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Stability and accuracy of a pseudospectral scheme for the Wigner function equation

A. Thomann, A. Borzì

Abstract

A pseudospectral scheme with centred time-differencing for solving the Wigner function equation is investigated. Stability, second-order accuracy in time, and spectral accuracy in space are proved for the Wigner function equation with a potential in a periodic setting. In addition, normalization and energy conservation properties, and Ehrenfest's theorem are discussed. Numerical experiments are presented to validate the theoretical results.

1 Introduction

In 1932, E. Wigner [30] introduced a representation of quantum mechanics on the basis of the so-called Wigner function that represents the joint quasiprobability density for space and momentum coordinates; see [18, 28, 29] for further pioneering contributions and [27] for a earlier review. This representation combines concepts that link quantum and classical mechanics allowing a convenient derivation of semiclassical methods. In particular, semiclassical schemes make it possible to model interaction between quantum mechanical and classical systems [8, 31]. Furthermore, they can be used to compute quantum corrections to classical results [19, 30]. Nowadays, the Wigner approach plays a central role in the investigation and application of open quantum systems; see, e.g., [32].

The evolution of the Wigner function is governed by the Wigner function (WF) equation, also known as the quantum Liouville equation. This equation appears in many fields of application including optics [1, 16], signal processing and pattern recognition [11], quantum transport [13, 24] and quantum tunneling phenomena [2, 10, 22].

Depending on specific application, different approximation schemes for the WF equation have been considered. In particular, in [15] first- and second-order finite difference schemes are investigated. For quantum transport problems Monte Carlo methods have been considered in [13, 23]. Further, cell-average spectral element schemes are discussed in [24], and finite-element WENO schemes are considered in [10]. In [22] a finite-difference spectral collocation method is analysed for simulation of quantum tunneling phenomena.

In these references a WF equation is considered with a Wigner potential energy term given by two nested infinite integrals. On the other hand, as discussed in [7, 12, 27], in the case where the confining potential V admits a Taylor expansion, the Wigner potential energy term can be rewritten in form of a series involving derivatives of V (Moyal's expansion), and of the Wigner function and powers of the reduced Planck constant $\hbar$. Our focus is the WF equation in the series formulation. This is a much less investigated model for which numerical analysis results are not available. For this model, we develop a leap-frog pseudospectral (LFPS) scheme and give an elegant proof of second-order accuracy in time and spectral accuracy in the phase space. We remark that the series representation is advantageous to investigate the influence of quantum perturbations to a classical model with different orders of the reduced Planck constant. Moreover, in the case of polynomial potentials the series becomes a finite sum and the infinite integral and the series representation are equivalent.

While we focus on a periodic setting, we remark that in application, e.g., [13, 14, 20], different boundary conditions are of interest, see, e.g., [9]. For this purpose, further investigation is required that may focus on pseudospectral schemes with orthogonal polynomials [6] and the approach in [25], where a windowed Fourier pseudospectral method is presented

that is coupled with a convolution algorithm in the physical space enabling the treatment of inflow/outflow boundary conditions.

The paper is organized in the following way. In the next section the quantum mechanical setting for the Wigner formalism is introduced and important properties of the Wigner function are discussed.

In Section 3, the Fourier pseudospectral scheme is illustrated including properties of the pseudospectral derivative and approximation estimates are given. This framework is used to develop and analyse the discretization of the space-momentum operators in the WF equation.

The main results of our work are presented in Section 4. In this section, the LFPS scheme is formulated and its stability and accuracy properties are investigated. We prove conditional stability of the LFPS scheme with a time-step size restriction that is explicitly given in terms of derivatives of the kinetic and potential energies. Further, subject to this restriction, we prove second-order accuracy in time and spectral accuracy in the phase-coordinates, taking care of the physical constants entering in the Wigner function model. In particular, our analysis accommodates any finite order of truncation of the Wigner potential series. Another important contribution of our work is given in Section 5. In this section, we prove that the LFPS scheme provides mass and energy conservation as in the continuous case. Also in Section 5, we discuss Ehrenfest's theorem in our pseudospectral Wigner framework.

In Section 6, we present results of numerical experiments. To demonstrate our accuracy estimates, we consider the case of V being the harmonic oscillator. This choice is motivated by the fact that in this case an exact solution to the WF equation is available. However, in this case no quantum perturbations appear. In a second series of experiments, in order to validate our LFPS scheme in the case where quantum perturbations are present, we consider a quartic double-well potential. In this case the Wigner potential term results in $\mathcal{O}(\hbar^2)$ perturbations. For this case, we compute the solution to the WF equation with two different values of $\hbar$ and compare these results with the solution of the unperturbed system. Further, we verify the conservation properties.

A section of conclusion completes this work.

2 The Wigner function equation

The WF equation governs the evolution of the quasiprobability distribution of a quantum mechanical system in phase space coordinates (q, p). In this phase space, it is possible to display motion simultaneously in the q and p variables. To introduce the Wigner function, we consider the quantum density matrix [12, 27]. For two position variables x, y, the density matrix $\rho(x, y)$, for a pure state, is defined as $\rho(x, y) = \Psi(x)\Psi^*(y)$, and for a mixed state, as $\rho(x, y) = \sum_k j_k \Psi_k(x)\Psi_k^*(y)$. The Ψ_k are states in which the electrons can exist in the position domain, and $j_k > 0$, $\sum_k j_k = 1$, is the corresponding probability that an electron can be found in that state. Using the density matrix, one can achieve the main goal of quantum mechanics, that is, calculating expectation values for physical observables.

To define the Wigner function, consider a phase space domain $\Omega = \mathbb{R} \times \mathbb{R}$ and $\Psi \in L^2(\Omega; \mathbb{C})$, $t \geq 0$. The Wigner function $W(q, p, t)$ is given by

$$W(q, p, t) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \rho(q + \frac{s}{2}, q - \frac{s}{2}, t) \mathrm{e}^{-\frac{ips}{\hbar}} \mathrm{d}s. \tag{1}$$

A direct consequence of the above definition is that $W(q, p, t)$ takes only real values [7]. Projecting the Wigner function on the q-axis gives the probability density in the position coordinate, and projecting the Wigner function on the p-axis gives the probability density in the momentum variable. We have

$$\int_{-\infty}^{\infty} W(q, p, t) \mathrm{d}p = \Psi(q, t)\Psi^*(q, t),$$
$$\int_{-\infty}^{\infty} W(q, p, t) \mathrm{d}q = \phi(p, t)\phi^*(p, t),$$

where Ψ denotes a wave function in position domain and ϕ a wave function in momentum domain.

The Wigner function is normalized in the phase space as follows

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} W(q,p,t)\mathrm{d}p\ \mathrm{d}q = 1.$$

Since the Wigner function can take on negative values, it is called a quasi probability density.

The inverse Weyl transform of a quantum operator $A(q,p)$ in the phase space is given by [12, 26]

$$A_W(q,p) = \int_{-\infty}^{\infty} A(q+\frac{s}{2}, q-\frac{s}{2})\mathrm{e}^{-\frac{ips}{\hbar}}\mathrm{d}s.$$

The expectation value of A is obtained by averaging $A_W(q,p)$ over the phase space as follows

$$\langle A\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} W(q,p,t)A_W(q,p)\mathrm{d}p\ \mathrm{d}q.$$

In particular, assuming that $\hat{H}(\hat{q},\hat{p}) = \hat{T}(\hat{p}) + \hat{V}(\hat{q})$, the Weyl transform of the quantum Hamiltonian operator $\hat{H}(\hat{p},\hat{q})$ is the classical Hamiltonian function $H(q,p)$ and thus the energy expectation value E is calculated by

$$E = \langle H\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} W(q,p,t)H(q,p)\mathrm{d}p\mathrm{d}q. \tag{2}$$

The time evolution of the Wigner function is derived from the following time-dependent Schrödinger equation

$$i\hbar\frac{\partial\Psi(q,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(q,t) + V(q)\Psi(q,t), \tag{3}$$

with a potential $V(q)$. Moreover, we have [27]

$$\begin{aligned}\frac{\partial\rho}{\partial t}(x,y,t) &= \sum_k j_k\frac{\partial}{\partial t}\Psi_k(x,t)\Psi_k^*(y,t)\\ &= \sum_k j_k\left(\frac{\partial\Psi_k(x,t)}{\partial t}\Psi_k^*(y,t) + \Psi_k(x,t)\frac{\partial\Psi_k^*(y,t)}{\partial t}\right).\end{aligned} \tag{4}$$

Inserting (3) into (4), we obtain

$$i\hbar\frac{\partial\rho}{\partial t}(x,y,t) = \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2}\right)\rho(x,y,t) + (V(x)-V(y))\,\rho(x,y,t). \tag{5}$$

Now, we consider a change of space coordinates from (x,y) to (q,s) under the transformation $q = \frac{1}{2}(x+y)$ and $s = x-y$. It follows that $x = q+\frac{s}{2}$ and $y = q-\frac{s}{2}$, and we obtain

$$\begin{aligned}\frac{\partial}{\partial x} &= \frac{1}{2}\frac{\partial}{\partial q} + \frac{\partial}{\partial s},\\ \frac{\partial}{\partial y} &= \frac{1}{2}\frac{\partial}{\partial q} - \frac{\partial}{\partial s},\\ \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} &= 2\frac{\partial^2}{\partial q\partial s}.\end{aligned}$$

With this transformation, the WF equation can be derived from (1) and (5) as follows

$$\frac{\partial W(q,p,t)}{\partial t} = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\frac{\partial\rho(q+s/2,q-s/2,t)}{\partial t}\mathrm{e}^{-ips/\hbar}\mathrm{d}s = A(\rho) + B(\rho),$$

where

$$A(\rho) = \left(-\frac{\hbar}{im}\right)\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\frac{\partial^2}{\partial q\partial s}\rho(q+\frac{s}{2},q-\frac{s}{2},t)\mathrm{e}^{-ips/\hbar}\mathrm{d}s$$
$$= \left(-\frac{\hbar}{im}\right)\frac{1}{2\pi\hbar}\frac{\partial}{\partial q}\int_{-\infty}^{\infty}\frac{\partial}{\partial s}\rho(q+\frac{s}{2},q-\frac{s}{2},t)\mathrm{e}^{-ips/\hbar}\mathrm{d}s.$$

Since

$$\frac{\partial}{\partial s}\left(\rho(q+\frac{s}{2},q-\frac{s}{2},t)\mathrm{e}^{-ips/\hbar}\right) = \left(\frac{\partial}{\partial s}\rho(q+\frac{s}{2},q-\frac{s}{2},t)\right)\mathrm{e}^{-ips/\hbar} - \frac{ip}{\hbar}\rho(q+\frac{s}{2},q-\frac{s}{2},t)\,\mathrm{e}^{-ips/\hbar},$$

and using (1), we have

$$\int_{-\infty}^{\infty}\frac{\partial}{\partial s}\left(\rho(q+\frac{s}{2},q-\frac{s}{2},t)\,\mathrm{e}^{-ips/\hbar}\right)\mathrm{d}s = \int_{-\infty}^{\infty}\left(\frac{\partial}{\partial s}\rho(q+\frac{s}{2},q-\frac{s}{2},t)\right)\mathrm{e}^{-ips/\hbar}\mathrm{d}s - \frac{ip}{\hbar}\,2\pi\hbar\,W(q,p,t)$$

For a wave function $\Psi(x)$, we require $\lim_{|x|\to\infty}\Psi(x)=0$ and thus $\lim_{|x|\to\infty}\rho(q+\frac{s}{2},q-\frac{s}{2},t)=0$. Therefore, with the fundamental theorem of calculus, we have

$$\int_{-\infty}^{\infty}\frac{\partial}{\partial s}\left(\rho(q+\frac{s}{2},q-\frac{s}{2},t)\,\mathrm{e}^{-ips/\hbar}\right)\mathrm{d}s = 0.$$

Hence, we obtain

$$A(\rho) = -\frac{p}{m}\frac{\partial}{\partial q}W(q,p,t).$$

Now, we analyse the term $B(\rho)$ [7]. We have

$$B(\rho) = \frac{1}{i\hbar}\,\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\left(V(q+\frac{s}{2})-V(q-\frac{s}{2})\right)\rho(q+\frac{s}{2},q-\frac{s}{2},t)\,\mathrm{e}^{-ips/\hbar}\mathrm{d}s.$$

Assume that the potential $V(q)$ is sufficiently regular such that it can be expanded in a power series of q. Then we can write

$$V(q+\frac{s}{2})-V(q-\frac{s}{2}) = 2\sum_{\nu=0}^{\infty}\frac{V^{(2\nu+1)}(q)}{2^{2\nu+1}(2\nu+1)!}s^{2\nu+1}. \tag{6}$$

Notice that

$$\frac{\partial^{2\nu+1}W(q,p)}{\partial p^{2\nu+1}} = \frac{1}{2\pi\hbar}\left(-\frac{i}{\hbar}\right)^{2\nu+1}\int_{-\infty}^{\infty}s^{2\nu+1}\rho(q+\frac{s}{2},q-\frac{s}{2},t)\,\mathrm{e}^{-ips/\hbar}\mathrm{d}s. \tag{7}$$

Combining (6) and (7), we have

$$B(\rho) = \sum_{\nu=0}^{\infty}\frac{(i\hbar)^{2\nu}}{2^{2\nu}(2\nu+1)!}\frac{\partial^{2\nu+1}V}{\partial q^{2\nu+1}}\frac{\partial^{2\nu+1}W}{\partial p^{2\nu+1}}.$$

Summarizing, the time evolution of the Wigner function is given by

$$\frac{\partial W}{\partial t} = -\frac{p}{m}\frac{\partial W}{\partial q} + \sum_{\nu=0}^{\infty}\frac{(-1)^{\nu}\,\hbar^{2\nu}}{2^{2\nu}(2\nu+1)!}\frac{\partial^{2\nu+1}V}{\partial q^{2\nu+1}}\frac{\partial^{2\nu+1}W}{\partial p^{2\nu+1}}. \tag{8}$$

We refer to [3, 21, 17] for functional analytic results on the WF equation. We remark that the infinite sum in (8) becomes finite for, e.g., potentials V that are polynomial functions of q.

In our investigation, we assume that the potentials of interest can be approximated by a finite series and the accuracy of this approximation can be 'controlled' by adding more terms in the series. Therefore we consider a truncated version of (8) with a partial sum up to $\nu = Q$. The particular choice of Q would depend on the features of the potential and on the purpose of the application.

3 The pseudospectral scheme

Our focus is the numerical solution of the WF equation in a setting that is common in applications [1, 5]. Specifically, we focus on a bounded phase space domain with periodic boundary conditions. Moreover, we assume that the potential $V(q)$ admits a Taylor series representation. For ease of notation, we focus our discussion on a two-dimensional phase space. However, we provide extension to higher dimensions.

To formulate our numerical approximation scheme for the WF equation, we need the following preparation.

Let Ω be a bounded domain with periodic boundary conditions, that is $\Omega \subset \mathbb{T}^2$, that is the 2-dimensional torus.

Definition 1 *A function u is called periodic on $\Omega = (-L, L) \times (-K, K)$ if $u(-L^+, \cdot) = u(L^-, \cdot)$ and $u(\cdot, -K^+) = u(\cdot, K^-)$.*

Let u be a periodic function defined on the domain $\Omega = (-L, L) \times (-K, K) \subset \mathbb{T}^2$. The domain is divided into NM subregions $(q_{j-1}, q_j) \times (p_{l-1}, p_l)$ of the length $h = q_j - q_{j-1} = \frac{2L}{N}$,$j = 1, \ldots, N$ and $k = p_l - p_{l-1} = \frac{2K}{M}$,$l = 1, \ldots, M$ respectively. The vertices of the mesh are denoted by (q_j, p_l) where $q_j = (j-1)h - L$ and $p_l = (l-1)k - K$.

Definition 2 *The discrete Fourier series of u in two dimensions is given by*

$$I_{N,M}u(q,p) := \sum_{r=-(N/2-1)}^{N/2} \sum_{s=-(M/2-1)}^{M/2} \tilde{u}_{r,s} \; e^{i2\pi(\frac{rq}{2L} + \frac{sp}{2K})}, \tag{9}$$

$$\tilde{u}_{r,s} := \frac{1}{MN} \sum_{j=1}^{N} \sum_{l=1}^{M} u(q_j, p_l) \; e^{-i2\pi(\frac{rq_j}{2L} + \frac{sp_l}{2K})}, \tag{10}$$

where $\tilde{u}_{r,s}$ are the Fourier coefficients.

The function $I_{N,M}u(q_j, p_l)$ is the trigonometric interpolant of u at the nodes q_j, $j = 1, \ldots, N$ and p_l, $l = 1, \ldots, M$.

The Fourier pseudospectral partial derivative of u with respect to q is defined by $D_q u := \frac{\partial}{\partial q}(I_{N,M}u)$; similarly, $D_p u := \frac{\partial}{\partial p}(I_{N,M}u)$; see [6]. Therefore, the ν-th pseudospectral derivative of u with respect to q is given by

$$D_q^\nu u(q,p) = \sum_{r=-(N/2-1)}^{N/2} \sum_{s=-(M/2-1)}^{M/2} \left(\frac{ir2\pi}{2L}\right)^\nu \tilde{u}_{r,s} \; \mathrm{e}^{i2\pi(\frac{rq}{2L} + \frac{sp}{2K})}. \tag{11}$$

Analogously, for the ν-th pseudospectral derivative of u with respect to p, we have

$$D_p^\nu u(q,p) = \sum_{r=-(N/2-1)}^{N/2} \sum_{s=-(M/2-1)}^{M/2} \left(\frac{is2\pi}{2K}\right)^\nu \tilde{u}_{r,s} \; \mathrm{e}^{i2\pi(\frac{rq}{2L} + \frac{sp}{2K})}. \tag{12}$$

For the purpose of our analysis, we introduce the following concepts.

Definition 3 *Let $u, v \in S_{N,M}$, where $S_{N,M} := span\left\{e^{i2\pi(\frac{rq}{2L} + \frac{sp}{2K})}, r \in \left\{-\frac{N}{2} + 1, \ldots, \frac{N}{2}\right\}, s \in \left\{-\frac{M}{2} + 1, \ldots, \frac{M}{2}\right\}\right\}$. Then the discrete $L^2(\Omega)$ inner product on the domain $\Omega = (-L, L) \times (-K, K)$ is defined as follows*

$$(u, v)_{N,M} = hk \sum_{j=1}^{N} \sum_{l=1}^{M} u(q_j, p_l) \overline{v(q_j, p_l)}, \tag{13}$$

and the corresponding norm is given by

$$\| u \| = \sqrt{(u, u)_{N,M}}.$$

Remark 4 The interpolation operator $I_{N,M}$ can be regarded as an orthogonal projection upon the space $S_{N,M}$ with respect to (13). Furthermore, we have $(u,v)_{N,M} = (u,v) := \int_\Omega u(q,p)\overline{v(q,p)}\mathrm{d}q\mathrm{d}p$ for all $u,v \in S_{N,M}$.

Notice that all pseudospectral partial derivatives that appear in the WF equation are skew symmetric. This is stated by the following lemma, see [6].

Lemma 5 *Let u,v be as above. Then all odd pseudospectral partial derivatives are skew symmetric in the discrete $L^2(\Omega)$ inner product. We have*

$$(D_q^\nu u, v)_{N,M} = -(u, D_q^\nu v)_{N,M},$$
$$(D_p^\nu u, v)_{N,M} = -(u, D_p^\nu v)_{N,M},$$

with $\nu = 2k+1$, for $k \in \mathbb{N}_0$.

Proof. The proof is done for the case $\nu = 1$ and the partial derivative with respect to q. All other cases can be proven analogously.

$$\begin{aligned}
(D_q u, v)_{N,M} &= hk \sum_{j=1}^{N}\sum_{l=1}^{M} D_q u(q_j,p_l)\overline{v(q_j,p_l)} = hk \sum_{j=1}^{N}\sum_{l=1}^{M} \overline{v(q_j,p_l)}\,\frac{\partial}{\partial q} I_{N,M} u(q,p)|_{q_j,p_l} \\
&= hk \sum_{j=1}^{N}\sum_{l=1}^{M} \overline{v(q_j,p_l)} \sum_{r=-(N/2-1)}^{N/2}\sum_{s=-(M/2-1)}^{M/2} \left(\frac{ir2\pi}{2L}\right) \tilde{u}_{r,s} \mathrm{e}^{i2\pi\left(\frac{rq_j}{2L}+\frac{sp_l}{2K}\right)} \\
&= hk \sum_{j=1}^{N}\sum_{l=1}^{M} \overline{v(q_j,p_l)} \times \\
&\quad \sum_{r=-(N/2-1)}^{N/2}\sum_{s=-(M/2-1)}^{M/2} \left(\frac{ir2\pi}{2L}\right) \left[\frac{1}{MN}\sum_{n=1}^{N}\sum_{m=1}^{M} u(q_n,p_m)\ \mathrm{e}^{-i2\pi\left(\frac{rq_n}{2L}+\frac{sp_m}{2K}\right)}\right] \mathrm{e}^{i2\pi\left(\frac{rq_j}{2L}+\frac{sp_l}{2K}\right)} \\
&= -hk \sum_{n=1}^{N}\sum_{m=1}^{M} u(q_n,p_m) \times \\
&\quad \overline{\sum_{r=-(N/2-1)}^{N/2}\sum_{s=-(M/2-1)}^{M/2} \left(\frac{ir2\pi}{2L}\right) \left[\frac{1}{MN}\sum_{j=1}^{N}\sum_{l=1}^{M} v(q_j,p_l)\ \mathrm{e}^{-i2\pi\left(\frac{rq_j}{2L}+\frac{sp_l}{2K}\right)}\right] \mathrm{e}^{i2\pi\left(\frac{rq_n}{2L}+\frac{sp_m}{2K}\right)}} \\
&= -hk \sum_{n=1}^{N}\sum_{m=1}^{M} u(q_n,p_m)\ \overline{\sum_{r=-(N/2-1)}^{N/2}\sum_{s=-(M/2-1)}^{M/2} \left(\frac{ir2\pi}{2L}\right) \tilde{v}_{r,s} \mathrm{e}^{i2\pi\left(\frac{rq_n}{2L}+\frac{sp_m}{2K}\right)}} \\
&= -hk \sum_{n=1}^{N}\sum_{m=1}^{M} u(q_n,p_m)\,\overline{D_q v(q_n,p_m)} = -(u, D_q v)_{N,M}.
\end{aligned}$$

□

In the following lemma, the operator norm $\| D_q \| = \sup_{u\in S_{N,M}\setminus\{0\}} \frac{\|D_q u\|}{\|u\|}$ is used.

Lemma 6 *Let D_q and D_p be the pseudospectral partial derivatives with respect to q and p respectively. Then the following estimates hold*

$$\| D_q^\nu \| \leq c_{q,\nu} N^\nu \qquad \textit{and} \qquad \| D_p^\nu \| \leq c_{p,\nu} M^\nu,$$

with $\nu \in \mathbb{N}$.

Proof. The proof is done for the partial derivative with respect to q. The other cases are proven analogously.

We start with

$$\| D_q u \|^2 = hk \sum_{j=1}^{N} \sum_{l=1}^{M} D_q u(q_j, p_l) \overline{D_q u(q_j, p_l)}.$$

Now, we use (11), with $\nu = 1$, and the following

$$\overline{D_q u(q,p)} = - \sum_{r'=-(N/2-1)}^{N/2} \sum_{s'=-(M/2-1)}^{M/2} \left(\frac{i r' 2\pi}{2L} \right) \overline{\tilde{u}_{r',s'}} \; \mathrm{e}^{-i2\pi(\frac{r'q}{2L} + \frac{s'p}{2K})}.$$

Further, we use the orthogonality condition

$$\sum_{j=1}^{N} \sum_{l=1}^{M} \mathrm{e}^{i2\pi(\frac{(r-r')q_j}{2L} + \frac{(s-s')p_l}{2K})} = NM \, \delta_{r,r'} \, \delta_{s,s'},$$

where $\delta_{r,r'}$ and $\delta_{s,s'}$ are the Kronecker delta of the integers r, r' and s, s', respectively. Thus, we obtain

$$\| D_q u \|^2 = hk \left(\frac{\pi}{L} \right)^2 NM \sum_{r=-(N/2-1)}^{N/2} \sum_{s=-(M/2-1)}^{M/2} |\tilde{u}_{r,s}|^2 \, r^2.$$

Now, notice that $|r| \leq N/2$ and, using similar calculation to compute $\| u \|^2$, we obtain

$$\| D_q u \|^2 \leq \left(\frac{\pi}{2L} \right)^2 N^2 \; \| u \|^2,$$

which proves the lemma with $c_q = c_{q,1} = \frac{\pi}{2L}$. For the ν-th derivative, we have $c_{q,\nu} = \left(\frac{\pi}{2L}\right)^\nu$, and the same holds for $c_{p,\nu}$. □

4 Stability and accuracy of the LFPS scheme

Consider the truncated WF equation on the interval $[0, T]$ with a discretization of the time-step size $\delta t = T/P$ and $t_n = n\delta t, \; n = 1, \ldots, P$. We assume that W is periodic in Ω. The function W at time step n is denoted by W^n.

The time derivative is approximated by a second-order central-difference quotient. For the partial derivatives in space and momentum, the Fourier pseudospectral partial derivatives are applied. We consider the time evolution of the Wigner function for a Hamiltonian function $H(q,p) = T(p) + V(q)$. Thereby $V = V(q) \in L^\infty(-L, L)$ is a real potential and smooth in q and its partial derivatives $\frac{\partial^\nu V}{\partial q^\nu} \in L^\infty(-L, L)$ and $T = T(p) \in L^2(-K, K)$ real.

The LFPS scheme for the truncated WF equation is given by

$$\begin{aligned} \frac{W^{n+1} - W^{n-1}}{2\delta t} &= -\frac{\partial H}{\partial p} D_q W^n + \sum_{\nu=0}^{Q} \frac{(-1)^\nu \hbar^{2\nu}}{2^{2\nu}(2\nu+1)!} \frac{\partial^{2\nu+1} H}{\partial q^{2\nu+1}} D_p^{2\nu+1} W^n, \\ W^0 &= W^0(q,p), \\ W^1 &= W^1(q,p). \end{aligned} \tag{14}$$

We remark that in the case of open quantum systems, additional relaxation and decoherence terms would appear in the truncated version of (8) that can be accommodated in the scheme (14).

Theorem 7 *(Stability). The LFPS scheme (14) is stable in the sense that for all n and $0 < \varepsilon < 1$, we have*

$$\|W^n\|^2 \leq \frac{2-\varepsilon}{\varepsilon} \left(\|W^1\|^2 + \|W^0\|^2 \right),$$

under the condition

$$\delta t \leq \frac{1-\varepsilon}{\| \frac{\mathrm{d}T}{\mathrm{d}p} \|_\infty c_q N + \sum_{\nu=0}^{Q} \hbar^{2\nu} \| \frac{\mathrm{d}^{2\nu+1} V}{\mathrm{d}q^{2\nu+1}} \|_\infty c_{p,\nu} M^{2\nu+1}}. \tag{15}$$

Proof. It is $\frac{\partial H}{\partial p} = \frac{\mathrm{d}T}{\mathrm{d}p}$ and $\frac{\partial^{2\nu+1} H}{\partial q^{2\nu+1}} = \frac{\mathrm{d}^{2\nu+1} V}{\mathrm{d}q^{2\nu+1}}$. Define $\tilde{p} = \frac{\mathrm{d}T}{\mathrm{d}p}$, $\tilde{V}_\nu(q) = \frac{1}{2^{2\nu}(2\nu+1)!}\frac{\mathrm{d}^{2\nu+1}V(q)}{\mathrm{d}q^{2\nu+1}}$, $\nu = 0, \ldots, Q$. Equation (14) can be rewritten in the following form

$$W^{n+1} - W^{n-1} = -2\delta t \tilde{p} D_q W^n + 2\delta t \sum_{\nu=0}^{Q} (-1)^\nu \hbar^{2\nu} \tilde{V}_\nu D_p^{2\nu+1} W^n.$$

Considering the inner product with $W^{n+1} + W^{n-1}$ gives the following

$$\begin{aligned}\|W^{n+1}\|^2 - \|W^{n-1}\|^2 = &-2\delta t(\tilde{p} D_q W^n, W^{n+1} + W^{n-1}) \\ &+2\delta t \sum_{\nu=0}^{Q} (-1)^\nu \hbar^{2\nu} (\tilde{V}_\nu D_p^{2\nu+1} W^n, W^{n+1} + W^{n-1}).\end{aligned}$$

Adding and subtracting $\|W^n\|^2$ and expanding the inner product gives

$$\begin{aligned}\|W^{n+1}\|^2 + \|W^n\|^2 - (\|W^n\|^2 + \|W^{n-1}\|^2) = \\ &- 2\delta t(\tilde{p} D_q W^n, W^{n+1}) - 2\delta t(\tilde{p} D_q W^n, W^{n-1}) \\ &+ 2\delta t \sum_{\nu=0}^{Q} (-1)^\nu \hbar^{2\nu} (\tilde{V}_\nu D_p^{2\nu+1} W^n, W^{n+1}) \\ &+ 2\delta t \sum_{\nu=0}^{Q} (-1)^\nu \hbar^{2\nu} (\tilde{V}_\nu D_p^{2\nu+1} W^n, W^{n-1}).\end{aligned}$$

Define E^n as follows

$$\begin{aligned}E^n :&= \|W^{n+1}\|^2 + \|W^n\|^2 + 2\delta t(\tilde{p} D_q W^n, W^{n+1}) - 2\delta t \sum_{\nu=0}^{Q} (-1)^\nu \hbar^{2\nu} (\tilde{V}_\nu D_p^{2\nu+1} W^n, W^{n+1}) \\ &= \|W^n\|^2 + \|W^{n-1}\|^2 + 2\delta t(\tilde{p} D_q W^{n-1}, W^n) - 2\delta t \sum_{\nu=0}^{Q} (-1)^\nu \hbar^{2\nu} (\tilde{V}_\nu D_p^{2\nu+1} W^{n-1}, W^n) \\ &= E^{n-1},\end{aligned}$$

where Lemma 5 is used. Notice that the recursion $E^n = E^{n-1} = \cdots = E^1 = E^0$ holds. Next, we define $\|V_\nu\|_\infty = \max_{q\in(-L,L)} |(-1)^\nu \tilde{V}_\nu(q)|$, $\nu = 0, \ldots, Q$ and $\|\tilde{p}\| = \max_{p\in(-K,K)} |\tilde{p}|$.

For $0 < \varepsilon < 1$, choose δt such that the following inequality holds

$$\delta t(\|\tilde{p}\|_\infty \|D_q\| + \sum_{\nu=0}^{Q} \hbar^{2\nu} \|V_\nu\|_\infty \|D_p^{2\nu+1}\|) \le (1-\varepsilon).$$

Using the Cauchy-Schwarz inequality, we have

$$\begin{aligned}&|2\delta t((\tilde{p} D_q - \sum_{\nu=0}^{Q} (-1)^\nu \hbar^{2\nu} \tilde{V}_\nu D_p^{2\nu+1}) W^n, W^{n+1})| \\ &\le 2\delta t \|\tilde{p} D_q - \sum_{\nu=0}^{Q} (-1)^\nu \hbar^{2\nu} \tilde{V}_\nu D_p^{2\nu+1}\| \|W^n\| \|W^{n+1}\| \\ &\le 2\delta t(\|\tilde{p}\|_\infty \|D_q\| + \sum_{\nu=0}^{Q} \hbar^{2\nu} \|V_\nu\|_\infty \|D_p^{2\nu+1}\|) \|W^n\| \|W^{n+1}\| \\ &\le 2(1-\varepsilon)\|W^n\| \|W^{n+1}\|.\end{aligned}$$

Using the inequality derived above, we obtain

$$\begin{aligned}E^n &\ge \|W^{n+1}\|^2 + \|W^n\|^2 - 2(1-\varepsilon)\|W^n\| \|W^{n+1}\| \\ &\ge \|W^{n+1}\|^2 + \|W^n\|^2 - (1-\varepsilon)\|W^n\|^2 - (1-\varepsilon)\|W^{n+1}\|^2 \\ &= \varepsilon(\|W^{n+1}\|^2 + \|W^n\|^2).\end{aligned}$$

This leads to the following

$$
\begin{aligned}
\|W^{n+1}\|^2 + \|W^n\|^2 \leq \frac{E^n}{\varepsilon} = \frac{E^0}{\varepsilon} \\
&= \frac{1}{\varepsilon}(\|W^1\|^2 + \|W^0\|^2 + 2\delta t((\tilde{p}D_q - \sum_{\nu=0}^{Q}(-1)^\nu \hbar^{2\nu}\tilde{V}_\nu D_p^{2\nu+1})W^0, W^1)) \\
&\leq \frac{1}{\varepsilon}(\|W^1\|^2 + \|W^0\|^2 + 2(1-\varepsilon)\|W^0\|\|W^1\|) \\
&\leq \frac{1}{\varepsilon}(\|W^1\|^2 + \|W^0\|^2 + (1-\varepsilon)\|W^0\|^2 + (1-\varepsilon)\|W^1\|^2 \\
&\leq \frac{2-\varepsilon}{\varepsilon}(\|W^0\|^2 + \|W^1\|^2).
\end{aligned}
$$

Using Lemma 6, the stability result is obtained under the constraint that δt satisfies the following condition

$$
\delta t \leq \frac{1-\varepsilon}{\|\frac{\mathrm{d}T}{\mathrm{d}p}\|_\infty c_q N + \sum_{\nu=0}^{Q} \hbar^{2\nu}\|\frac{\mathrm{d}^{2\nu+1}V}{\mathrm{d}q^{2\nu+1}}\|_\infty c_{p,\nu} M^{2\nu+1}},
$$

where $c_{p,\nu} = \frac{c}{2^{2\nu}(2\nu+1)!}$, where c is a positive constant from the estimate in Lemma 6. □

From the result of Theorem 7, we conclude that the LFPS scheme is conditionally stable and we see that the restriction to the time-step size depends on N, M and on $\hbar$.

Remark 8 *(Classical limit)* We remark that the stability condition (15) on the time-step size allows to analyse the classical limit $\hbar \to 0$.

Remark 9 *(Extension to d dimensions).* The pseudospectral framework can be extended to several dimensions. Let $\Omega = (-L, L)^d \times (-K, K)^d \subseteq \mathbb{R}^d \times \mathbb{R}^d$, and consider $(\mathbf{q}, \mathbf{p}) = ((q_1, \cdots, q_d), (p_1, \cdots, p_d)) \in \Omega$. Since Ω is the Cartesian product of d copies of the interval $(-L, L) \times (-K, K)$, as an orthogonal system in $L^2(\Omega)$, one can use the tensor product of an orthogonal system in $L^2((-L, L) \times (-K, K))$. We have

$$
\phi_{\mathbf{r},\mathbf{s}}(\mathbf{q}, \mathbf{p}) = \mathrm{e}^{i2\pi\left(\frac{\mathbf{rq}}{2L} + \frac{\mathbf{sp}}{2K}\right)}, \tag{16}
$$

and

$$
S_{N,M} = span\left\{\phi_{\mathbf{r},\mathbf{s}}(\mathbf{q}, \mathbf{p}) | \mathbf{r}_j \in \left\{-\frac{N}{2}+1, \ldots, \frac{N}{2}\right\}, \mathbf{s}_l \in \left\{-\frac{M}{2}+1, \ldots, \frac{M}{2}\right\}\right\}. \tag{17}
$$

With the multi-index notation, that is, $\mathbf{j} = (j_1, \ldots, j_d)$, $\mathbf{r} = (r_1, \ldots, r_d)$, $\mathbf{l} = (l_1, \ldots, l_d)$, $\mathbf{s} = (s_1, \ldots, s_d)$ the interpolation operator is defined as follows

$$
I_{N,M}u(\mathbf{q}, \mathbf{p}) := \sum_{\mathbf{r}=-(N/2-1)}^{N/2} \sum_{\mathbf{s}=-(M/2-1)}^{M/2} \tilde{u}_{\mathbf{r},\mathbf{s}}\ \mathrm{e}^{i2\pi(\frac{\mathbf{r}\ \mathbf{q}}{2L} + \frac{\mathbf{s}\ \mathbf{p}}{2K})}, \tag{18}
$$

$$
\tilde{u}_{\mathbf{r},\mathbf{s}} := \frac{1}{M^d N^d} \sum_{\mathbf{j}=1}^{N} \sum_{\mathbf{l}=1}^{M} u(\mathbf{q_j}, \mathbf{p_l})\ \mathrm{e}^{-i2\pi(\frac{\mathbf{r}\ \mathbf{q_j}}{2L} + \frac{\mathbf{s}\ \mathbf{p_l}}{2K})}. \tag{19}
$$

The inner product on the space $S_{N,M}$ is given by

$$
(u, v)_{N,M} = h^d k^d \sum_{\mathbf{j}=1}^{N} \sum_{\mathbf{l}=1}^{M} u(\mathbf{q_j}, \mathbf{p_l})\overline{v(\mathbf{q_j}, \mathbf{p_l})}. \tag{20}
$$

The error estimates for the pseudospectral partial derivatives are given by the following

$$
\|D_q^\nu\| \leq d^{\nu/2} c_{q,\nu} N^\nu \tag{21}
$$

$$
\|D_p^\nu\| \leq d^{\nu/2} c_{p,\nu} M^\nu, \tag{22}
$$

with $c_{q,\nu}$, $c_{p,\nu}$ from Lemma 6. Thus the LFPS scheme is stable under the condition

$$
\delta t \leq \frac{1-\varepsilon}{\|\frac{\mathrm{d}T}{\mathrm{d}p}\|_\infty d^{1/2} c_q N + \sum_{\nu=0}^{Q} \hbar^{2\nu}\|\frac{\mathrm{d}^{2\nu+1}V}{\mathrm{d}q^{2\nu+1}}\|_\infty d^{(2\nu+1)/2} c_{p,\nu} M^{2\nu+1}}, \quad 0 < \varepsilon < 1. \tag{23}
$$

Next, we consider the accuracy of the LFPS scheme. For this purpose, we first have to define the truncation error of this scheme. Denote with W_{jl}^n the solution of the LFPS scheme at the point (q_j, p_l, t_n) and $e_{jl} := W_{jl}^n - \hat{W}_{jl}^n$ the error at each time step between the continuous solution $W(q_j, p_l, t_n)$, denoted by $\hat{W}_{jl}^n$, and the approximate solution W_{jl}^n. The truncation error of the scheme (14) is given by

$$\tau_{jl}^n = D_t \hat{W}_{jl}^n + \left(\frac{\mathrm{d}T}{\mathrm{d}p}\right)_l D_q \hat{W}_{jl}^n - \sum_{\nu=0}^{Q} (-1)^\nu \frac{\hbar^{2\nu}}{2^{2\nu}(2\nu+1)!} \left(\frac{\mathrm{d}^{2\nu+1}V}{\mathrm{d}q^{2\nu+1}}\right)_j D_p^{2\nu+1} \hat{W}_{jl}^n, \tag{24}$$

where $D_t \hat{W}_{jl}^n = (\hat{W}_{jl}^{n+1} - \hat{W}_{jl}^{n-1})/2\delta t$ denotes the central difference quotient.

For the analytical solution at the point (q_j, p_l, t_n) it follows

$$0 = \left(\frac{\partial}{\partial t}\hat{W} + \frac{\mathrm{d}T}{\mathrm{d}p}\frac{\partial}{\partial q}\hat{W} - \sum_{\nu=0}^{Q} (-1)^\nu \frac{\hbar^{2\nu}}{2^{2\nu}(2\nu+1)!} \frac{\mathrm{d}^{2\nu+1}V}{\mathrm{d}q^{2\nu+1}} \frac{\partial^{2\nu+1}}{\partial p^{2\nu+1}}\hat{W} \right)\Big|_{jl}^n. \tag{25}$$

Subtracting equation (25) from equation (24), we have

$$\begin{aligned}\tau_{jl}^n = &\left(D_t \hat{W}_{jl}^n - \frac{\partial}{\partial t}\hat{W}\Big|_{jl}^n \right) + \left(\frac{\mathrm{d}T}{\mathrm{d}p}\right)_l \left(D_q \hat{W}_{jl}^n - \frac{\partial}{\partial q}\hat{W}\Big|_{jl}^n \right) \\ &- \sum_{\nu=0}^{Q} (-1)^\nu \frac{(\hbar)^{2\nu}}{2^{2\nu}(2\nu+1)!} \left(\frac{\mathrm{d}^{2\nu+1}V}{\mathrm{d}q^{2\nu+1}}\right)_j \left(D_p^{2\nu+1} \hat{W}_{jl}^n - \frac{\partial^{2\nu+1}}{\partial p^{2\nu+1}}\hat{W}\Big|_{jl}^n \right).\end{aligned}$$

In order to estimate the truncation error, we need the following approximation properties.

Lemma 10 *Let $\hat{W} \in C^3([0,T]; H^m)$ with $m \geq 2\nu+1$, where $H^m(\Omega)$ is the m-order Sobolev space with periodic boundary conditions. Then the following inequalities hold*

$$\|\frac{\partial \hat{W}}{\partial t} - D_t \hat{W}\| \leq c_0 \delta t^2, \tag{26}$$

$$\|\frac{\partial}{\partial q}\hat{W} - D_q \hat{W}\| \leq c_1 N^{1-m} \|\frac{\partial^m}{\partial q^m}\hat{W}\|, \qquad m \geq 1, \tag{27}$$

$$\|\frac{\partial^{2\nu+1}}{\partial p^{2\nu+1}}\hat{W} - D_p^{2\nu+1}\hat{W}\| \leq \tilde{c}_\nu M^{(2\nu+1)-m} \|\frac{\partial^m}{\partial p^m}\hat{W}\|, \qquad m \geq 2\nu+1, \tag{28}$$

$\nu = 0, \ldots, Q$, $Q \in \mathbb{N}$.

Proof. Assume that $\hat{W} \in C^3([0,T]; L^2(\Omega))$ and from the Taylor expansion, we obtain

$$D_t \hat{W}_{jl}^n = \frac{\partial \hat{W}}{\partial t}\Big|_{jl}^n + \frac{\delta t^2}{2!}\frac{\partial^3 \hat{W}}{\partial t^3}\Big|_{jl}^n + \mathcal{O}(\delta t^3),$$

and hence

$$\|\frac{\partial \hat{W}}{\partial t} - D_t \hat{W}\| \leq \frac{1}{2!}\|\hat{W}\|_{C^3} \delta t^2 = c_0 \delta t^2.$$

The estimates (27) and (28) can be obtained from the Bernstein inverse inequality, see [6]. ∎

With Lemma 10, the norm of the truncation error is estimated by

$$
\begin{aligned}
\|\tau^n\| \leq & \|D_t\hat{W} - \frac{\partial}{\partial t}\hat{W}\| + \|\frac{\mathrm{d}T}{\mathrm{d}p}\left(D_q\hat{W} - \frac{\partial}{\partial q}\hat{W}\right)\| \\
& + \sum_{\nu=0}^{Q}\|\frac{\hbar^{2\nu}}{2^{2\nu}(2\nu+1)!}\frac{\mathrm{d}^{2\nu+1}V}{\mathrm{d}q^{2\nu+1}}\left(D_p^{2\nu+1}\hat{W}_{jl}^n - \frac{\partial^{2\nu+1}}{\partial p^{2\nu+1}}\hat{W}\right)\| \\
\leq & c_0\delta t^2 + c_1\|\frac{\mathrm{d}T}{\mathrm{d}p}\|_\infty N^{1-m}\|\frac{\partial^m}{\partial q^m}\hat{W}\| \\
& + \sum_{\nu=0}^{Q}\tilde{c}_\nu\|\frac{\hbar^{2\nu}}{2^{2\nu}(2\nu+1)!}\frac{\mathrm{d}^{2\nu+1}V}{\mathrm{d}q^{2\nu+1}}\|_\infty M^{(2\nu+1)-m}\|\frac{\partial^m}{\partial p^m}\hat{W}\| \\
\leq & c\left(\delta t^2 + \|\frac{\mathrm{d}T}{\mathrm{d}p}\|_\infty N^{1-m}\|\frac{\partial^m}{\partial q^m}\hat{W}\|\right. \\
& \left. + \sum_{\nu=0}^{Q}\|\frac{\hbar^{2\nu}}{2^{2\nu}(2\nu+1)!}\frac{\mathrm{d}^{2\nu+1}V}{\mathrm{d}q^{2\nu+1}}\|_\infty M^{(2\nu+1)-m}\|\frac{\partial^m}{\partial p^m}\hat{W}\|\right),
\end{aligned}
\tag{29}
$$

with $c = \max\{c_0, c_1, \tilde{c}_0, \ldots, \tilde{c}_Q\}$.

Theorem 11 *(Accuracy). Assume that $\hat{W} \in C^3([0,T]; H^m)$ with $m \geq 2\nu+1$, $\nu = 1, \ldots, Q$, be a solution of (14) and let W_{jl}^n be its LFPS approximation at (q_j, p_l, t_n). Assume that the time-step size satisfies the stability condition of Theorem 7, given by (15). Then there exist constants k_1, k_2 and k_3, such that the following estimate holds*

$$
\|W^n - \hat{W}^n\|^2 \leq \mathrm{e}^{k_1 T}\left[k_2\left(\|W^1 - \hat{W}^1\|^2 + \|W^0 - \hat{W}^0\|^2\right) + k_3 T\left(\delta t^2 + \tilde{C}_{N,M,\hbar}\right)^2\right], \tag{30}
$$

for $n = 2, \ldots, P$, and

$$
\tilde{C}_{N,M,\hbar} := \|\tilde{p}\|_\infty N^{1-m}\|\frac{\partial^m}{\partial q^m}\hat{W}\| + \sum_{\nu=0}^{Q}\hbar^{2\nu}\|V_\nu\|_\infty M^{(2\nu+1)-m}\|\frac{\partial^m}{\partial p^m}\hat{W}\|. \tag{31}
$$

Proof. Analogous to the proof of Theorem 7, define $\tilde{p} = \frac{\mathrm{d}T}{\mathrm{d}p}$, $\tilde{V}_\nu(q) = \frac{1}{2^{2\nu}(2\nu+1)!}\frac{\mathrm{d}^{2\nu+1}V(q)}{\mathrm{d}q^{2\nu+1}}$, $\nu = 0, \ldots, Q$. Set

$$
B^n = \|e^{n+1}\|^2 + \|e^n\|^2 + 2\delta t((-\tilde{p}D_q + \sum_{\nu=0}^{Q}(-1)^\nu\hbar^{2\nu}\tilde{V}_\nu D_p^{2\nu+1})e^n, e^{n+1}).
$$

With the constant $c_{p,\nu} = \frac{c}{2^{2\nu}(2\nu+1)!}$ from the proof of Theorem 7, it follows that

$$
\begin{aligned}
& |2\delta t((-\tilde{p}D_q + \sum_{\nu=0}^{Q}(-1)^\nu\hbar^{2\nu}\tilde{V}_\nu D_p^{2\nu+1})e^n, e^{n+1})| \\
& \leq 2\delta t|((-\tilde{p}D_q + \sum_{\nu=0}^{Q}(-1)^\nu\hbar^{2\nu}\tilde{V}_\nu D_p^{2\nu+1})e^n, e^{n+1})| \\
& \leq 2\delta t\|-\tilde{p}D_q + \sum_{\nu=0}^{Q}(-1)^\nu\hbar^{2\nu}\tilde{V}_\nu D_p^{2\nu+1}\|\|e^n\|\|e^{n+1}\| \\
& \leq 2\delta t(\|\tilde{p}\|_\infty\|D_q\| + \sum_{\nu=0}^{Q}\hbar^{2\nu}\|V_\nu\|_\infty\|D_p^{2\nu+1}\|)\|e^n\|\|e^{n+1}\| \\
& \leq 2\delta t(\|\tilde{p}\|_\infty c_q N + \sum_{\nu=0}^{Q}\hbar^{2\nu}\|V_\nu\|_\infty c_{p,\nu}M^{2\nu+1})\|e^n\|\|e^{n+1}\| \\
& \leq \delta t C_{N,M,\hbar}(\|e^n\|^2 + \|e^{n+1}\|^2),
\end{aligned}
$$

with the constant $C_{N,M,\hbar} := \|\tilde{p}\|_\infty c_q N + \sum_{\nu=0}^{Q} \hbar^{2\nu} \|V_\nu\|_\infty c_{p,\nu} M^{2\nu+1}$, depending on N and powers of M and $\hbar$. Therefore, we have

$$|B^n| \leq (1 + \delta t C_{N,M,\hbar})(\|e^n\|^2 + \|e^{n+1}\|^2).$$

Analogously, it follows that

$$\begin{aligned} B^n &\geq \|e^{n+1}\|^2 + \|e^n\|^2 + 2\delta t((-\tilde{p}D_q + \sum_{\nu=0}^{Q}(-1)^\nu \hbar^{2\nu} \tilde{V}_\nu D_p^{2\nu+1})e^n, e^{n+1}) \\ &\geq (1 - \delta t C_{N,M,\hbar})(\|e^n\|^2 + \|e^{n+1}\|^2). \end{aligned}$$

Since $\delta t\, C_{N,M,\hbar} \leq 1 - \varepsilon < 1$ because of the stability condition (15), B^n is a positive function and we obtain

$$(1 - \delta t C_{N,M,\hbar})(\|e^n\|^2 + \|e^{n+1}\|^2) \leq B^n \leq (1 + \delta t C_{N,M,\hbar})(\|e^n\|^2 + \|e^{n+1}\|^2). \tag{32}$$

We use the relation between the truncation and the solution error given by

$$-\tau_{jl}^n = D_t e_{jl}^n - \tilde{p} D_q e_{jl}^n + \sum_{\nu=0}^{Q}(-1)^\nu \hbar^{2\nu} \tilde{V}_\nu D_p^{2\nu+1} e_{jl}^n. \tag{33}$$

Multiplying (33) by $\overline{e_{jl}^{n+1} + e_{jl}^{n-1}}$ and since $D_t e_{jl}^n = (e_{jl}^{n+1} - e_{jl}^{n-1})/2\delta t$, we have

$$\begin{aligned} -(\tau^n, e^{n+1} + e^{n-1}) =& \frac{1}{2\delta t}(\|e^{n+1}\|^2 - \|e^{n-1}\|^2 + (e^{n+1}, e^{n-1}) - (e^{n-1}, e^{n+1})) \\ &- (\tilde{p} D_q e^n, e^{n+1} + e^{n-1}) + \sum_{\nu=0}^{Q}(-1)^\nu \hbar^{2\nu}(\tilde{V}_\nu D_p^{2\nu+1} e^n, e^{n+1} + e^{n-1}). \end{aligned}$$

Considering the real part multiplied by $2\delta t$ and adding and subtracting $\|e^n\|^2$, we obtain

$$\begin{aligned} &-2\delta t(\tau^n, e^{n+1} + e^{n-1}) \\ &\quad = \|e^{n+1}\|^2 + \|e^n\|^2 - 2\delta t(\tilde{p} D_q e^n, e^{n+1}) + 2\delta t \sum_{\nu=0}^{Q}(-1)^\nu \hbar^{2\nu}(\tilde{V}_\nu D_p^{2\nu+1} e^n, e^{n+1}) \\ &\quad - \left(\|e^n\|^2 + \|e^{n-1}\|^2 - 2\delta t(\tilde{p} D_q e^{n-1}, e^n) + 2\delta t \sum_{\nu=0}^{Q}(-1)^\nu \hbar^{2\nu}(\tilde{V}_\nu D_p^{2\nu+1} e^{n-1}, e^n) \right) \\ &\quad = B^n - B^{n-1}. \end{aligned}$$

Taking repeated sum from 1 to P gives the following result

$$B^P - B^0 = -\sum_{n=1}^{P} 2\delta t(\tau^n, e^{n+1} + e^{n-1}). \tag{34}$$

From this, we have the following

$$\begin{aligned} B^P \leq& B^0 + \sum_{n=1}^{P} 2\delta t|(\tau^n, e^{n+1} + e^{n-1})| \leq B^0 + \delta t \sum_{n=1}^{P} \|\tau^n\|^2 + \|e^{n+1} + e^{n-1}\|^2 \\ \leq& B^0 + \delta t \sum_{n=1}^{P} \|e^{n+1}\|^2 + \|e^{n-1}\|^2 + \delta t \sum_{n=1}^{P} \|\tau^n\| \\ \leq& B^0 + \delta t \sum_{n=1}^{P} \|e^{n+1}\|^2 + \frac{\delta t}{2}(2\|e^0\|^2 + \|e^1\|^2 + \sum_{n=1}^{P} \|e^n\|^2 + \sum_{n=1}^{P} \|e^{n+1}\|^2) + \delta t \sum_{n=1}^{P} \|\tau^n\|^2. \end{aligned}$$

Using the estimate for the truncation error from equation (29), we have

$$
\begin{aligned}
B^P \leq & B^0 + \delta t \sum_{n=1}^{P} \|e^{n+1}\|^2 + \frac{\delta t}{2}(2\|e^0\|^2 + \|e^1\|^2 + \sum_{n=1}^{P} \|e^n\|^2 + \sum_{n=1}^{P} \|e^{n+1}\|^2) \\
& + \sum_{n=1}^{P} \delta t c^2 (\delta t^2 + \|\tilde{p}\|_\infty N^{1-m} \|\frac{\partial^m}{\partial q^m} \hat{W}\| + \sum_{\nu=0}^{Q} \hbar^{2\nu} \|V_\nu\|_\infty M^{(2\nu+1)-m} \|\frac{\partial^m}{\partial p^m} \hat{W}\|)^2 \\
\leq & B^0 + Tc^2(\delta t^2 + \tilde{C}_{N,M,\hbar})^2 + \delta t(\|e^0\|^2 + \|e^1\|^2) \\
& + \frac{3\delta t}{2} \sum_{n=1}^{P} (\|e^n\|^2 + \|e^{n+1}\|^2).
\end{aligned}
$$

With equation (32), this inequality can be rewritten as follows

$$
\begin{aligned}
& (1 - \delta t C_{N,M,\hbar})(\|e^P\|^2 + \|e^{P+1}\|^2) \\
& \qquad \leq (1 + \delta t(1 + C_{N,M,\hbar}))(\|e^0\|^2 + \|e^1\|^2) + Tc^2(\delta t^2 + \tilde{C}_{N,M,\hbar})^2 \\
& \qquad\quad + \frac{3\delta t}{2(1 - \delta t C_{N,M,\hbar})} \sum_{n=1}^{P} (\|e^n\|^2 + \|e^{n+1}\|^2)(1 - \delta t C_{N,M,\hbar}).
\end{aligned}
$$

Applying the Gronwall's inequality, we obtain

$$
\begin{aligned}
& (1 - \delta t C_{N,M,\hbar})(\|e^P\|^2 + \|e^{P+1}\|^2) \\
& \qquad \leq \left[(1 + \delta t(1 + C_{N,M,\hbar}))(\|e^0\|^2 + \|e^1\|^2) + Tc^2(\delta t^2 + \tilde{C}_{N,M,\hbar})^2\right] \\
& \qquad\quad \times \exp\left(\frac{3T}{2(1 - \delta t C_{N,M,\hbar})}\right).
\end{aligned}
$$

Therefore, we have

$$
\|e^P\|^2 \leq e^{k_1 T} \left[k_2(\|e^0\|^2 + \|e^1\|^2) + k_3 T \left(\delta t^2 + \tilde{C}_{N,M,\hbar}\right)^2\right], \tag{35}
$$

with

$$
k_1 := \frac{3}{2(1 - \delta t C_{N,M,\hbar})},\ k_2 := \frac{(1 + \delta t(1 + C_{N,M,\hbar}))}{1 - \delta t C_{N,M,\hbar}},\ k_3 := \frac{c^2}{1 - \delta t C_{N,M,\hbar}}.
$$

□

From estimate (30), we can see that the LFPS scheme provides second-order accuracy in time and spectral accuracy in space.

5 Conservation laws

Among the important properties of the Wigner function are normalization and energy conservation in the phase space. We prove that the LFPS solutions of the WF equation posses the discrete analogues of these properties. The following theorem considers the normalization of the Wigner function.

Theorem 12 *The LFPS scheme (14) preserves the normalization of the Wigner function.*

Proof. Since the discrete inner product coincides with the inner product in L^2 for functions in $S_{N,M}$ and using the notation of the proof of Theorem 11 and Lemma 5, we have

$$\begin{aligned}
hk\sum_{j=1}^{N}\sum_{l=1}^{M}W_{jl}^{n+1} &= (W^{n+1},1)\\
&= (W^{n-1},1) - 2\delta t(\tilde{p}\ D_qW^n,1) + 2\delta t\sum_{\nu=0}^{Q}(-1)^{\nu}\hbar^{2\nu}(\tilde{V}_{\nu}\ D_p^{2\nu+1}W^n,1)\\
&= (W^{n-1},1) - 2\delta t(D_qW^n,\tilde{p}) + 2\delta t\sum_{\nu=0}^{Q}(-1)^{\nu}\hbar^{2\nu}(D_p^{2\nu+1}W^n,\tilde{V}_{\nu})\\
&= (W^{n-1},1) + 2\delta t(W^n,D_q\tilde{p}) - 2\delta t\sum_{\nu=0}^{Q}(-1)^{\nu}\hbar^{2\nu}(W^n,D_p^{2\nu+1}\tilde{V}_{\nu})\\
&= hk\sum_{j=1}^{N}\sum_{l=1}^{M}W_{jl}^{n-1}.
\end{aligned}$$

Since the initial conditions $W^0(q,p)$ and $W^1(q,p)$ are assumed to be normalized over the phase space, and by repetition of the above result, we have

$$\begin{aligned}
hk\sum_{j=1}^{N}\sum_{l=1}^{M}W_{jl}^{n+1} &= hk\sum_{j=1}^{N}\sum_{l=1}^{M}W_{jl}^{0} = 1, \quad \text{if n is odd;}\\
hk\sum_{j=1}^{N}\sum_{l=1}^{M}W_{jl}^{n+1} &= hk\sum_{j=1}^{N}\sum_{l=1}^{M}W_{jl}^{1} = 1, \quad \text{if n is even.}
\end{aligned}$$

□

The energy expectation value in the phase space is calculated according to (2). The LFPS scheme preserves the discrete energy functional, as proven in the following theorem.

Theorem 13 *Let $H(q,p) = \frac{p^2}{2m} + V(q)$ be a Hamilton function on the phase space. Then the LFPS scheme (14) preserves the energy*

$$E = hk\sum_{j=1}^{N}\sum_{l=1}^{M}W_{jl}^{n}\,H(q_j,p_l). \tag{36}$$

Proof. In this proof Lemma 5 is used. We have

$$\begin{aligned}
hk\sum_{j=1}^{N}\sum_{l=1}^{M}W_{jl}^{n+1}\,H(q_j,p_l) &= (W^{n+1},H)\\
&= (W^{n-1},H) - 2\delta t\,(\frac{p}{m}D_qW^n,H) + 2\delta t\sum_{\nu=0}^{Q}(-1)^{\nu}\hbar^{2\nu}\,(\tilde{V}_{\nu}D_p^{2\nu+1}W^n,H)\\
&= (W^{n-1},H) + 2\delta t\,(\frac{p}{m}W^n,D_qH) - 2\delta t\sum_{\nu=0}^{Q}(-1)^{\nu}\hbar^{2\nu}\,(\tilde{V}_{\nu}W^n,D_p^{2\nu+1}H)\\
&= (W^{n-1},H) + 2\delta t\,(\frac{p}{m}W^n,D_qV) - 2\delta t\,(\frac{dV}{\mathrm{d}q}W^n,D_p\frac{p^2}{2m})\\
&= (W^{n-1},H) = hk\sum_{j=1}^{N}\sum_{l=1}^{M}W_{jl}^{n-1}\,H(q_j,p_l).
\end{aligned}$$

Since the initial conditions $W^0(q,p)$ and $W^1(q,p)$ are assumed to result in the same energy and by repetition of the above result, we have

$$\begin{aligned}
(W^{n+1},H) &= (W^0,H) = E, \quad \text{if n is odd;}\\
(W^{n+1},H) &= (W^1,H) = E, \quad \text{if n is even.}
\end{aligned}$$

□

We conclude this section discussing the result of Ehrenfest's theorem in our pseudospectral framework.

In [4], it was proven that a pseudospectral approximation provides an exact counterpart to the commutation relation. Now, consider a function $f \in S_{N,M}$ in phase space. As we have done for the energy, we can define its expectation value as follows

$$\langle f \rangle^n = hk \sum_{j=1}^{N} \sum_{l=1}^{M} W_{jl}^n f_{jl},$$

where $f_{jl} = f(q_j, p_l)$. The leap-frog time derivative of this quantity is given by

$$D_t \langle f \rangle^n = hk \sum_{j=1}^{N} \sum_{l=1}^{M} D_t(W_{jl}^n) f_{jl}$$

Now, we use (14) to obtain

$$\begin{aligned} D_t \langle f \rangle^n &= hk \sum_{j=1}^{N} \sum_{l=1}^{M} \left(-\frac{\partial H}{\partial p} D_q W^n + \frac{\partial H}{\partial q} D_p W^n + \sum_{\nu=1}^{Q} \frac{(-1)^{2\nu} \hbar^{2\nu}}{2^{2\nu}(2\nu+1)!} \frac{\partial^{2\nu+1} H}{\partial q^{2\nu+1}} D^{2\nu+1} W^n \right)_{jl} f_{jl} \\ &= hk \sum_{j=1}^{N} \sum_{l=1}^{M} \left(D_q f \frac{\partial H}{\partial p} - D_p f \frac{\partial H}{\partial q} \right)_{jl} W_{jl}^n \\ &- hk \sum_{j=1}^{N} \sum_{l=1}^{M} \left(\sum_{\nu=1}^{Q} \frac{(-1)^{2\nu} \hbar^{2\nu}}{2^{2\nu}(2\nu+1)!} \frac{\partial^{2\nu+1} H}{\partial q^{2\nu+1}} D_p^{2\nu+1} f \right)_{jl} W_{jl}^n. \end{aligned} \tag{37}$$

For this calculation, we use Lemma 5 and require that $\frac{\partial^{2\nu+1} H}{\partial q^{2\nu+1}}$ does not depend on p. Notice that (37) responds to the continuous evolution equation

$$\langle \dot{f} \rangle = \langle \{\{f, H\}\} \rangle, \tag{38}$$

where $\{\{\cdot,\cdot\}\}$ denotes the Moyal brackets.

Now, in the case of $f(q,p) = q$ and $H(q,p) = \frac{p^2}{2m} + V(q)$, we obtain

$$D_t \langle q \rangle^n = \frac{1}{m} \langle p \rangle, \tag{39}$$

and, with $f(q,p) = p$, we have

$$D_t \langle p \rangle^n = -\left\langle \frac{\partial V(q)}{\partial q} \right\rangle. \tag{40}$$

The results (39) and (40) correspond to the statement of Ehrenfest's Theorem [26].

6 Numerical experiments

In this section, results of numerical experiments are presented to validate our theoretical statements on the computational performance of the LFPS scheme.

We start considering the model of a harmonic oscillator. Correspondingly, we have the following Hamiltonian function

$$H(q,p) = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2.$$

For $V(q) = \frac{m\omega^2}{2m} q^2$, we have $\frac{\mathrm{d}^k V}{\mathrm{d}q^k} = 0,\ k \geq 3$. Therefore, the time evolution of the Wigner function is given by

$$\frac{\partial W}{\partial t} = -\frac{p}{m} \frac{\partial W}{\partial q} + m\omega^2 q \frac{\partial W}{\partial p}. \tag{41}$$

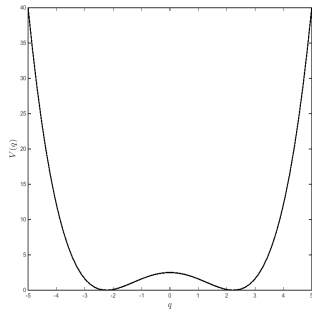

Figure 1: Double well potential, $V(q) = aq^4 - bq^2$ with $a = 1, b = 0.1$.

A solution to (41) is given by the following Wigner function

$$W(q,p,t) = \frac{1}{\pi}\left(2\sqrt{m\omega\hbar}\left(q\cos(\omega_{10}t) - \frac{p}{m\omega}\sin(\omega_{10}t)\right) + \frac{1}{m\omega}p^2 + m\omega q^2\right) \times \mathrm{e}^{-\frac{1}{m\omega\hbar}p^2}\mathrm{e}^{-\frac{m\omega}{\hbar}q^2}, \tag{42}$$

where $w_{10} = (E_1 - E_0)/\hbar$. This function is obtained as a superposition of eigenfunctions of the ground state and of the first excited state of the harmonic oscillator as follows

$$\Psi(q,t) = \frac{1}{\sqrt{2}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(\mathrm{e}^{iE_0t/\hbar} + \left(\frac{m\omega}{\hbar}\right)^{1/2} q\mathrm{e}^{iE_1t/\hbar}\right)\mathrm{e}^{-\frac{m\omega}{2\hbar}q^2}. \tag{43}$$

One can verify that $\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} W(q,p)\mathrm{d}p\mathrm{d}q = 1$ and the energy for the harmonic oscillator is given by $E = (E_0 + E_1)/2 = \hbar\omega$. The expectation value of the energy in phase space can be calculated from $\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} W(q,p)H(q,p)\mathrm{d}p\mathrm{d}q = \hbar\omega$. For the numerical calculation on the domain $\Omega = (-5,5)^2$, we set $m = 1, \hbar = 1$ and $\omega = 1$. As initial conditions for the LFPS scheme, we take $W^0 = W(q,p,-\delta t)$ and $W^1 = W(q,p,0)$.

Further, we consider the WF equation with a quartic symmetric double-well potential. In this case, the Hamiltonian function is given by

$$H(q,p) := \frac{p^2}{2m} + aq^4 - bq^2, \tag{44}$$

with constants $a, b \in \mathbb{R}$. The quartic symmetric double well potential V is illustrated in Figure 1.

With this setting the WF equation is given by

$$\frac{\partial W}{\partial t} = -\frac{p}{m}\frac{\partial W}{\partial q} + \frac{\partial H}{\partial q}\frac{\partial W}{\partial p} - \hbar^2\frac{1}{24}\frac{\partial^3 H}{\partial q^3}\frac{\partial^3 W}{\partial p^3}. \tag{45}$$

As initial condition, we take the Wigner function (42) at $t = -\delta t$ and $t = 0$. Notice that this function is not a solution to the WF equation (45).

We investigate the LFPS accuracy in solving (41) and (45) and report the corresponding results in Figure 2 and 3. In Figure 2, the convergence behaviour of the LFPS scheme depending on the number of points N, M is depicted. In Figure 2 (left), we report the convergence performance of the LFPS scheme, in terms of the L^2 norm of the solution error, in the case of an harmonic potential for which the exact solution (42) is available. In Figure 2 (right), we depict the convergence behaviour with respect to a reference numerical solution W_{ref} computed with a finer discretization ($N, M = 512$, $\delta t = 10^{-7}$). In both cases, we see that as the number of discrete points increases the error decreases showing spectral convergence. In Figure 3, we report results of numerical experiments that show second-order convergence in time.

As discussed in Section 5, the LFPS scheme provides conservation of normalization of the Wigner function in the phase space. In Table 1 the normalization error is computed at different time steps in the time interval $[0,1]$ for the harmonic setting. In the same table, we verify that the LFPS scheme also preserves the energy with high accuracy.

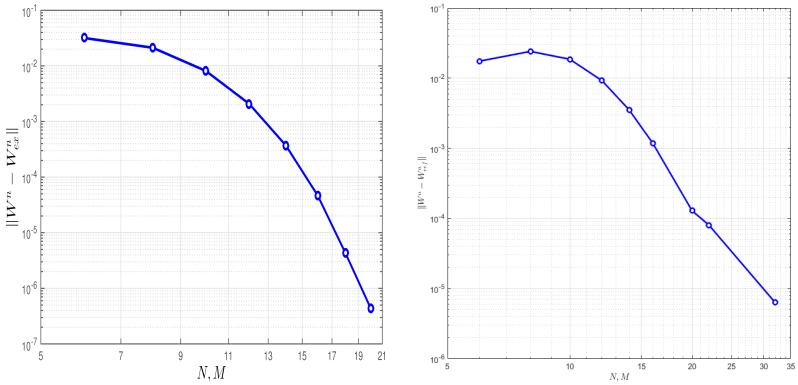

Figure 2: Convergence behaviour of the LFPS scheme depending on N, M with $T = 0.1$ and $\delta t = 10^{-4}$ when solving (41) (left) and $\delta t = 10^{-7}$ for solving (45) (right).

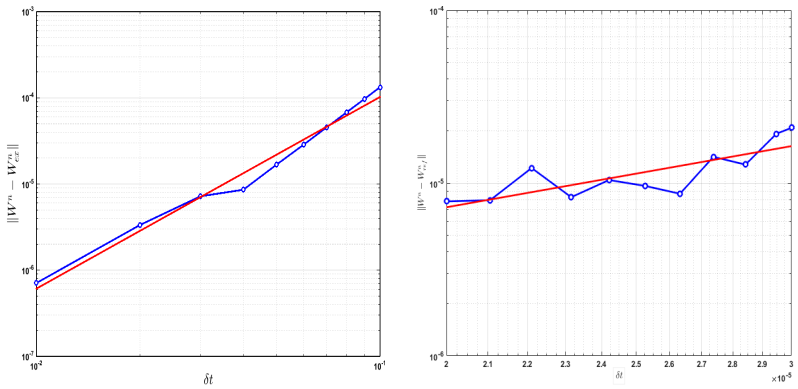

Figure 3: Convergence behaviour of the LFPS scheme depending on δt with $T = 0.1$ and $N, M = 128$ for (41) (left, comparison with W_{ex}) and for (45) (right, comparison with W_{ref}). The red graph (straight line) is the best-fit line with a slope of 2.2240 for (41) and 2.0087 for (45).

t	$(\eta_{cl} - \eta^0_{cl})/\eta^0_{cl}$	$(E_{cl} - E^0_{cl})/E^0_{cl}$
0.1	$1.7837842317 \cdot 10^{-11}$	$1.9428413970 \cdot 10^{-10}$
0.2	$1.2325278577 \cdot 10^{-9}$	$1.0876361904 \cdot 10^{-8}$
0.3	$1.0154207365 \cdot 10^{-8}$	$7.3865939221 \cdot 10^{-8}$
0.4	$1.0154207365 \cdot 10^{-8}$	$7.3865939221 \cdot 10^{-8}$
0.5	$3.0154873380 \cdot 10^{-8}$	$1.8665803360 \cdot 10^{-7}$
0.6	$9.6998593616 \cdot 10^{-9}$	$7.1202841409 \cdot 10^{-8}$
0.7	$1.4544413453 \cdot 10^{-9}$	$2.7312704559 \cdot 10^{-8}$
0.8	$8.6312501603 \cdot 10^{-10}$	$2.3517853277 \cdot 10^{-8}$
0.9	$2.3803289343 \cdot 10^{-9}$	$4.1091949695 \cdot 10^{-8}$
1.0	$4.7128412291 \cdot 10^{-9}$	$4.2260307692 \cdot 10^{-8}$

Table 1: Relative error values with respect to the initial value for normalization $\eta_{cl} := \int W_{cl} \mathrm{d}p\mathrm{d}q$ and energy E_{cl} for (41) with $\delta t = 10^{-4}$ and $N, M = 128$.

In Table 2, we report the error relative to normalization and conservation of energy for the case with quartic potential and $\hbar = 1$. In this case, the Wigner function has higher oscillation than the solution corresponding to the harmonic case and therefore larger numerical errors affect the computation of the integrals. On the other hand, we see that these errors are relatively small and do not grow with time.

The influence of the quantum mechanical perturbation on the classical model is considered in $\Omega = (-5, 5)^2$ with different values of $\hbar = 0, 0.5, 1$. In Figure 4, the LFPS time

t	$(\eta_{qm} - \eta^0_{qm})/\eta^0_{qm}$	$(E_{qm} - E^0_{qm})/E^0_{qm}$
0.5	$8.7695756212 \cdot 10^{-8}$	$1.2692411141 \cdot 10^{-6}$
1.0	$4.6309574109 \cdot 10^{-7}$	$1.4362297706 \cdot 10^{-5}$
1.5	$4.4018099576 \cdot 10^{-7}$	$2.1039245725 \cdot 10^{-5}$
2.0	$4.3262192917 \cdot 10^{-7}$	$1.1219491864 \cdot 10^{-5}$

Table 2: Relative error values with respect to the initial values of normalization $\eta_{qm} = \int W_{qm} \mathrm{d}p\mathrm{d}q$ and energy conservation E_{qm} with $\delta t = 10^{-6}, N, M = 128$ and $\hbar = 1$.

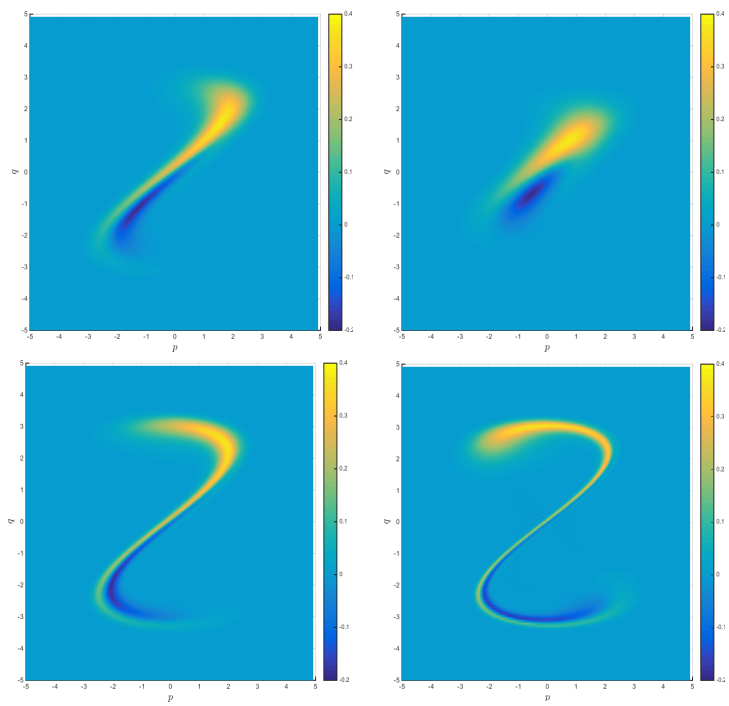

Figure 4: Time evolution of the Wigner function (42) in the classical case with $N, M = 128, \delta t = 10^{-4}$, plotted at $T = 0.5$ (top left), $T = 1.0$ (top right), $T = 1.5$ (bottom left) and $T = 2.0$ (bottom right).

evolution of the Wigner function with quartic potential and $\hbar = 0$ in (45) at $t = 0.5, 1.0, 1.5$ and $t = 2.0$ is depicted. In fact, in this figure no quantum mechanical perturbation effects can be seen.

To better understand this picture, notice that the initial wave function is mostly supported at the well of the potential V, which is at $(0, 0)$. As the time evolves, the wave package begins to spread and moves towards the two minima of the double well potential. After the wave package has passed the minima, the potential increases and thus the wave package is reflected back. The counter clockwise rotation of the Wigner function corresponds to the resulting time evolution of the momentum.

Next, we solve (45) for different non zero values of $\hbar$. The resulting time evolution with quantum mechanical perturbation can be seen in Figures 5 ($\hbar = 0.5$) and 6 ($\hbar = 1$). These snap-shots of the solution are taken at $t = 0.5, 1.0, 1.5, 2.0$. We remark that the quantum mechanical influence is clearly visible. As time progresses, the Wigner function results scattered other than in the $\hbar = 0$ case. Furthermore, we see that the quantum mechanical perturbations decrease with the decrease of $\hbar$, as expected in the classical limit [7].

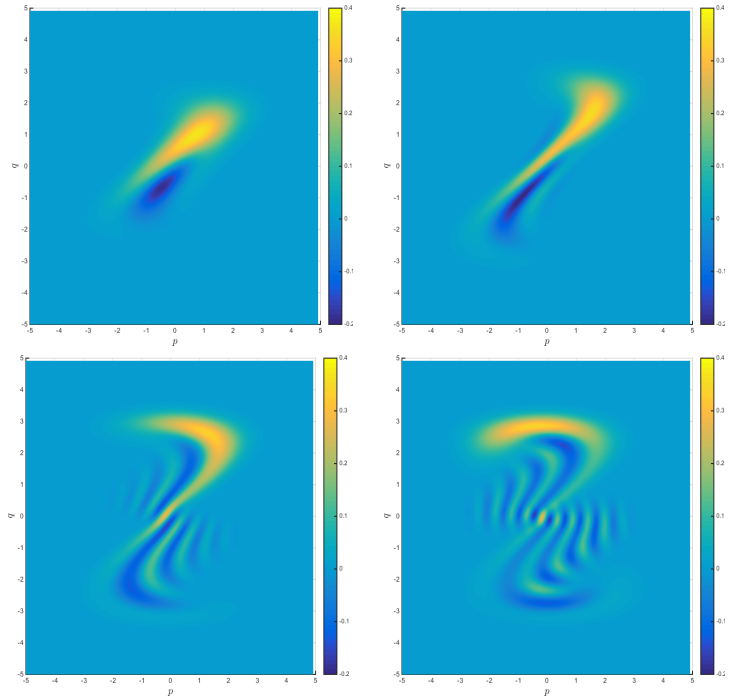

Figure 5: Time evolution of the Wigner function (42) with quantum mechanical perturbation $\hbar = 0.5$ with $N, M = 128, \delta t = 10^{-6}$, plotted at $T = 0.5$ (top left), $T = 1.0$ (top right), $T = 1.5$ (bottom left) and $T = 2.0$ (bottom right).

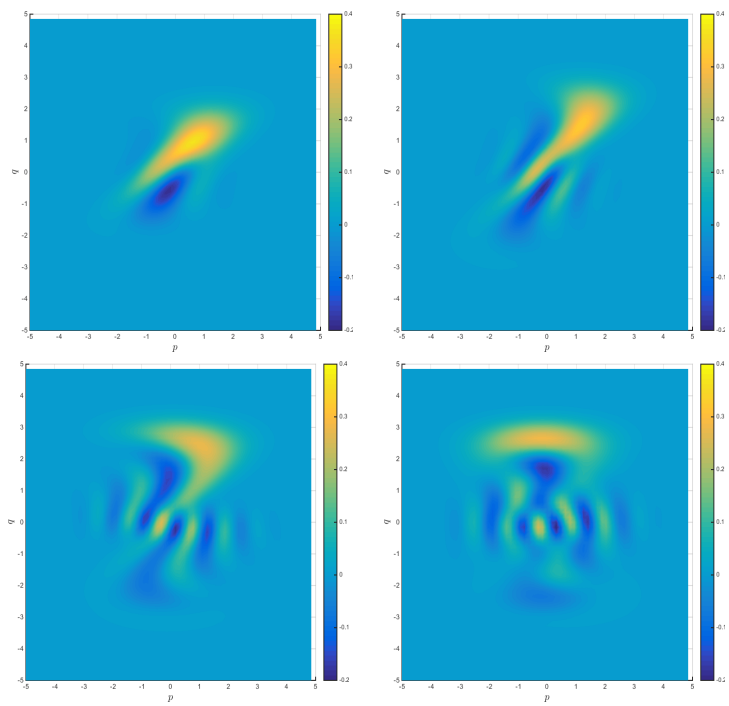

Figure 6: Time evolution of the Wigner function (42) with quantum mechanical perturbation $\hbar = 1$ with $N, M = 64, \delta t = 10^{-6}$, plotted at $T = 0.5$ (top left), $T = 1.0$ (top right), $T = 1.5$ (bottom left) and $T = 2.0$ (bottom right).

7 Conclusion

A numerical analysis of a leap-frog pseudospectral scheme for the time evolution of the Wigner function was presented. The stability of this scheme subject to a stability condition for the time step size was proved. Spectral accuracy in space and second-order accuracy in time were proven, together with the conservation of the normalization and energy values. Results of numerical experiments with different potentials were reported that validated the theoretical findings.

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