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THE PHASE–SPACE APPROACH TO TIME EVOLUTION OF QUANTUM STATES IN CONFINED SYSTEMS: THE SPECTRAL SPLIT–OPERATOR METHOD

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Using the phase space approach, we consider the quantum dynamics of a wave packet in an isolated confined system with three different potential energy profiles. We solve the Moyal equation of motion for the Wigner function with the highly efficient spectral split-operator method. The main aim of this study is to compare the accuracy of the employed algorithm through analysis of the total energy expectation value, in terms of deviation from its exact value. This comparison is performed for the second and fourth order factorizations of the time evolution operator.

Keywords: Wigner distribution function, Moyal dynamics, spectral split-operator method.

1. Introduction

The theory of quanta revolutionized the way of thinking about physical phenomena in the microscopic world and introduced an abstract mathematical formalism based on some concepts of functional analysis. The structure of quantum theory is determined by a set of independent axioms which incorporates the probabilistic aspect of measurements of dynamical variables. Thereby quantum theory has a statistical character. Usually, we assume that states of a physical system are represented by abstract vectors $|\psi(t)\rangle$ in the Hilbert space. Nevertheless, in some physical situations, the description of the system states in terms of the abstract vectors is not sufficient because the states are known only statistically. To meet these challenges, quantum-statistical theory offers a more general approach in which the state of a system is described by the density operator $\hat{\rho}(t)$. Its form, in the spectral representation, is given by a convex combination of the rank-one orthogonal projection operators onto the abstract vectors (Ter Haar, 1961), i.e.,

$$\hat{\rho}(t) = \sum_n p_n \left|\phi_n(t)\right\rangle \left\langle\phi_n(t)\right|, \tag{1}$$

where p_n is the probability of finding the system in a pure state $|\phi_n(t)\rangle$ at time instant t. Time evolution of the density operator is governed by the von Neumann equation,

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}(t) = \left[\hat{H}(\hat{x},\hat{p}), \hat{\rho}(t)\right], \tag{2}$$

where the symbol $[\cdot,\cdot]$ stands for the commutator of two operators, $\hbar$ is the reduced Planck constant, and i is the imaginary unit.

The above equation of motion describes the non-dissipative evolution of the density operator for an isolated (closed) system which is characterized by the one-particle Hamiltonian in the form

$$\hat{H}(\hat{x},\hat{p}) = \frac{\hat{p}^2}{2m} + U(\hat{x}), \tag{3}$$

where m is the mass of a particle, while $\hat{x}$ and $\hat{p}$ are respectively the noncommuting position and the momentum operators obeying the following commutation relation:

$$[\hat{x},\hat{p}] = i\hbar\hat{1}, \tag{4}$$

where the symbol $\hat{1}$ denotes the unit operator. Moreover, $U(\hat{x})$ is the operator of the potential energy.

The expectation value of any dynamical observable which is represented by a Hermitian operator $\hat{A}$ is obtained by the formula

$$\langle A(t)\rangle = \mathrm{Tr}\Big\{\hat{\rho}(t)\hat{A}\Big\}, \tag{5}$$

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where the symbol $\mathrm{Tr}\{\cdot\}$ indicates the trace of the operator. Hence it can be concluded that the density operator in the quantum-statistical description of the system plays a similar role as the probability distribution function over the phase space in the statistical description of a classical system.

The relationship between the density operator and the function of phase-space variables was established by Wigner (1932), who applied the Weyl transform (Pool, 1966; Ozorio de Almeida, 1998) to the density operator. As a result, the following c-number function (Baker, 1958; Tatarskiĭ, 1983; Hillery *et al*., 1984; Balazs and Jennings, 1984; Lee, 1995), which depends on the position and momentum coordinates, is obtained:

$$\varrho(x,p;t) = \frac{1}{2\pi\hbar}\int \mathrm{d}X \left\langle x+\frac{X}{2}\right| \hat{\rho}(t) \left| x-\frac{X}{2}\right\rangle \times \exp\left[-\frac{ipX}{\hbar}\right]. \quad (6)$$

Nowadays this function is known as the Wigner distribution function (WDF). In fact, it can take negative values in some regions of the phase space, and therefore it is regarded as a quasi-probability density in this space. It is worth mentioning that the negativity of the WDF exhibits non-classical properties of the state and can be used as an indicator of quantum phenomena in the system (Benedict and Czirják, 1999; Kenfack and Życzkowski, 2004; Sadeghi *et al*., 2010; Kenfack, 2016; Khademi *et al*., 2016). It should be also emphasized that the WDF plays the role of a state in the so-called phase-space formulation of quantum mechanics (Baker, 1958; Curtright and Zachos, 2012; Błaszak and Domański, 2010), in which a non-commutative algebra of smooth observables represented by ordinary c-number functions is generated by the Groenewold star-product

$$* = \exp\left[\frac{i\hbar}{2}\left(\overleftarrow{\partial_x}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_x}\right)\right], \quad (7)$$

where the arrows indicate in which direction the derivatives act.

In practice, this product may be evaluated through translation of the argument of the phase-space function in the following way:

$$(f*g)(x,p) = f\left(x+\frac{i\hbar}{2}\overrightarrow{\partial_p}, p-\frac{i\hbar}{2}\overrightarrow{\partial_x}\right) g(x,p). \quad (8)$$

Hence, one can conclude that the star-product of two such functions is described by a power series in the form

$$(f*g)(x,p) = (fg)(x,p) + \frac{i\hbar}{2}\{f,g\}(x,p) + O(\hbar^2), \quad (9)$$

where the first term in the series is the pointwise product, and the second term is the Poisson bracket.

The aforementioned expression suggests that the quantum mechanics in the phase space may be regarded as a deformation theory of classical mechanics (Bayen *et al*., 1977; 1978a; 1978b). Presently, this formulation is exploited in some branches of modern physics and chemistry, i.e., it is applied in quantum-statistical studies of transport processes (Xue and Prodan, 2012; Leung and Prodan, 2013), quantum optics (Isar and Scheid, 2004), or quantum field theory (Lechner, 2011), and it is also very inspiring for some branches of mathematics such as deformation of the Lie algebras (Delius and Hüffmann, 1996), or non-commutative or symplectic geometry (Castellani, 2000).

The subject of this report is the exploration of two variants of the spectral split-operator method in application to the phase-space propagation of the quantum state in small confined systems. Originally, the spectral split-operator method was proposed to solve the Schrödinger equation (Feit *et al*., 1982). Then this method was adapted to the solution of the Liouville equation (Torres-Vega and Frederick, 1982; Dattoli *et al*., 1995; Gómez *et al*., 2014), and it is often used to simulate the dynamics of states in molecular systems. We performed comparative studies of this numerical method in the second and fourth orders. For this purpose we consider the initially localized WDF and its dynamics in the harmonic potential and the class of the power-exponential potentials (Ciurla *et al*., 2002). These dynamics are generated by Moyal's equation of motion.

The paper is organized as follows. In Section 2 we present the theoretical background of quantum mechanics in the phase space, i.e., basic concepts and notation for the Moyal dynamics in the phase space. Then we introduce some elements of the spectral split-operator method of the second and fourth order applied to the Moyal equation. Section 3.1 contains the results of calculations and their discussion, and conclusions are presented in Section 4.

2. Theory

In the phase-space formulation of quantum mechanics, the system considered is characterized by the Weyl symbol of the Hamiltonian, which can be written in the position representation as follows (Baker, 1958; Tatarskiĭ, 1983):

$$H_W(x,p) = \int \mathrm{d}X \left\langle x+\frac{X}{2}\right| \hat{H}(\hat{x},\hat{p}) \left| x-\frac{X}{2}\right\rangle \times \exp\left[-\frac{ipX}{\hbar}\right], \quad (10)$$

where $\hat{H}(\hat{x},\hat{p})$ corresponds to the Hermitian Hamiltonian in the form given by Eqn. (3). As mentioned at the beginning, the state of the system in the phase space is given by the WDF. In turn, its unitary evolution in time can be described by the equation of motion in the Moyal

form (Hiley, 2015),

$$\frac{\partial \varrho(x,p;t)}{\partial t} = \hat{\mathcal{L}}_M \varrho(x,p;t), \tag{11}$$

where the operator $\hat{\mathcal{L}}_M$ is given by the Moyal bracket which is defined, for a given Weyl symbol of the Hamiltonian, as a skew-symmetric part of the star-product, i.e.,

$$\begin{aligned}\hat{\mathcal{L}}_M \varrho(x,p;t) &= \frac{1}{i\hbar}\left[H_W(x,p) * \varrho(x,p;t)\right. \\ &\quad \left. - \varrho(x,p;t) * H_W(x,p)\right] \\ &= \left\{H_W(x,p), \varrho(x,p;t)\right\}_M . \end{aligned} \tag{12}$$

This means that the Moyal bracket emerges as a generator of quantum dynamics of the state in the phase space.

The Moyal equation (11) with an appropriate boundary condition generates the continuous dynamical system $(\mathbb{R}^2, \hat{\mathcal{U}}(t))$, where $\mathbb{R}^2$ is the phase space, and the evolution operator $\hat{\mathcal{U}}(t)$ is defined by the relation

$$\varrho(x,p;t) = \hat{\mathcal{U}}(t)\varrho(x,p;0). \tag{13}$$

The explicit form of the evolution operator $\hat{\mathcal{U}}(t)$ is given by the formula $\hat{\mathcal{U}}(t) = \exp\left[i\hat{\mathcal{L}}_M t\right]$. This formulation of the dynamical problem considered seems to be more adequate for dynamical systems theory regarded as a branch of mathematics (Luenberger, 1979; Walker, 1980), which has applications to a wide variety of fields such as control theory, for example (Berkovitz, 1974; Sontag, 1990; Polderman and Willems, 1998).

An important property of the Moyal bracket is that it becomes the Poisson bracket in the classical limit ($\hbar \to 0$). This implies that the Moyal equation becomes the Liouville equation for the classical phase-space distribution function. The Moyal equation can be written in the alternative form as follows (Kubo, 1964):

$$\begin{aligned}i\hbar\partial_t \varrho(x,p;t) = &\left[H_W\left(x + \frac{i\hbar}{2}\overrightarrow{\partial_p}, p - \frac{i\hbar}{2}\overrightarrow{\partial_x}\right)\right. \\ &\left. - H_W\left(x - \frac{i\hbar}{2}\overrightarrow{\partial_p}, p + \frac{i\hbar}{2}\overrightarrow{\partial_x}\right)\right] \\ &\times \varrho(x,p;t),\end{aligned} \tag{14}$$

owing to the ansatz given by Eqn. (8). Just as the Schrödinger equation, the Moyal equation (14) can be written in a more abstract form, i.e., independent of a particular representation. It was shown by Bondar *et al.* (2013), who defined the Hilbert phase space in which every state of the quantum system, which in general can be mixed, is represented by an abstract vector $|\rho(t)\rangle$, and its time evolution is given by the equation

$$\begin{aligned}i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\rho(t)\rangle = &\left[\frac{\hbar}{m}\hat{p}\hat{\lambda} + U\left(\hat{x} - \frac{\hbar}{2}\hat{\theta}\right) - U\left(\hat{x} + \frac{\hbar}{2}\hat{\theta}\right)\right] \\ &\times |\rho(t)\rangle ,\end{aligned} \tag{15}$$

where the operators $\hat{\lambda}$, $\hat{\theta}$, $\hat{p}$, and $\hat{x}$ belong to a six-operator algebra with respect to the following commutation relations:

$$\begin{aligned}&\left[\hat{x},\hat{\theta}\right] = \hat{0}, \qquad [\hat{x},\hat{p}] = \hat{0}, \qquad \left[\hat{x},\hat{\lambda}\right] = i\hat{1}, \\ &\left[\hat{p},\hat{\theta}\right] = i\hat{1}, \qquad \left[\hat{p},\hat{\lambda}\right] = \hat{0}, \qquad \left[\hat{\lambda},\hat{\theta}\right] = \hat{0}.\end{aligned} \tag{16}$$

In the $\langle xp|$ representation where

$$\hat{x} = x, \qquad \hat{p} = p, \qquad \hat{\lambda} = -i\partial_x, \qquad \hat{\theta} = -i\partial_p, \tag{17}$$

we obtain the WDF as it turns out that $\langle xp|\,\rho(t)\rangle = \varrho(x,p,t)$ and Eqn. (15) boils down to Eqn. (14).

Equation (15) has the same form as the well-known time evolution equation for the abstract state vector in the Hilbert space,

$$i\hbar\,|\psi(t)\rangle = \hat{H}\,(\hat{x},\hat{p})\,|\psi(t)\rangle\,, \tag{18}$$

but in the Hilbert phase space the dynamics are induced by the operator

$$\begin{aligned}\hat{H}_{HPS}\left(\hat{x},\hat{\theta},\hat{p},\hat{\lambda}\right) = &\hat{H}\left(\hat{x} - \frac{\hbar}{2}\hat{\theta}, \hat{p} + \frac{\hbar}{2}\hat{\lambda}\right) \\ &- \hat{H}\left(\hat{x} + \frac{\hbar}{2}\hat{\theta}, \hat{p} - \frac{\hbar}{2}\hat{\lambda}\right),\end{aligned} \tag{19}$$

which we will call the Hilbert phase space (HPS) Hamiltonian.

Knowing the state at time instant t_0, $|\rho(t_0)\rangle$, the solution of Eqn. (15) for arbitrary $t_0 + \Delta t$ can be written in the form $|\rho(t_0 + \Delta t)\rangle = \hat{\mathcal{U}}(\Delta t)\,|\rho(t_0)\rangle$, where

$$\begin{aligned}\hat{\mathcal{U}}(\Delta t) = \exp\left\{-\frac{i}{\hbar}\left[\frac{\hbar}{m}\hat{p}\hat{\lambda} + U\left(\hat{x} - \frac{\hbar}{2}\hat{\theta}\right)\right.\right. \\ \left.\left. - U\left(\hat{x} + \frac{\hbar}{2}\hat{\theta}\right)\right]\Delta t\right\}\end{aligned} \tag{20}$$

is called the time evolution operator, which can be written in more concise form as

$$\hat{\mathcal{U}}(\Delta t) = \exp\left[-\frac{i}{\hbar}\left(\hat{T} + \hat{U}\right)\Delta t\right]. \tag{21}$$

In this notation, the operator

$$\hat{T} = \frac{\hbar}{m}\hat{p}\hat{\lambda} \tag{22}$$

represents the kinetic part, whereas the operator

$$\hat{U} = U\left(\hat{x} - \frac{\hbar\hat{\theta}}{2}\right) - U\left(\hat{x} + \frac{\hbar\hat{\theta}}{2}\right) \tag{23}$$

represents the potential part. Importantly, these two operators do not commute.

It should be noted that in the $\langle \lambda p|$ representation, where

$$\hat{x} = i\partial_\lambda, \quad \hat{p} = p, \quad \hat{\lambda} = \lambda, \quad \hat{\theta} = -i\partial_p, \tag{24}$$

operator $\hat{T}$ is a multiplication operator. Similarly, in the $\langle x\theta|$ representation, where

$$\hat{x} = x, \quad \hat{p} = i\partial_\theta, \quad \hat{\lambda} = -i\partial_x, \quad \hat{\theta} = \theta, \tag{25}$$

operator $\hat{U}$ is a multiplication operator. Transformations between different representations of the state vector $|\rho(t)\rangle$ are realized by the Fourier transforms, i.e.,

$$\begin{aligned}
\langle x\theta|\ \rho\rangle &= \int \mathrm{d}p e^{-ip\theta} \langle xp|\ \rho\rangle\,, \\
\langle \lambda p|\ \rho\rangle &= \frac{1}{2\pi} \int \mathrm{d}x\, \mathrm{d}\theta e^{i(p\theta - \lambda x)} \langle x\theta|\ \rho\rangle\,, \\
\langle xp|\ \rho\rangle &= \frac{1}{2\pi} \int \mathrm{d}\theta e^{ix\lambda} \langle \lambda p|\ \rho\rangle\,.
\end{aligned} \tag{26}$$

The core of the spectral split-operator method is factorization of the time evolution operator (21) as a product of operators dependent only on $\hat{T}$ and only on $\hat{U}$. Each of them can be easily realized numerically as a multiplication in an adequate representation, while the transformations between various representations can be efficiently realized by the fast Fourier transform.

We consider two factorizations of time evolution operator (21): the widely used second order factorization,

$$\begin{aligned}
\hat{\mathcal{U}}_2(\Delta t) = \exp\left[-\frac{i}{2\hbar}\hat{T}\Delta t\right] \exp\left[-\frac{i}{\hbar}\hat{U}\Delta t\right] \\
\times \exp\left[-\frac{i}{2\hbar}\hat{T}\Delta t\right],
\end{aligned} \tag{27}$$

and the fourth-order factorization,

$$\begin{aligned}
\hat{\mathcal{U}}_4(\Delta t) = \exp\left[-\frac{i}{6\hbar}\hat{U}\Delta t\right] \exp\left[-\frac{i}{2\hbar}\hat{T}\Delta t\right] \\
\times \exp\left[-\frac{2i}{3\hbar}\hat{W}\Delta t\right] \exp\left[-\frac{i}{2\hbar}\hat{T}\Delta t\right] \\
\times \exp\left[-\frac{i}{6\hbar}\hat{U}\Delta t\right],
\end{aligned} \tag{28}$$

where

$$\hat{\mathcal{U}}(\Delta t) = \hat{\mathcal{U}}_k(\Delta t) + O\left(\Delta t^{k+1}\right) \tag{29}$$

for $k = 2, 4$ and

$$\hat{W} = \hat{U} - \left[\hat{U}, \left[\hat{T}, \hat{U}\right]\right] \frac{\Delta t^2}{48\hbar^2}, \tag{30}$$

which was originally derived by Chin (1997), and then applied to the Liouville equation. Later this factorization was also used for the Schrödinger equation (Chin and Chen, 2002). It can be clearly seen that the latter factorization requires $5/3$ times more operations, both multiplications and Fourier transforms. It can be shown that

$$\begin{aligned}
&\langle x\theta| \left[\hat{U}, \left[\hat{T}, \hat{U}\right]\right] |\rho(t)\rangle \\
&= \frac{\hbar^2}{m} \left\{ \left[U'\left(x - \frac{\hbar}{2}\theta\right)\right]^2 \right. \\
&\quad \left. - \left[U'\left(x + \frac{\hbar}{2}\theta\right)\right]^2 \right\} \langle x\theta|\ \rho(t)\rangle\,,
\end{aligned} \tag{31}$$

where $U'(x)$ is the first derivative of the potential energy function $U(x)$, so the operator $\left[\hat{U}, \left[\hat{T}, \hat{U}\right]\right]$ is just a multiplication operator in the $\langle x\theta|$ representation.

The time shift of the WDF from the time instant t_0 to $t_0 + \Delta t$ can be realized in the following steps, respectively for the second-order factorization (27),

$$\begin{aligned}
\varrho(x, p, t_0 + \Delta t) \approx \mathcal{F}^{\lambda\to x} \exp\left[-\frac{i\Delta t}{2m} T(\lambda, p)\right] \mathcal{F}^{\theta\to p}_{x\to\lambda} \\
\times \exp\left[-\frac{i\Delta t}{\hbar} U(x, \theta)\right] \mathcal{F}^{\lambda\to x}_{p\to\theta} \\
\times \exp\left[-\frac{i\Delta t}{2m} T(\lambda, p)\right] \mathcal{F}_{x\to\lambda} \varrho(x, p, t_0),
\end{aligned} \tag{32}$$

and for the fourth-order factorization (28),

$$\begin{aligned}
\varrho(x, p, t_0 + \Delta t) \approx \mathcal{F}^{\theta\to p} \exp\left[-\frac{i\Delta t}{6\hbar} U(x, \theta)\right] \mathcal{F}^{\lambda\to x}_{p\to\theta} \\
\times \exp\left[-\frac{i\Delta t}{2m} T(\lambda, p)\right] \mathcal{F}^{\theta\to p}_{x\to\lambda} \\
\times \exp\left[-\frac{2i\Delta t}{3\hbar} W(x, \theta)\right] \mathcal{F}^{\lambda\to x}_{p\to\theta} \\
\times \exp\left[-\frac{i\Delta t}{2m} T(\lambda, p)\right] \mathcal{F}^{\theta\to p}_{x\to\lambda} \\
\times \exp\left[-\frac{i\Delta t}{6\hbar} U(x, \theta)\right] \mathcal{F}_{p\to\theta} \varrho(x, p, t_0).
\end{aligned} \tag{33}$$

In Eqns. (32) and (33), $\mathcal{F}_{a\to b}$ denotes the ordinary Fourier transform defined by the relation

$$\mathcal{F}_{a\to b} f(a) = \int \mathrm{d}a e^{-iab} f(a) = \widetilde{f}(b), \tag{34}$$

where $\mathcal{F}^{b\to a}$ is used for the inverse Fourier transform

$$\mathcal{F}^{b\to a} g(b) = \frac{1}{2\pi} \int \mathrm{d}b e^{iba} g(b) = \widetilde{g}(a), \tag{35}$$

and $\mathcal{F}^{c\to d}_{a\to b}$ is equivalent to the successive application of ordinary Fourier transforms in one variable and the inverse Fourier transform in the other variable according to

$$\mathcal{F}^{c\to d}_{a\to b} h(a, c) = \mathcal{F}^{c\to d} \mathcal{F}_{a\to b} h(a, c) = \widetilde{h}(b, d). \tag{36}$$

In numerical calculations we can obtain the WDF time evolution by successive application of the time evolution operator (20) with a given time step Δt. We use the computational box of size $[-L_x, L_x] \times [-L_p, L_p]$ with the $N_x \times N_p$ grid, and discretize the position and momentum in the following way:

$$x_m = -L_x + m\Delta x, \quad p_n = -L_p + n\Delta p, \tag{37}$$

where $\Delta x = 2L_x/N_x$ and $\Delta p = 2L_p/N_p$. For the variables θ and λ we define

$$\Delta\lambda = \frac{\pi}{L_x}, \quad \Delta\theta = \frac{\pi}{L_p}, \quad L_\lambda = \frac{N_x\Delta\lambda}{2}, \quad L_\theta = \frac{N_p\Delta\theta}{2}. \tag{38}$$

Unlike for x and p, the discretizations of variables θ and λ have to be shifted due to the properties of the discrete Fourier transform,

$$\lambda_k = \begin{cases} -L_\lambda + \left(k + \frac{N_x}{2}\right)\Delta\lambda, & k = 0, 1, \ldots, \frac{N_x}{2} - 1, \\ -L_\lambda + \left(k - \frac{N_x}{2}\right)\Delta\lambda, & k = \frac{N_x}{2}, \ldots, N_x - 1 \end{cases} \tag{39}$$

and

$$\theta_l = \begin{cases} -L_\theta + \left(l + \frac{N_p}{2}\right)\Delta\theta, & l = 0, 1, \ldots, \frac{N_p}{2} - 1, \\ -L_\theta + \left(l - \frac{N_p}{2}\right)\Delta\theta, & l = \frac{N_p}{2}, \ldots, N_p - 1. \end{cases} \tag{40}$$

For numerical simulation according to Eqns. (32) and (33), one has to discretize functions $T(\lambda, p)$, $U(x, \theta)$ and $W(x, \theta)$ on appropriate grids and apply the discrete Fourier transforms that are defined as usual, respectively for the ordinary and the inverse transform,

$$F_k = \sum_{n=0}^{N-1} f_n e^{-i2\pi kn/N}, \quad f_n = \frac{1}{N}\sum_{n=0}^{N-1} F_k e^{i2\pi kn/N}, \tag{41}$$

for efficient computations implemented as fast Fourier transforms.

An interesting observation is that the approximate time evolution operators given by Eqns. (27) and (28) for the Moyal equation (14) have the form of the Floquet operator, which is the time evolution operator over a single period for a quantum system periodically perturbed by the delta distribution kicks. It is shown in Section A1 of Appendix that the second-order factorization of the time evolution operator (27) has exactly the same form as the Floquet operator of a periodically kicked system with a time-dependent Hamiltonian defined as follows:

$$\hat{H}^{(2)}(\hat{x}, \hat{p}; t) = \frac{\hat{p}^2}{2m} + U(\hat{x})\Delta t \times \sum_{n=-\infty}^{\infty} \delta\left(t - \left(n + \frac{1}{2}\right)\Delta t\right). \tag{42}$$

Similarly, in Section A2 of Appendix it is shown that the fourth-order factorization of the time evolution operator (28) has the same form as the Floquet operator of a periodically kicked system whose time-dependent Hamiltonian has the following form:

$$\hat{H}^{(4)}(\hat{x}, \hat{p}; t) = \frac{\hat{p}^2}{2m} + \frac{1}{3}U(\hat{x})\Delta t \sum_{n=-\infty}^{\infty} \delta(t - n\Delta t) + \frac{2}{3}\left[U(\hat{x})\Delta t - [U'(\hat{x})]^2 \frac{\Delta t^3}{48m}\right] \times \sum_{n=-\infty}^{\infty} \delta\left(t - \left(n + \frac{1}{2}\right)\Delta t\right). \tag{43}$$

In general, we can say that the spectral split-operator method approximates a quantum system of particles in a constant potential with a quantum system of periodically kicked free particles. As the time step decreases, the kicks get weaker but more frequent, thus better mimicking the original constant potential (assuming that the time step is not too short for the employed arithmetic precision, as this would lead to accumulation of round-off errors).

3. Results and a discussion

3.1. Initial condition and potential energies considered. The presented algorithm based on the spectral split-operator method for a given initial WDF at time instant $t = 0$ allows one to find the time evolution of the WDF via successive application of the time evolution operator. We take the initial condition in the Wigner form of the Gaussian wave packet centered around some point $(0, p_0)$ in the phase space (Kaczor *et al.*, 2016),

$$\varrho(x, p; 0) = \frac{1}{\pi\hbar}\exp\left\{-\frac{2\delta_x^2(p - p_0)^2}{\hbar^2} - \frac{x^2}{2\delta_x^2}\right\}, \tag{44}$$

where δ_x^2 is the initial variance of the wave packet.

Owing to the WDF at successive time instants, we can determine evolution of some dynamical observables that are characteristic for the systems considered. In the general case, the expectation value of any dynamical variable can be calculated in accordance with the formula

$$\langle A(t)\rangle = \int \mathrm{d}x\,\mathrm{d}p\; A_W(x, p)\varrho(x, p; t), \tag{45}$$

where $A_W(x, p)$ is the Weyl symbol of the quantum-mechanical operator of a dynamical variable $\hat{A}$ in the position representation,

$$A_W(x, p) = \int \mathrm{d}X \left\langle x + \frac{X}{2}\right| \hat{A}(\hat{x}, \hat{p}) \left| x - \frac{X}{2}\right\rangle \times \exp\left[-\frac{ipX}{\hbar}\right]. \tag{46}$$

From these expressions we can simply derive the formula for temporary changes of the expectation value of the total energy associated with the WDF moving in the potential considered. Inasmuch it can be shown that for an arbitrary natural value of l, $x_W^l = x^l$ and $p_W^l = p^l$, that formula can be expressed in the following form:

$$\langle E(t)\rangle = \int \mathrm{d}x\,\mathrm{d}p\,\left[\frac{p^2}{2m} + U(x)\right]\varrho(x,p;t). \tag{47}$$

Because the analyzed systems are closed, the expectation value of the total energy is constant throughout the motion, and deviations from this value serve us as a measure of algorithm precision. For this purpose, we define the following formulas:

$$\mathrm{error}(E;t,\Delta t) = E^{\mathrm{num}}(t,\Delta t) - E^{\mathrm{exact}}, \tag{48}$$

$$\mathrm{error}(E;\Delta t) = \max_t \left|\mathrm{error}(E;t,\Delta t)\right|, \tag{49}$$

which will be used in further subsections.

Potential energy profiles that are considered are the simple harmonic oscillator,

$$U_{\mathrm{SHO}}(x) = \frac{1}{2}m\omega^2 x^2, \tag{50}$$

the Gaussian well,

$$U_{\mathrm{G}}(x) = U_0\left[1 - \exp\left(-\frac{x^2}{2\sigma_x^2}\right)\right] \tag{51}$$

and the power-exponential well,

$$U_{\mathrm{PE}}(x) = U_0\left\{1 - \exp\left[-\left(\frac{x}{\sqrt{2}\sigma_x}\right)^{2n}\right]\right\}, \tag{52}$$

which is considered for $n = 2$. It should be noted that the potential energy $U_G(x)$ is a special case of the power-exponential function (52) for $n = 1$. In Eqns. (50)–(52), m is the mass of the particle, ω is the angular frequency of the harmonic oscillator, U_0 is the depth of the potential well, and σ_x is related to the width of the potential well. Figure 1 shows the potential energy profiles for the employed values of the parameters that will be specified in the following subsections.

Given the initial WDF (44) and three above forms of the potential energy, one can calculate the analytic forms of the total energy expectation values from Eqn. (47), namely,

$$E_{\mathrm{SHO}}^{\mathrm{exact}} = \frac{1}{2m}\left(\frac{\hbar^2}{4\delta_x^2} + p_0^2\right) + \frac{m\omega^2}{2}\delta_x^2, \tag{53}$$

$$E_{\mathrm{G}}^{\mathrm{exact}} = \frac{1}{2m}\left(\frac{\hbar^2}{4\delta_x^2} + p_0^2\right) + U_0\left(1 - \sqrt{\frac{\sigma_x^2}{\sigma_x^2+\delta_x^2}}\right), \tag{54}$$

$$E_{\mathrm{PE}}^{\mathrm{exact}} = \frac{1}{2m}\left(\frac{\hbar^2}{4\delta_x^2} + p_0^2\right) + U_0\left[1 - \frac{\sigma_x^2}{2\pi\delta_x^2}\exp\left(\frac{\sigma_x^4}{8\delta_x^4}\right) \times K_{\frac{1}{4}}\left(\frac{\sigma_x^4}{8\delta_x^4}\right)\right], \tag{55}$$

where $K_\nu(x)$ is the modified Bessel function of the second kind. Furthermore, time evolution of the WDF in the case of the harmonic oscillator can be determined analytically. In this case we introduce another measure to monitor deviation of the numerical WDF from the exact

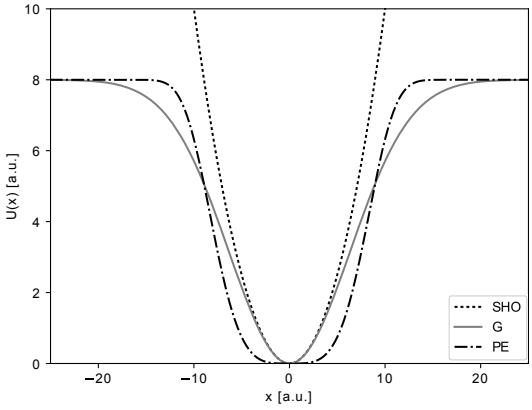

Fig. 1. Discussed profiles of the potential energy: harmonic oscillator (SHO), Gaussian (G), and power-exponential (PE).

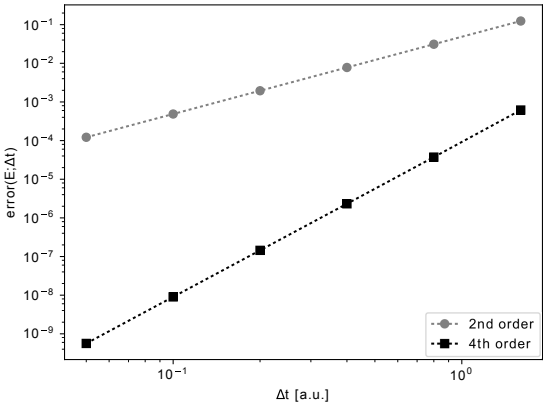

Fig. 2. Maximum value of the error of total energy during simulation for various time steps in the case of the second- and fourth-order algorithms applied to the potential of the harmonic oscillator.

one during time evolution, namely,

$$\text{error}(\varrho;\Delta t)=\max_t\left\{\hbar\sum_{ij}\left[\varrho_{ij}^{\text{exact}}(t)-\varrho_{ij}^{\text{num}}(t;\Delta t)\right]^2\Delta x\Delta p\right\}^{\frac{1}{2}}. \quad (56)$$

This is the square root of the mean square error of the WDF and the $\hbar$ constant was introduced to guarantee that the measure considered is dimensionless.

All calculations were performed in the atomic units (a.u.), i.e. $\hbar = m_e = 1$, where m_e is the electron rest mass.

3.2. Harmonic oscillator potential. In all our calculations we use the potential energy (50) with $m = 1$ a.u. and $\omega = 1/\sqrt{5}$ a.u. The initial WDF (44) assumes that $p_0 = 1$ a.u. and $\delta_x^2 = 0.25$ a.u. Then the expectation value of the total energy (53) is $E_{\text{HO}}^{\text{exact}} = 1.025$ a.u. The maxima of the total energy error for both factorizations of the time evolution operator are presented in Fig. 2 as a function of the employed time step Δt. It shows that for the shortest time step $\Delta t = 0.05$ a.u. the fourth-order method produces an error which is five orders of magnitude smaller than for the second-order method. Even at the longest tested $\Delta t = 1.6$ a.u. the error of the fourth-order method is similar to that of the second-order method with the shortest Δt.

Time dependence of the total energy error for two sample time steps for each method is shown in Fig. 3.

The only visible difference between the plots for both time steps is scaling, but the shape is virtually the same. The same is true for all other time steps considered.

In the case of the harmonic oscillator potential the Moyal equation can be solved analytically and the solution is

$$\varrho(x,p,t)=\varrho\left(x\cos\omega t-\frac{p}{m\omega}\sin\omega t, p\cos\omega t+m\omega x\sin\omega t\right). \quad (57)$$

For the initial WDF in the form given by Eqn. (44) the above formula leads to the following time evolution of the WDF:

$$\varrho_{\text{SHO}}(x,p,t)=\frac{1}{\pi\hbar}\exp\left[-\frac{\left(x\cos\omega t-\frac{p}{m\omega}\sin\omega t\right)^2}{2\delta_x^2}-\frac{2\delta_x^2(p\cos\omega t+m\omega x\sin\omega t-p_0)^2}{\hbar^2}\right]. \quad (58)$$

The maxima of the WDF error for both factorizations of the time evolution operator are presented in Fig. 4 as a function of the employed time step Δt. This shows that for the shortest time step $\Delta t = 0.05$ a.u. the fourth-order method produces an error which is five orders of magnitude smaller than for the second-order method. Even at the longest tested $\Delta t = 1.6$ a.u. the error of the fourth-order method is similar of the second-order method with the shortest Δt. The error of the WDF behaves just like that of total energy in Fig. 2, apart from a little deviation from linear dependence in the log-log scale for the longest time step in the case of the second-order factorization.

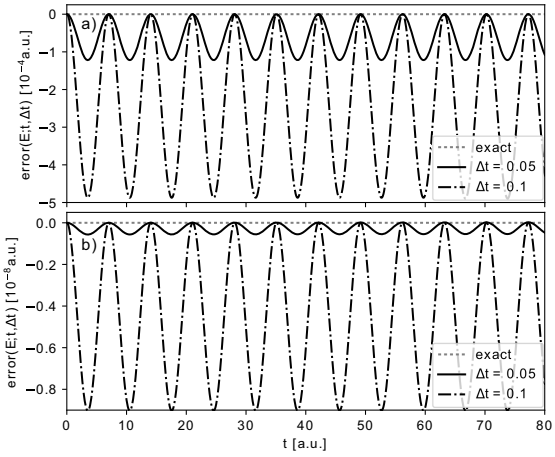

Fig. 3. Total energy error time dependence for time steps: $\Delta t = 0.05$ a.u. (solid line) and $\Delta t = 0.1$ a.u. (dash-dotted line) for the second-order algorithm (a) and the fourth-order algorithm (b), both for the harmonic oscillator potential.

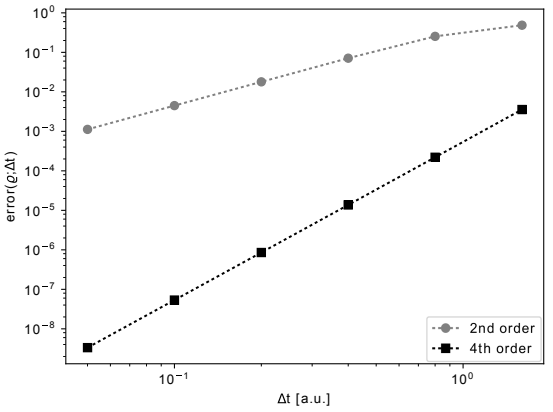

Fig. 4. Maximum value of the error of the WDF during simulation for various time steps in the case of the second- and fourth-order algorithms applied to the harmonic oscillator potential.

3.3. Gaussian potential. In our calculations we use the potential energy (51) with $U_0 = 8$ a.u. and $\sigma_x^2 = 40$ a.u. The initial WDF (44) assumes the following parameters: $p_0 = 1$ a.u. and $\delta_x^2 = 0.25$ a.u. Then the expectation value of the total energy (54) is $E_G^{\text{exact}} = 1.024883$ a.u. The maxima of the total energy error for both factorizations of the time evolution operator presented in Fig. 5 turn out to be pretty similar to the results obtained previously for the harmonic oscillator potential. Analogically, for the time step $\Delta t = 0.05$ a.u. the fourth-order method produces an error which is five orders of magnitude smaller than the error of the second order method. Also for the longest tested $\Delta t = 1.6$ a.u. the error of the fourth order method is comparable to that of the second-order method for the shortest $\Delta t = 0.5$ a.u.

Time dependence of the total energy error (Fig. 6) differs from the case of the harmonic oscillator (Fig. 3), since the amplitude of oscillations is decreasing.

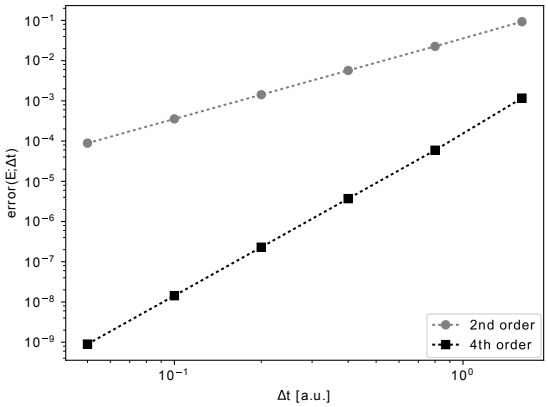

Fig. 5. Maximum value of the error of total energy during simulation for various time steps in the case of the second- and fourth-order algorithms applied to the Gaussian potential.

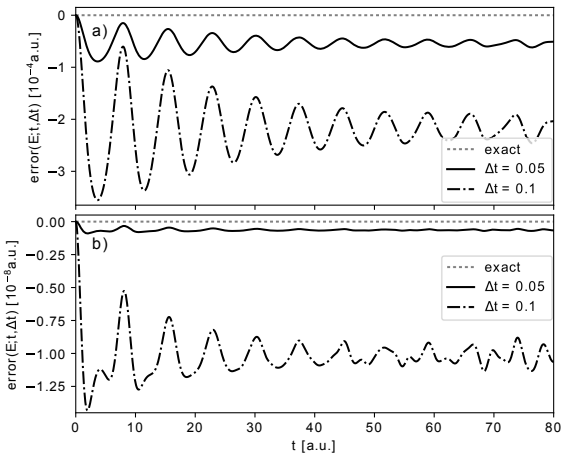

Fig. 6. Total energy error time dependence for time steps: $\Delta t = 0.05$ a.u. (solid line) and $\Delta t = 0.1$ a.u. (dash-dotted line) for the second-order algorithm (a) and the fourth-order algorithm (b) in the Gaussian well case.

3.4. Power-exponential potential. In our calculations we use the potential energy (52) with $U_0 = 8$ a.u. and $\sigma_x^2 = 40$ a.u. The initial WDF (44) is taken with $p_0 = 1$ a.u. and $\delta_x^2 = 0.25$ a.u. The expectation value of the total energy (55) is $E_{PE}^{\text{exact}} = 1.000234$ a.u. The maxima of the total energy error for both factorizations of the time evolution operator presented in Fig. 7 exhibit very similar behavior to the results presented in Figs. 2 and 5 for the harmonic oscillator potential and the Gaussian well potential, respectively, and the time dependence of the total energy error (Fig. 8) exhibits an analogous characteristic as for the Gaussian potential (Fig. 6).

4. Conclusions

We studied the phase space dynamics of a quantum particle in three different confined systems according to the Moyal equation determining the time evolution of the Wigner function. We analyzed the precision of the algorithm based on the spectral split-operator method for various time steps and for the second- and fourth-order factorizations of the time evolution operator. The fourth-order factorization was used for the first time for Wigner function dynamics in the quantum phase space. The influence of the boundaries on the dynamics of the Wigner function was neglected because the extents of the computational box were suitably adjusted to avoid this effect. Also the employed grid size 1024×1024 was large enough to keep errors related to the phase space discretization much smaller than those resulting from the analyzed lengths of the time step.

As a measure of precision, we used the deviation of the total energy from its exact value. For every profile of the potential energy we have obtained similar dependencies of the total energy error as a function of the time step length. These dependencies are very close to linear in the log-log scale, which means that they are power relations. More precisely, regardless of the potential energy form, the total energy error is approximately proportional to some power of the time step, which turned out to be equal to the order of the used factorization method.

For a given time evolution operator factorization and a given potential energy profile, the error is a function displaying a very similar shape regardless of the time step used, but it is scaled approximately by the ratio of two time steps considered raised to the power of the factorization order of the time evolution operator.

Additionally, in the case of the harmonic oscillator we also analyzed the square root of the mean squared error of the numerical WDF in relation to the analytical one. The behavior and scaling of that parameter closely mimic the results obtained for the total energy error.

After running all of the calculations we can undoubtedly state that the fourth-order factorization scheme of the time evolution operator is far superior to the second-order one. It requires only $5/3$ times more calculations for a single time step but provides results several orders of magnitude more precise for the same time step length. Additionally, we showed that applying the split-operator method to the quantum dynamics induced by the time-independent Hamiltonian effectively means that the system considered is replaced by a free particle periodically perturbed by delta distribution kicks and the period is equal to the time step length.

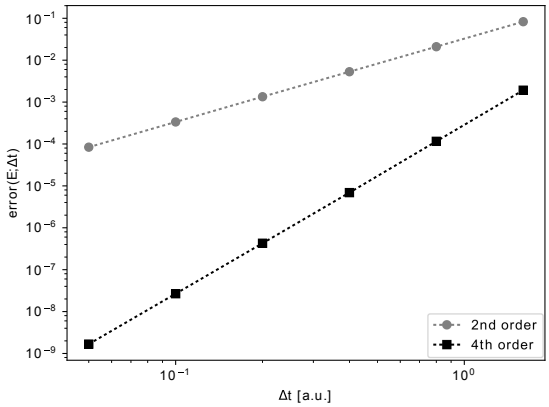

Fig. 7. Maximum value of the error of total energy during simulation for various time steps in the case of the second- and fourth-order algorithms applied to the power-exponential potential.

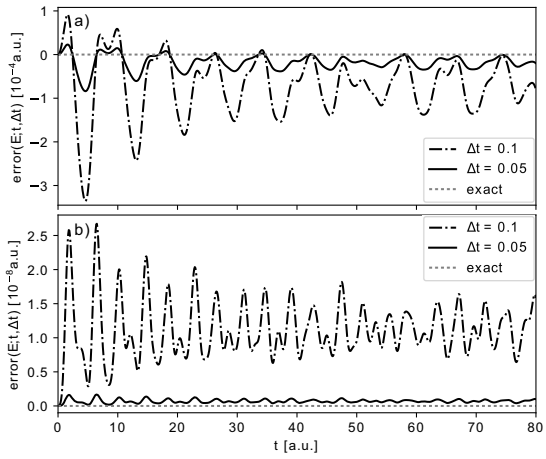

Fig. 8. Total energy error time dependence for time steps: $\Delta t = 0.05$ a.u. (solid line) and $\Delta t = 0.1$ a.u. (dash-dotted line) for the second-order algorithm (a) and the fourth-order algorithm (b) in the power-exponential well case.

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References

Baker, G.A. (1958). Formulation of quantum mechanics based on the quasi-probability distribution induced on phase space, *Physical Review* **109**(6): 2198–2206, DOI: 10.1103/PhysRev.109.2198.

Balazs, N.L. and Jennings, B.K. (1984). Wigner's function and other distribution functions on Mock phase spaces, *Physics Reports* **104**(6): 347–391, DOI: 10.1016/0370-1573(84)90151-0.

Bayen, F., Flato, M., Fronsdal, C., Lichnerowicz, A. and Sternheimer, D. (1977). Quantum mechanics as a deformation of classical mechanics, *Letters in Mathematical Physics* **1**(6): 521–530, DOI: 10.1007/BF00399745.

Bayen, F., Flato, M., Fronsdal, C., Lichnerowicz, A. and Sternheimer, D. (1978a). Deformation theory and quantization. I: Deformation of symplectic structures, *Annals of Physics* **111**(1): 61–110, DOI: 10.1016/0003-4916(78)90224-5.

Bayen, F., Flato, M., Fronsdal, C., Lichnerowicz, A. and Sternheimer, D. (1978b). Deformation theory and quantization. II: Physical applications, *Annals of Physics* **111**(1): 111–151, DOI: 10.1016/0003-4916(78)90225-7.

Benedict, M.G. and Czirják, A. (1999). Wigner functions, squeezing properties, and slow decoherence of a mesoscopic superposition of two-level atoms, *Physical Review A* **60**(5): 4034–4044, DOI: 10.1103/PhysRevA.60.4034.

Berkovitz, L.D. (1974). *Optimal Control Theory*, Springer-Verlag, New York, NY.

Błaszak, M. and Domański, Z. (2010). Phase space quantum mechanics, *Annals of Physics* **327**(2): 167–211, DOI: 10.1016/j.aop.2011.09.006.

Bondar, D.I., Cabrera, R., Zhdanov, D.V. and Rabitz, H.A. (2013). Wigner phase-space distribution as a wave function, *Physical Review A* **88**(5): 052108–1–052108–6, DOI: 10.1103/PhysRevA.88.052108.

Castellani, L. (2000). Non-commutative geometry and physics: A review of selected recent results, *Classical and Quantum Gravity* **17**(17): 3377–3401, DOI: 10.1088/0264-9381/17/17/301.

Chin, S.A. (1997). Symplectic integrators from composite operator factorizations, *Physics Letters A* **226**(6): 344–348, DOI: 10.1016/S0375-9601(97)00003-0.

Chin, S.A. and Chen, C.R. (2002). Gradient symplectic algorithms for solving the Schrödinger equation with time-dependent potentials, *The Journal of Chemical Physics* **117**(4): 1409–1415, DOI: 10.1063/1.1485725.

Ciurla, M., Adamowski, J., Szafran, B. and Bednarek, S. (2002). Modelling of confinement potentials in quantum dots, *Physica E: Low-dimensional Systems and Nanostructures* **15**(4): 261–268, DOI: 10.1016/S1386-9477(02)00572-6.

Curtright, T.L. and Zachos, C.K. (2012). Quantum mechanics in phase space, *Asia-Pacific Physics Newsletter* **1**(1): 37–46, DOI: 10.1142/S2251158X12000069.

Dattoli, G., Giannessi, L., Ottaviani, P.L. and Torre, A. (1995). Split-operator technique and solution of Liouville propagation equations, *Physical Review E: Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics* **51**(1): 821–824, DOI: 10.1103/PhysRevE.51.821.

Delius, G.W. and Hüffmann, A. (1996). On quantum Lie algebras and quantum root systems, *Journal of Physics A: Mathematical and General* **29**(8): 1703–1722, DOI: 10.1088/0305-4470/29/8/018.

Feit, M.D., Fleck, J.A. and Steiger, A. (1982). Solution of the Schrödinger equation by a spectral method, *Journal of Computational Physics* **47**(3): 412–433, DOI: 10.1016/0021-9991(82)90091-2.

Gómez, E.A., Thirumuruganandham, S.P. and Santana, A. (2014). Split-operator technique for propagating phase space functions: Exploring chaotic, dissipative and relativistic dynamics, *Computer Physics Communications* **185**(1): 136–143, DOI: 10.1016/j.cpc.2013.08.025.

Hiley, B.J. (2015). On the relationship between the Wigner–Moyal approach and the quantum operator algebra of von Neumann, *Journal of Computational Electronics* **14**(4): 869–878, DOI: 10.1007/s10825-015-0728-7.

Hillery, M., O'Connell, R.F., Scully, M.O. and Wigner, E.P. (1984). Distribution functions in physics: Fundamentals, *Physics Reports* **106**(3): 121–167, DOI: 10.1016/0370-1573(84)90160-1.

Isar, A. and Scheid, W. (2004). Deformation of quantum oscillator and of its interaction with environment, *Physica A: Statistical Mechanics and Its Applications* **335**(1–2): 79–93, DOI: 10.1016/j.physa.2003.12.017.

Kaczor, U., Klimas, B., Szydłowski, D., Wołoszyn, M. and Spisak, B. (2016). Phase-space description of the coherent state dynamics in a small one-dimensional system, *Open Physics* **14**(1): 354–359, DOI: 10.1515/phys-2016-0036.

Kenfack, A. (2016). Comment on Nonclassicality indicator for the real phase-space distribution functions, *Physical Review A* **93**(3): 036101-1–036101-2, DOI: 10.1103/PhysRevA.93.036101.

Kenfack, A. and Życzkowski, K. (2004). Negativity of the Wigner function as an indicator of non-classicality, *Journal of Optics B Quantum and Semiclassical Optics* **6**(10): 396–404, DOI: 10.1088/1464-4266/6/10/003.

Khademi, S., Sadeghi, P. and Nasiri, S. (2016). Reply to Comment on Nonclassicality indicator for the real phase-space distribution functions, *Physical Review A* **93**(3): 036102-1–036102-2, DOI: 10.1103/PhysRevA.93.036102.

Kołaczek, D., Spisak, B.J. and Wołoszyn, M. (2018). Phase-space approach to time evolution of quantum states in confined systems. The spectral split-operator method, *in* P. Kulczycki *et al.* (Eds), *Contemporary Computational Science*, AGH-UST Press, Cracow, p. 5.

Kołaczek, D., Spisak, B.J. and Wołoszyn, M. (2020). Phase-space approach to time evolution of quantum states in confined systems. The spectral split-operator method, *in* P. Kulczycki *et al.* (Eds), *Information Technology, Systems Research, and Computational Physics*, Springer, Cham, pp. 307–320.

Kubo, R. (1964). Wigner representation of quantum operators and its applications to electrons in a magnetic field, *Journal of the Physical Society of Japan* **19**(11): 2127–2139, DOI: 10.1143/JPSJ.19.2127.

Lechner, G. (2011). Deformations of quantum field theories and integrable models, *Communications in Mathematical Physics* **312**(1): 265–302, DOI: 10.1007/s00220-011-1390-y.

Lee, H.-W. (1995). Theory and application of the quantum phase-space distribution functions, *Physics Reports* **259**(3): 147–211, DOI: 10.1016/0370-1573(95)00007-4.

Leung, B. and Prodan, E. (2013). A non-commutative formula for the isotropic magneto-electric response, *Journal of Physics A: Mathematical and Theoretical* **46**(15): 085205-1–085205-14, DOI: 10.1088/1751-8113/46/8/085205.

Luenberger, D.G. (1979). *Introduction to Dynamic Systems, Theory, Models, and Applications*, John Wiley & Sons, Inc., New York, NY.

Ozorio de Almeida, A.M. (1998). The Weyl representation in classical and quantum mechanics, *Physics Reports* **295**(6): 265–342, DOI: 10.1016/S0370-1573(97)00070-7.

Polderman, J.W. and Willems, J.C. (1998). *Introduction to Mathematical Systems Theory. A Behavioral Approach*, Springer-Verlag, New York, NY.

Pool, J.C.T. (1966). Mathematical aspects of the Weyl correspondence, *Journal of Mathematical Physics* **7**(1): 66–76, DOI: 10.1063/1.1704817.

Sadeghi, P., Khademi, S. and Nasiri, S. (2010). Nonclassicality indicator for the real phase-space distribution functions, *Physical Review A* **83**(1): 012102-1–012102-8, DOI: 10.1103/PhysRevA.82.012102.

Sontag, E.D. (1990). *Mathematical Control Theory. Deterministic Finite Dimensional Systems*, Springer-Verlag, New York, NY.

Tatarskiĭ, V.I. (1983). The Wigner representation of quantum mechanics, *Soviet Physics Uspekhi* **26**(4): 311–327, DOI: 10.1070/PU1983v026n04ABEH004345.

Ter Haar, D. (1961). Theory and applications of the density matrix, *Reports on Progress in Physics* **24**(1): 304–362, DOI: 10.1088/0034-4885/24/1/307.

Torres-Vega, G. and Frederick, J.H. (1982). Numerical method for the propagation of quantum-mechanical wave functions in phase space, *Physical Review Letters* **67**(19): 2601–2604, DOI: 10.1103/PhysRevLett.67.2601.

Walker, J.A. (1980). *Dynamical Systems and Evolution Equations. Theory and Applications*, Plenum Press, New York, NY.

Wigner, E. (1932). On the quantum correction for thermodynamic equilibrium, *Physical Review* **40**(5): 749–759, DOI: 10.1103/PhysRev.40.749.

Xue, Y. and Prodan, E. (2012). The noncommutative Kubo formula: Applications to transport in disordered topological insulators with and without magnetic fields, *Physical Review. B: Condensed Matter* **86**(15): 155445-1–155445-17, DOI: 10.1103/PhysRevB.86.155445.

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Appendix

Floquet operators for periodically kicked quantum systems

It will be shown that approximate time evolution operators for time-independent systems, obtained by the spectral split-operator method of the second and fourth orders, are equivalent to the exact Floquet operators of relevant periodically kicked systems. In the case of the time-dependent HPS Hamiltonian, the time evolution operator, which evolves the state from time instant t_1 to t_2, has the following form:

$$\hat{\mathcal{U}}\left(t_2,t_1\right)=\hat{\mathcal{T}}\exp\left[-\frac{i}{\hbar}\int_{t_1}^{t_2}\hat{H}_{HPS}\left(t\right)\,\mathrm{d}t\right], \tag{A1}$$

where $\hat{\mathcal{T}}$ is the time-ordering operator. The time evolution operator obeys the following composition rule:

$$\hat{\mathcal{U}}\left(t_3,t_1\right)=\hat{\mathcal{U}}\left(t_3,t_2\right)\hat{\mathcal{U}}\left(t_2,t_1\right), \tag{A2}$$

where $t_3>t_2>t_1$.

A1. Second order factorization

The HPS Hamiltonian corresponding to the Hamiltonian (42) can be written as follows:

$$\hat{H}^{(2)}_{\mathrm{HPS}}(t)=\hat{T}+\hat{U}\Delta t\sum_{n=-\infty}^{\infty}\delta\left(t-t_{n+\frac{1}{2}}\right), \tag{A3}$$

where the notation $t_n\equiv n\Delta t$ is used. The corresponding Floquet operator (time evolution operator over a single period), according to the composition rule (A2), can be factorized to

$$\begin{aligned}\hat{\mathcal{U}}^{(2)}\left(t_{n+1},t_n\right)=\hat{\mathcal{T}}&\exp\left[-\frac{i}{\hbar}\int_{t_{n+\frac{1}{2}}+\epsilon}^{t_{n+1}}\hat{H}_{HPS}\left(t\right)\,\mathrm{d}t\right]\\&\times\exp\left[-\frac{i}{\hbar}\int_{t_{n+\frac{1}{2}}-\epsilon}^{t_{n+\frac{1}{2}}+\epsilon}\hat{H}_{HPS}\left(t\right))\,\mathrm{d}t\right]\\&\times\exp\left[-\frac{i}{\hbar}\int_{t_n}^{t_{n+\frac{1}{2}}-\epsilon}\hat{H}_{HPS}\left(t\right))\,\mathrm{d}t\right],\end{aligned} \tag{A4}$$

where $0<\epsilon<\Delta t/2$ is an arbitrary constant. Using Eqn. (A3), we get

$$\begin{aligned}\hat{\mathcal{U}}^{(2)}\left(t_{n+1},t_n\right)=\exp&\left[-\frac{i}{\hbar}\hat{T}\int_{t_{n+\frac{1}{2}}+\epsilon}^{t_{n+1}}\mathrm{d}t\right]\\&\times\exp\left[-\frac{i}{\hbar}\hat{T}\int_{t_{n+\frac{1}{2}}-\epsilon}^{t_{n+\frac{1}{2}}+\epsilon}\mathrm{d}t\right.\\&\left.+\hat{U}\Delta t\int_{t_{n+\frac{1}{2}}-\epsilon}^{t_{n+\frac{1}{2}}+\epsilon}\delta(t-t_{n+\frac{1}{2}})\,\mathrm{d}t\right]\end{aligned}$$

$$\times \exp\left[-\frac{i}{\hbar}\hat{T}\int_{t_n}^{t_{n+\frac{1}{2}}-\epsilon} \mathrm{d}t\right]$$
$$= \exp\left[-\frac{i}{\hbar}\left(\frac{\Delta t}{2}-\epsilon\right)\hat{T}\right]$$
$$\times \exp\left[-\frac{i}{\hbar}\left(2\epsilon\hat{T}+\hat{U}\Delta t\right)\right]$$
$$\times \exp\left[-\frac{i}{\hbar}\left(\frac{\Delta t}{2}-\epsilon\right)\hat{T}\right]. \quad \text{(A5)}$$

Letting $\epsilon \to 0^+$, we finally get

$$\hat{\mathcal{U}_2}^{(2)}(\Delta t) = \exp\left[-\frac{i}{2\hbar}\hat{T}\Delta t\right]\exp\left[-\frac{i}{\hbar}\hat{U}\Delta t\right]$$
$$\times \exp\left[-\frac{i}{2\hbar}\hat{T}\Delta t\right], \quad \text{(A6)}$$

so Eqn. (27) is recovered.

A2. Fourth-order factorization

The HPS Hamiltonian corresponding to the Hamiltonian (43) is

$$\hat{H}^{(4)}_{HPS}(t) = \hat{T} + \frac{1}{3}\hat{U}\Delta t\sum_{n=-\infty}^{\infty}\delta\left(t-t_n\right)$$
$$+\frac{2}{3}\hat{W}\Delta t\sum_{n=-\infty}^{\infty}\delta\left(t-t_{n+\frac{1}{2}}\right), \quad \text{(A7)}$$

where the previously introduced notation $t_n \equiv n\Delta t$ is used.

In this case, kicks of the strength $\hat{U}\Delta t/3$ occur right at the border of two neighbouring time steps. To overcome this difficulty, we start with considering the shifted Floquet operator $\hat{\mathcal{U}}^{(4)}(t_{n+1}+\mu, t_n+\mu)$, where $0<\mu<\Delta t/2$. Introducing another constant $0<\epsilon<\Delta t/4$, obeying also $\epsilon+\mu<\Delta t/2$, and $\epsilon<\mu$, the Floquet operator can be factorized according to the composition rule (A2) in the following way:

$$\hat{\mathcal{U}}^{(4)}(t_{n+1}+\mu, t_n+\mu)$$
$$= \hat{\mathcal{T}}\exp\left[-\frac{i}{\hbar}\int_{t_{n+1}+\epsilon}^{t_{n+1}+\mu}\hat{H}_{\text{HPS}}(t)\,\mathrm{d}t\right]$$
$$\times \exp\left[-\frac{i}{\hbar}\int_{t_{n+1}-\epsilon}^{t_{n+1}+\epsilon}\hat{H}_{\text{HPS}}(t)\,\mathrm{d}t\right]$$
$$\times \exp\left[-\frac{i}{\hbar}\int_{t_{n+\frac{1}{2}}+\epsilon}^{t_{n+1}-\epsilon}\hat{H}_{\text{HPS}}(t)\,\mathrm{d}t\right]$$
$$\times \exp\left[-\frac{i}{\hbar}\int_{t_{n+\frac{1}{2}}-\epsilon}^{t_{n+\frac{1}{2}}+\epsilon}\hat{H}_{\text{HPS}}(t)\,\mathrm{d}t\right]$$
$$\times \exp\left[-\frac{i}{\hbar}\int_{t_n+\mu}^{t_{n+\frac{1}{2}}-\epsilon}\hat{H}_{\text{HPS}}(t)\,\mathrm{d}t\right]. \quad \text{(A8)}$$

Using Eqn. (A7), we get

$$\hat{\mathcal{U}}^{(4)}(t_{n+1}+\mu, t_n+\mu)$$
$$= \exp\left[-\frac{i}{\hbar}\hat{T}\int_{t_{n+1}+\epsilon}^{t_{n+1}+\mu}\mathrm{d}t\right]$$
$$\times \exp\left[-\frac{i}{\hbar}\left(\hat{T}\int_{t_{n+1}-\epsilon}^{t_{n+1}+\epsilon}\mathrm{d}t\right.\right.$$
$$\left.\left.+\frac{1}{3}\hat{U}\Delta t\int_{t_{n+1}-\epsilon}^{t_{n+1}+\epsilon}\delta(t-t_{n+1})\,\mathrm{d}t\right)\right]$$
$$\times \exp\left[-\frac{i}{\hbar}\hat{T}\int_{t_{n+\frac{1}{2}}+\epsilon}^{t_{n+1}-\epsilon}\mathrm{d}t\right]$$
$$\times \exp\left[-\frac{i}{\hbar}\left(\hat{T}\int_{t_{n+\frac{1}{2}}-\epsilon}^{t_{n+\frac{1}{2}}+\epsilon}\mathrm{d}t\right.\right.$$
$$\left.\left.+\frac{2}{3}\hat{W}\Delta t\int_{t_{n+\frac{1}{2}}-\epsilon}^{t_{n+\frac{1}{2}}+\epsilon}\delta\left(t-t_{n+\frac{1}{2}}\right)\,\mathrm{d}t\right)\right]$$
$$\times \exp\left[-\frac{i}{\hbar}\hat{T}\int_{t_n+\mu}^{t_{n+\frac{1}{2}}-\epsilon}\mathrm{d}t\right]. \quad \text{(A9)}$$

Calculating the integrals leads to

$$\hat{\mathcal{U}}^{(4)}(t_{n+1}+\mu, t_n+\mu)$$
$$= \exp\left[-\frac{i}{\hbar}(\mu-\epsilon)\hat{T}\right]$$
$$\times \exp\left[-\frac{i}{\hbar}\left(2\epsilon\hat{T}+\frac{1}{3}\hat{U}\Delta t\right)\right]$$
$$\times \exp\left[-\frac{i}{\hbar}\left(\frac{\Delta t}{2}-\epsilon\right)\hat{T}\right]$$
$$\times \exp\left[-\frac{i}{\hbar}\left(2\epsilon\hat{T}+\frac{2}{3}\hat{W}\Delta t\right)\right]$$
$$\times \exp\left[-\frac{i}{\hbar}\left(\frac{\Delta t}{2}-\mu-\epsilon\right)\hat{T}\right]. \quad \text{(A10)}$$

Letting $\epsilon, \mu \to 0^+$, we get

$$\hat{\mathcal{U}}^{(4)}\left(t_{n+1}+0^+, t_n+0^+\right)$$
$$= \exp\left[-\frac{i}{3\hbar}\hat{U}\Delta t\right]\exp\left[-\frac{i}{2\hbar}\hat{T}\Delta t\right]$$
$$\times \exp\left[-\frac{2i}{3\hbar}\hat{W}\Delta t\right]\exp\left[-\frac{i}{2\hbar}\hat{T}\Delta t\right]. \quad \text{(A11)}$$

The notation t_n+0^+ means that it is the time instant right after the delta kick that happened at time instant t_n. If we assume that time instant t_n is right in the middle of the kick, we have to split the operator $\exp\left[-i\hat{U}\Delta t/(3\hbar)\right]$

into two halves, which finally leads to

$$\begin{aligned}\hat{\mathcal{U}}^{(4)}\left(t_{n+1},t_n\right) &= \exp\left[-\frac{i}{6\hbar}\hat{U}\Delta t\right]\exp\left[-\frac{i}{2\hbar}\hat{T}\Delta t\right]\\ &\times\exp\left[-\frac{2i}{3\hbar}\hat{W}\Delta t\right]\exp\left[-\frac{i}{2\hbar}\hat{T}\Delta t\right]\\ &\times\exp\left[-\frac{i}{6\hbar}\hat{U}\Delta t\right],\end{aligned}\tag{A12}$$

so that Eqn. (28) is recovered.

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