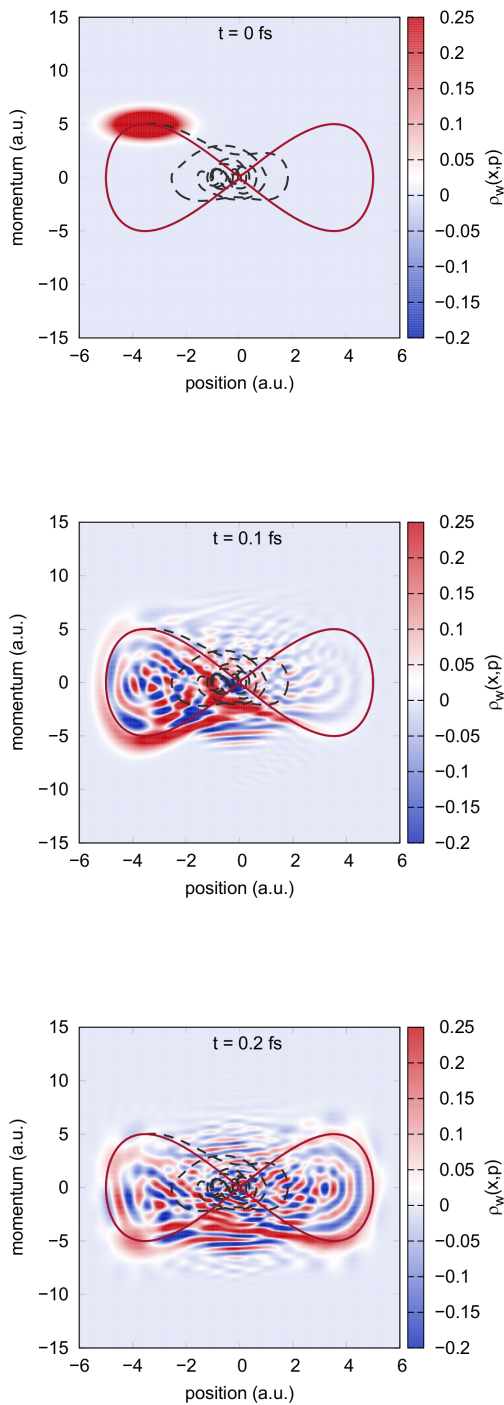


Figure 3: Color maps showing the WDF at $t = 0$, $t = 0.1$ fs, and $t = 0.2$ fs, in case of $p_0 = 5$ a.u. The quantum trajectory (dashed line), the classical trajectory (red solid line). In this case, the classical trajectory exhibits a constriction in the vicinity of 0.

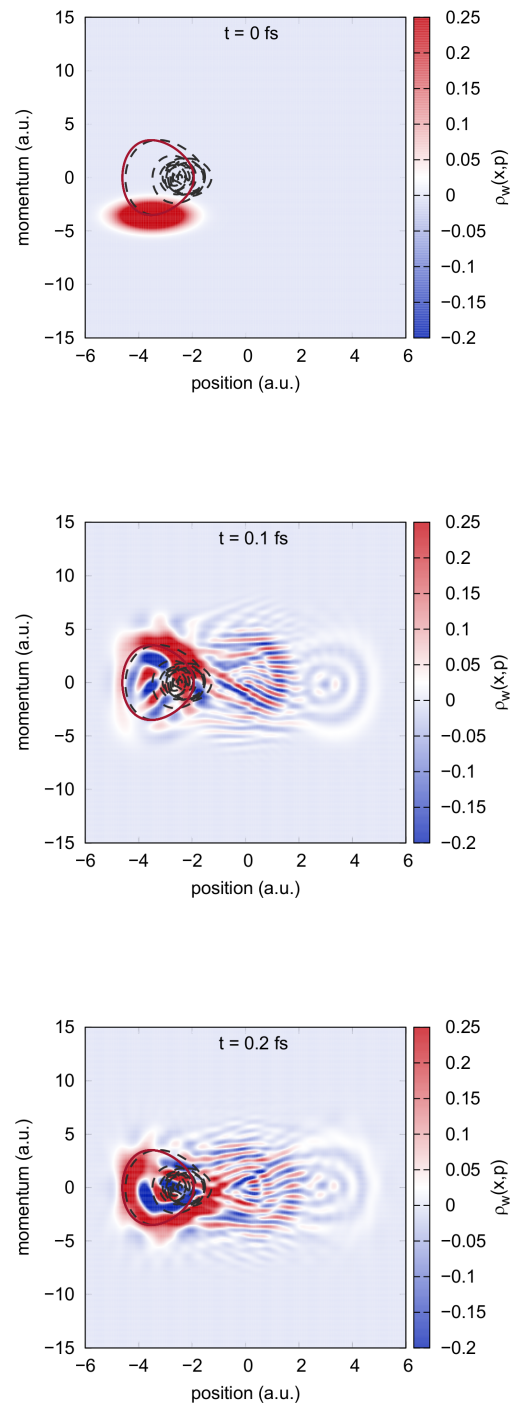


Figure 4: Color maps showing the WDF at $t = 0$, $t = 0.1$ fs, and $t = 0.2$ fs, in case of $p_0 = -3.5$ a.u. The quantum trajectory (dashed line), the classical trajectory (red solid line).

of the phase space occupied by the WDF increases. Simultaneously, the negative values of the WDF emerge as a re-

sult of the quantum correlations between different pieces of the state in the phase space [27]. It stems from the fact that the information from the off-diagonal terms in Eq. (1) represented by X variable is transferred to the WDF via the momentum p .

Apart from the trajectories, we also determine the autocorrelation function of the WDF which is defined as [28]

$$C(t) = \text{Tr}\{\varrho_W(x, p; 0)\varrho_W(x, p; t)\}, \quad (11)$$

where Tr refers to the trace in the phase space. The quantity allows us to extract some additional information on the WDF's dynamics in the considered potential. We performed appropriate calculations of the function $C(t)$ for the same initial momenta of the WDF for which we generated the classical and quantum trajectories in the phase space. The results of the calculations are displayed in Fig. 5. For comparison, we also display in Fig. 5 the classical autocorrelation function which is generated by the classical evolution of the coherent state. For this purpose we solve the Liouville equation with the initial condition in the form (6).

In general, we can state that the details of the autocorrelation function depend not only on the form of the confining potential of the small system, but also on the initial momentum of the WDF. However, the autocorrelation function possesses some universal properties, namely this function almost always exhibits a finite sequence of regular peaks with magnitudes decreasing in time. The consecutive peaks in the autocorrelation function are associated with the return of the WDF to the vicinity of the initial location, whereas an irregular part of the function $C(t)$ is generated by some parts of the WDF which travel forth and back across an available region of the phase space. Finally, this fractional recurrences lead to occupation of the bounded region of the phase space which is always larger than the region occupied by the initial quantum state. This observation suggests that the autocorrelation function contains information on the properties of the dynamical localization of the WDF during its time evolution. Regardless of this observation, the degree of localization of the quantum state in the phase space can be investigated in terms of the Husimi function [27] which is defined as the convolution of the Wigner distribution function and a window function with the resolution corresponding to the minimum result from the uncertainty principle.

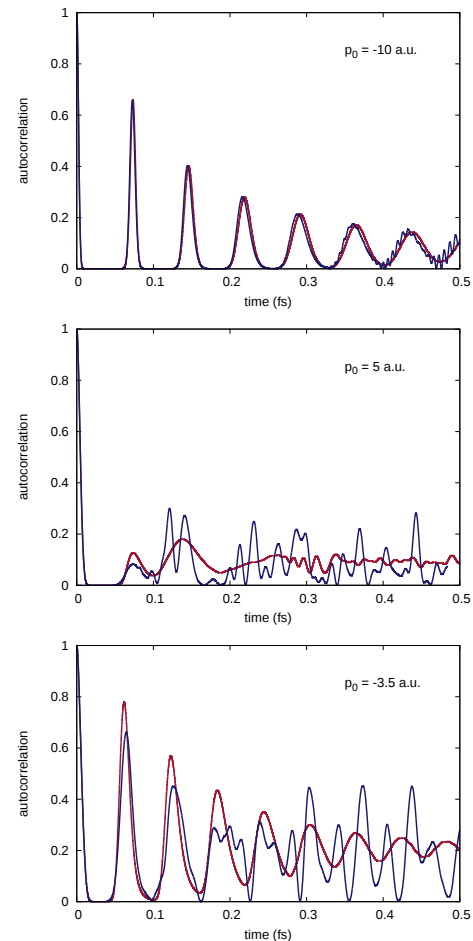


Figure 5: The autocorrelation function of the WDF generated by the Moyal equation (blue line) and the Liouville equation (red line) for three different initial momenta.

4 Conclusion

As a result of our computational studies we present the analysis of the quantum trajectories in the phase space generated by the time evolution of the Wigner distribution function. We compare the trajectories for different kinetic energies of the initially localized Wigner distribution function with the classical counterparts, which are obtained from the solution of the Hamilton's equations. This strategy allows us to visualize the differences between the both types of trajectories and discuss reasons for such discrepancy. The results presented are also supported by calculations of the autocorrelation function of the Wigner distribution function for different initial momenta.

Acknowledgment

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