
Giovanni Russo\(^a\),* Peter Smereka\(^b\)

\(^a\) Department of Mathematics and Computer Science, University of Catania, Catania, Italy
\(^b\) Department of Mathematics, University of Michigan, Ann Arbor, MI 48109, United States

**Abstract**

A Gaussian wave packet transform is developed for the efficient computation of the semi-classical limit of the multidimensional Schrödinger equation with smooth potential. This transformation, based on Gaussian wave packets, yields a Schrödinger-type equation that is very amenable to numerical solution in the semi-classical limit. The transformed Schrödinger equation is solved with a 4th order splitting method. The wave function can be reconstructed from the transformed wave function whereas some expectation values can easily be evaluated directly. The number of grid points needed per degree of freedom is small enough that computations in dimension of up to 4 or 5 are feasible without the use of any basis thinning procedures.

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1. Introduction

In this paper, we develop an efficient computational approach for the semi-classical limit of the Schrödinger equation in the case of many degrees of freedom. Our approach is based on an extension of the Gaussian Wave Packet Transform developed in Ref. [16] for the one dimensional case. This formulation transforms the Schrödinger equation into another partial differential equation which is much more amenable to computation in the semi-classical limit. This is a challenging problem that has many applications in chemistry (e.g. [17]).

To better understand the computational issues at hand, let us consider the scattering of a Carbon atom of 1 eV from some sort of scattering potential. Ideally we would like to bring the particle in from infinity, have it scatter, and follow it as it moves back out to infinity. Intermolecular forces have ranges on the order of several angstroms, therefore for this problem we would need to consider a computational domain that is at least 10 to 20 angstroms in size.

According to de Broglie, the wavelength of a particle with momentum \( P_0 \) is

\[
\lambda = \frac{h}{P_0},
\]

where \( h \) is Planck’s constant \((h = 6.626 \times 10^{-34} \text{ kg m}^2/\text{sec})\). Now for a free particle, \( P_0 = \sqrt{2mE_0} \) where \( E_0 \) is its energy and \( m \) is its mass. Therefore

\[
\lambda = \frac{h}{\sqrt{2mE_0}}.
\]

The mass of Carbon is \( m = 1.9985 \times 10^{-26} \text{ kg} \) and if we take \( E_0 = 1 \text{ eV} (1.60217 \times 10^{-19} \text{ kg m}^2/\text{sec}^2) \) then

\[
\lambda = 8.24 \times 10^{-12} \text{ m} = 0.0824 \text{ Å}.
\]

* Corresponding author.

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If we wish to compute the scattering problem by directly solving the Schrödinger equation then we will need approximately 10 grid points per wavelength. Therefore for a problem like this on a domain the size of 10 Å one would need at least $10^5$ grid points. This is quite manageable in one and two degree of freedom systems but for 3 or more it becomes prohibitively expensive.

Before we begin the discussion of the results of our paper it is useful to present the dimensionless form that will be used here.

1.1. Dimensionless form of the Schrödinger equation

We start with the Schrödinger equation with one degree of freedom:

$$i\hbar\psi_t = -\frac{\hbar^2}{2m}\psi_{xx} + U(X)\psi.$$  \hspace{1cm} (1)

where $\psi$ is the wave function, $\hbar=h/2\pi$ is the reduced Planck's constant, $m$ is the mass of the particle, and $U(X)$ is the potential energy. We shall let $\Lambda$ denote a length associated to the potential energy. For example, if $U(X)=e^{-X/\alpha}$ then $\Lambda=\alpha$. If $E_0$ is the total energy then $\sqrt{2mE_0}$ is a momentum scale and $T=\Lambda\sqrt{m/(2E_0)}$ is a time scale. The momentum scale is combined with the de Broglie formula to produce a quantum length scale $\lambda=h/\sqrt{2mE_0}$.

Notice that the uncertainty principle tells us

$$\Delta X \Delta P \geq \hbar/2,$$

where $\Delta X$ and $\Delta P$ are the uncertainties in position and momentum respectively. One can nondimensionalize the above relationship by dividing both sides by $\sqrt{2mE_0}$ and $\Lambda$ to obtain

$$\frac{\Delta X}{\Lambda\sqrt{2mE_0}} \frac{\Delta P}{\Delta p} \geq \frac{\hbar}{2\Lambda\sqrt{2mE_0}} \equiv \varepsilon/2,$$  \hspace{1cm} (2)

where $\Delta x$ and $\Delta p$ are the respective dimensionless uncertainties in position and momentum and

$$\varepsilon = \frac{\hbar}{\Lambda\sqrt{2mE_0}}.$$  \hspace{1cm} (3)

This is a dimensionless Planck’s constant. Finally, in view of the definition of the quantum length scale, $\lambda$, $\varepsilon$ can be written as

$$\varepsilon = \frac{\lambda}{2\pi\Lambda}. $$

A typical length scale for an intermolecular potential is about 2 Å. So for 1 eV Carbon atoms we have that $\varepsilon \approx 0.006$ which is small but not negligible.

The dimensionless Planck’s constant defined above also naturally comes out of the Schrödinger equation. To see this we will rescale both space $X=Lx$ and time $\tau=Tt$. The condition

$$1 = \int_{\mathbb{R}^N} |\Psi(X,0)|^2 \, dX = \int_{\mathbb{R}^N} |\psi(x,0)|^2 \, dx$$

suggests to set

$$\Psi(X,\tau) = \psi(x,t)L^{N/2}. $$

Applying the change of variables to (1), and dividing by $2E_0L^{N/2}$, one obtains

$$\frac{i\hbar}{2T' E_0} \psi_t = -\frac{\hbar^2}{4mL^2 E_0} \psi_{xx} + \frac{U(xL)}{2E_0} \psi.$$  \hspace{1cm} (4)

Now we choose

$$T = \Lambda\sqrt{m/(2E_0)} \quad \text{and} \quad L = \Lambda,$$

and find

$$i\varepsilon \psi_t = -\frac{\varepsilon^2}{2} \psi_{xx} + V(x) \psi,$$  \hspace{1cm} (5)

where $V(x) = U(x\Lambda)/(2E_0)$. The dimensionless momentum operator is $\hat{p} = -i\varepsilon \partial_x$. This is the dimensionless form of the Schrödinger equation we shall use in this paper.
1.2. The semi-classical problem

We are interested in problems where the resulting dynamics of the Schrödinger equation are such that the expectations of position and momentum are close to their classical counterparts. To that end, we consider wave packet type initial conditions

\[ \psi(x, 0) = \psi_0(x), \]

with the following properties

1. \( \Delta x = O(\sqrt{\varepsilon}) \),
2. \( \langle E \rangle = \langle \hat{p}^2/2 + V(x) \rangle = O(1) \).

Remarks.

1. The first condition implies, via the uncertainty principle, that \( \Delta p = O(\sqrt{\varepsilon}) \). Therefore this condition is natural if one supposes that the relative uncertainty in position and momentum are of the same order.
2. The second condition guarantees that there is enough energy in the system so that semi-classical behavior will take place.
3. The scaling \( \Delta x = O(\sqrt{\varepsilon}) \) is the same as the one used for a single Gaussian wave packet.
4. There has been considerable work in the semi-classical literature, especially by the applied mathematics community, on WKB type initial conditions for which \( \Delta x = O(1) \), \( \Delta p = O(\varepsilon) \) (e.g. \( \psi(x, 0) = (2\beta/\pi)^{1/4}\exp[-\beta(x-x_0)^2 + ip_0(x-x_0)/\varepsilon] \)). WKB initial data can be incorporated into the Gaussian beam framework by approximating the initial condition as superposition of Gaussian wave packets, each with \( \Delta x = O(\sqrt{\varepsilon}) \) and \( \Delta p = O(\varepsilon) \), using the so-called FBI transform [12,14].
5. It has been established that many important quantities can be computed using wave packet type solutions (e.g. Heller [6] or Tanner [17]).

1.2.1. A wave packet initial condition

A one dimensional version of wave packet initial condition that we shall make use of is

\[ \psi(x, 0) = \left( \frac{2\beta}{\pi \varepsilon} \right)^{1/4} \exp\left[ -\beta(x-x_0)^2/\varepsilon + ip_0(x-x_0)/\varepsilon \right], \tag{5} \]

where \( \beta > 0 \). Notice that, at \( t = 0 \), we have:

1. \( \int_{-\infty}^{\infty} \psi^* \psi \, dx = 1 \).
2. \( \langle x \rangle = x_0 \).
3. \( \langle \hat{p} \rangle = p_0 \).
4. \( \Delta x = (x-x_0)^2 = \frac{1}{2} \varepsilon / \beta \).
5. \( \Delta p = (p-p_0)^2 = \sqrt{\varepsilon} \beta \).
6. \( \Delta x \Delta p = \frac{\varepsilon}{4} \).

1.3. Dimensionless Schrödinger equation in N dimensions

Based on Eq. (4), we shall write the dimensionless Schrödinger equation in \( N \) dimensions in the following form,

\[ \psi_t = \sum_{j=1}^{N} \frac{i\varepsilon}{2m_j} \frac{\partial^2 \psi}{\partial x_j^2} - \frac{i}{\varepsilon} V(x) \psi, \tag{6} \]

where \( \psi = \psi(x, t) \in \mathbb{C} \) is the wave function, \( N \) is the number of degrees of freedom, \( x = (x_1, x_2, \ldots, x_N) \) is the spatial variable, \( t \) is time, \( V(x) \) is the potential (real valued), and \( m_j \) is the dimensionless mass associated with the \( j \)th degree of freedom. It is convenient for our purposes to write Eq. (6) in a slightly different form, namely

\[ \psi_t = \frac{i\varepsilon}{2} \text{Tr}(M^{-1} \nabla \nabla \psi) - \frac{i}{\varepsilon} V(x) \psi \tag{7} \]

where \( M = \text{diag}(m_1, m_2, \ldots, m_N) \) and \( \nabla \nabla \) is the Hessian operator.

We are interested in the case \( \varepsilon \ll 1 \). In this regime the solutions will be highly oscillatory in both space and time on a scale of \( O(\varepsilon) \).
1.4. Previous work

Even in one space dimension, the computation of the semi-classical limit of the Schrödinger equation is a challenging problem and has attracted considerable attention. However in high degree of freedom systems the problem is even more difficult. For this reason, much work in trying to solve the Schrödinger equation in the semi-classical limit has relied on asymptotic approximations, see for example the review by Jin et al. [9]. One of these approaches is formulated with Gaussian wave packets. It is based on the fact that one can construct a Gaussian wave packet solution that is an exact solution of the Schrödinger equation with a harmonic potential [6,4]. That this solution is also accurate, for non-harmonic potentials, when \( \varepsilon \ll 1 \) is the basis for the method of Gaussian beams. There are several papers that developed methods for the computation of the semi-classical limit of the Schrödinger equation using Gaussian beams, see for example [7,8,11,13,14]. However, the error estimates for these methods are asymptotic in nature [9,13] and as such have a small but uncontrollable error for fixed \( \varepsilon \). A more detailed discussion of this issue as well as a more comprehensive discussion of previous work on asymptotic methods can be found in Part 1 of this paper [16].

Recently, Faou, Gradinaru, and Lubich [3] proposed a numerical method based on Hagedorn’s wave packets [5]. The advantage of their approach is that it requires very few modes when \( \varepsilon \ll 1 \), meaning that fairly large dimensional systems \( (N = 12) \) become tractable. Importantly, the error can be controlled by increasing the resolution of the numerical scheme. One drawback of their approach is, quoting from their paper, “...we expect a phase error of order \( (\Delta t)^2 / \varepsilon \). If we compare the absolute values of the two solutions we have only the error of order \( (\Delta t)^2 \) and this is the quantity we plot...”. A large phase error can be quite problematic in quantum mechanics because it means that two wave packets might not interfere correctly.

1.5. Outline

In Part 1 [16] the Gaussian Wave Packet transform for the Schrödinger equation in one space dimension was introduced. This formulation, based on a transformation inspired by Gaussian wave packets, converts the Schrödinger equation into another Schrödinger equation, called the \( w \)-equation, which is much more amenable to be solved in the semi-classical limit. For example, it was shown that for \( \varepsilon = 10^{-3} \), using just 32 modes with this approach is more accurate than the Gaussian wave packet approximation by several orders of magnitude. Furthermore, it was demonstrated that this method is robust as \( \varepsilon \to 0 \). In addition the method is applicable to initial conditions which are not Gaussians.

In this paper, we extend Part 1 [16] to the case of an arbitrary number of dimensions. This is a non-trivial extension. First, we reformulate Heller’s wave packets for the \( N \) dimensional setting; this provides the starting point for the derivation of the Gaussian wave packet transform. By following the ideas exposed in Part 1 [16], we arrive at a transformed version of the Schrödinger equation in \( N \) dimensions. As in the one dimensional case, this new Schrödinger equation is another Schrödinger equation with a time dependent potential – the \( w \)-equation. Our approach relies on the potential having at least two derivatives. This assumption is actually true in several practical physical cases (e.g. [17]); furthermore it has been widely used by many authors in the field of semi-classical approximation, e.g. [3,6,8,11].

However, unlike the one dimensional case, the \( w \)-equation has a time dependent kinetic energy operator. Therefore it is necessary to extend the 4th order splitting method proposed by Chin and Chen [2] to numerically integrate the \( w \)-equation. It is also straightforward and efficient to reconstruct the wave function \( \psi \) from \( w \). Comparisons of the wave function computed from direct simulations of the Schrödinger equation with the reconstructed one show that we can obtain very accurate solutions using a small number of modes when \( \varepsilon \) is small. For example, in two dimensions using 16 modes in each direction we find that the relative error in \( L^2 \) is \( O(10^{-2}) \) for \( \varepsilon = 10^{-3} \) (see Fig. 3). In particular this indicates that a straightforward implementation of our method to 4 or 5 dimensions should be feasible. Indeed, we include an example of two interacting particles, each moving in two space dimensions, meaning the Schrödinger equation must be solved in 4 dimensions. Finally, we mention that we did not observe \( O((\Delta t)^2 / \varepsilon) \) phase errors such as those reported in Ref. [3].

2. Gaussian wave packets in \( N \) dimensions

Heller [6] introduced the approach of solving the semi-classical limit of the Schrödinger equation by representing a solution as sum of Gaussian wave packets. This extends quite nicely to \( N \) degrees of freedom as follows. Let

\[
\psi_G(x, t) = e^{i\theta c / \varepsilon},
\]

where \( \theta c = \xi^TA\xi + p^TA\xi + \gamma(t) \), \( \xi = x - q \), \( A \) is a complex-valued symmetric \( N \times N \) matrix, \( p(t) \in \mathbb{R}^N \), \( q(t) \in \mathbb{R}^N \) and \( \gamma(t) \) is a complex number. \( \Im(\gamma(0)) \) is chosen so that

\[
\int_{\mathbb{R}^N} |\psi(x, 0)|^2 dx = 1.
\]

It will be shown below that (8) is a solution of the Schrödinger equation provided the potential \( V \) is harmonic and
\[ \dot{q} = M^{-1}p, \quad \dot{p} = -\nabla V(q), \quad \dot{\xi} = \frac{i}{\epsilon} \left( \xi^T \dot{A} \xi - 2 \xi^T A \dot{q} + \xi^T \dot{\xi} p - \frac{1}{2} p^T \dot{p} \xi + \gamma \right), \]

and

\[ e^{-i\epsilon/\xi} \frac{\partial}{\partial t} \psi_G = \frac{i}{\epsilon} (\xi^T \dot{A} \xi - 2 \xi^T A \dot{q} + \xi^T \dot{\xi} p - p^T \dot{p} \xi + \gamma). \]

Since

\[ \text{Tr}(M^{-1}(2A\xi + p)(2A\xi + p)^T) = (2A\xi + p)^T M^{-1}(2A\xi + p) \]

we find

\[ e^{-i\epsilon/\xi} \frac{i\epsilon}{2} \text{Tr}(M^{-1} \nabla \nabla \psi_G) = -\left( \text{Tr}(M^{-1} A) + \frac{2i}{\epsilon} \left[ \xi^T A M^{-1} A \xi + \xi^T A M^{-1} p + \frac{1}{4} p^T M^{-1} p \right] \right). \]

This can be established by first showing

\[ e^{-i\epsilon/\xi} \frac{i\epsilon}{2} \text{Tr}(M^{-1} \nabla \nabla \psi_G) = -\left( \text{Tr}(M^{-1} A) + \frac{2i}{\epsilon} \left[ \xi^T A M^{-1} A \xi + \xi^T A M^{-1} p + \frac{1}{4} p^T M^{-1} p \right] \right). \]

Now to guarantee that \( \psi_G \) is a solution, we use Eqs. (13), (15), and (16) in (7) and equate powers of \( \xi \) obtaining

\[ \xi^0: \, \dot{\gamma} - p^T \dot{q} = i \epsilon \text{Tr}(M^{-1} A) - \frac{1}{2} p^T M^{-1} p - V(q), \]

\[ \xi^1: \, \dot{p} - 2A\dot{q} = -2A M^{-1} p - \nabla V(q), \]

\[ \xi^2: \, \dot{A} = -2A M^{-1} A - \frac{1}{2} \nabla \nabla V(q). \]

Things will vanish at each order if (9)–(12) are satisfied.

It should be pointed out that another way of formulating the above calculations is due to Hagedorn [4] and this approach is sometimes called Gaussian beams. For our purposes, Heller’s formulation is more convenient.

### 3. Gaussian wave packet transformation

In this section the Gaussian wave packet transformation for the Schrödinger equation in \( N \) dimensions will be presented. The approach will follow the formulation described in Part 1 [16], however there are some important differences. We begin with the following expression

\[ \psi_W(x, t) = W(\xi, t) e^{i\theta/\epsilon}, \]

where \( \theta = \xi^T A_R \xi + \xi^T p(t) + \gamma_2(t), \xi = x - q, \) and \( A_R \) is real valued symmetric matrix. This should be compared with Eq. (16) in Part 1. As pointed out in Part 1, unless \( A_R \) is purely real the resulting equation for \( W \) will be ill-posed. However, as we shall see, the evolution equation for the complex matrix \( A \) will be the same as for the Gaussian wave packets.

Our plan is to substitute (17) into the Schrödinger equation (7) to find a partial differential equation for \( W \) so that (17) is a solution of (7).

A direct calculation shows that

\[ e^{-i\theta/\epsilon} \frac{i\epsilon}{2} \text{Tr}(M^{-1} \nabla \nabla \psi_W) = -\text{Tr}(M^{-1} A_R W) + \frac{i\epsilon}{2} \text{Tr}(M^{-1} \nabla \nabla W) - \frac{1}{2} (2A_R \xi + p)^T M^{-1} \nabla W - \frac{i}{2\epsilon} (2A_R \xi + p)^T M^{-1} (2A_R \xi + p) W. \]

We will use these expressions later, but for now, motivated by one dimensional formulation of Part 1 [16], we demand that
\begin{align}
\dot{q} & = M^{-1}p, \\
\dot{p} & = -\nabla V(q), \\
\gamma_2 & = \frac{1}{2} B^T M^{-1} p - V(q) + i\epsilon \text{Tr}(M^{-1}A_R), \\
\dot{A} & = -2AM^{-1}A - \frac{1}{2} \nabla \nabla V(q),
\end{align}
where $A = A_R + iA_I$. These equations are very similar to ordinary differential equations derived in Part 1 (see with Eqs. (22)-(25) of Part 1). In fact if one considers the case $N = 1$ and $m_1 = 1$ then Eqs. (20)-(23) will be the same as those in Part 1. Also, notice that these equations are identical to (9)-(12) with the exception of Eq. (22) where $A$ is replaced by $A_R$. In particular, the evolution equation for $A$ is the same.

We substitute (17) into (7), using (18) and (19), while enforcing (20)-(23) to arrive at:
\begin{equation}
W_t = \frac{i\epsilon}{2} \text{Tr}(M^{-1} \nabla \nabla W) - 2\xi^T A_R M^{-1} \nabla W - \frac{i}{\epsilon} (V_2 + 2\xi^T A_I M^{-1} A_I \xi) W, \tag{24}
\end{equation}
where
\begin{equation}
V_2(q, \xi) = V(q + \xi) - V(q) - \xi^T \nabla V(q) - \frac{1}{2} \xi^T \nabla \nabla V(q) \xi. \tag{25}
\end{equation}
Therefore, if $W$ satisfies (24) and if the ordinary differential equations given by (9)-(12) are also satisfied, then (17) is a solution of the Schrödinger equation. Eq. (24) should be compared with Eq. (21) of Part 1.

Now it is useful to make one last change of variables. We let $w(\eta, t) = W(\xi, t)$ where
\begin{equation}
\eta = B\xi/\sqrt{\epsilon}, \tag{26}
\end{equation}
where $B$ is a real-valued $N \times N$ matrix that will be determined below.

An important difference between this derivation and the one in Part 1 is that here there is no advantage in rescaling time. In Part 1, by rescaling time we were able to make the kinetic energy operator time independent. This is not possible in the $N$ dimensional setting and for this reason no rescaling of time will be used. The transformation given by (26) should be compared to Eq. (26) of Part 1.

With the change of variables given by (26) one finds that (24) becomes
\begin{equation}
w_t + (\nabla_\eta w)^T B \nabla^{-1}_B \eta + 2(\nabla_\eta w)^T B M^{-1} A_R B^{-1} \eta = \frac{i}{2} \text{Tr}(M^{-1} B^T \nabla_\eta \nabla_\eta w B) - \frac{i}{\epsilon} U w, \tag{27}
\end{equation}
where
\begin{equation}
U(\eta, t) = 2\epsilon \eta^T B^{-T} A_I M^{-1} A_I B^{-1} \eta + V_2(q, \sqrt{\epsilon} B^{-1} \eta). \tag{28}
\end{equation}
Clearly, if we demand
\begin{equation}
\dot{B} = -2BM^{-1}A_R, \tag{29}
\end{equation}
then the above equation will simplify to
\begin{equation}
w_t = \frac{i}{2} \text{Tr}(M^{-1} B^T \nabla_\eta \nabla_\eta w B) - \frac{i}{\epsilon} U(\eta, t) w. \tag{30}
\end{equation}
It follows from (23) that
\begin{equation}
\dot{A}_I = -2(A_I M^{-1} A_R + A_R M^{-1} A_I). \tag{31}
\end{equation}
Left multiplying Eq. (28) by $B^T$ one has
\begin{equation}
B^T \dot{B} = -2B^T BM^{-1} A_R, \tag{32}
\end{equation}
while taking the transpose and multiplying by $B$ we have
\begin{equation}
\dot{B}^T B = -2A_R M^{-1} B^T B. \tag{33}
\end{equation}
Summing up the two equations one obtains
\begin{equation}
\frac{d}{dt}(B^T B) = -2(B^T BM^{-1} A_R + A_R M^{-1} B^T B), \tag{34}
\end{equation}
i.e. $B^T B$ satisfies the same Eq. (30) as $A_I$. This implies that if we take $B(0) = \sqrt{A_I(0)}$ then

$$A_I = B^T B \quad \text{for all } t \geq 0.$$  

(32)

The reader should note that even though $B(0)$ is symmetric, $B(t)$ will not necessarily be. In particular, if $B(0)$ and $A_R(0)$ do not commute then $B(t)$ will not be symmetric for $t > 0$. In addition, we point out that $A_I$ is positive definite for all $t > 0$ (e.g. Ralston [15]) which means that $B$ must be invertible. Eq. (32) further implies that we can rewrite $U$ as

$$U(\eta, t) = 2\epsilon \eta^T B M^{-1} B^T \epsilon + V_2(q, \sqrt{\epsilon} B^{-1} \eta).$$  

(33)

We shall refer to Eq. (29) with $U$ defined by (33) as the w-equation. Eq. (29) is comparable with Eq. (27) of Part 1. It should be noted, however, that the kinetic energy operator of the w-equation is now time dependent unlike the one dimensional case.

The linear transformation (26) induced by matrix $B$, together with the time-dependent kinetic energy appearing in the w-equation (29), make the extension from one to several degrees of freedom non-trivial; for example this requires, among other things, a generalization of the original Chin and Chen fourth order splitting scheme (see Section 4.1.2).

It is our assertion, that in the semi-classical limit it is extremely efficient to solve the $w$-equation and then reconstruct $\psi$ from $w$. This assertion was verified in one dimension in Part 1 [16]. In Section 5 we shall establish that this formulation also works in higher dimensions as well. But before we do that, several other issues need to be addressed, the first one being how the initial conditions for $w$ are determined.

3.1. Initial conditions

In this paper we use Gaussian wave packet initial conditions which take the form

$$\psi(x, 0) = e^{-\xi^T C_I \xi / \sqrt{\epsilon}} e^{i(\xi^T C_R \xi + \xi^T p_0 + \delta) / \sqrt{\epsilon}},$$  

(34)

where $\xi = x - x_0$, $C_I$ is a symmetric positive definite matrix, $C_R$ is a symmetric matrix and $\delta$ is complex with $\text{Im}(\delta)$ chosen so that

$$\int_{\mathbb{R}^N} |\psi(x, t)|^2 dx = 1.$$  

Then, it follows from (17) and (26) that the initial condition for $w$ is given by

$$w(\eta, 0) = e^{-\eta^T B^{-T}(0) C_I B^{-1}(0) \eta}.$$  

Consequently, if we choose $B(0) = \sqrt{C_I}$ then

$$w(\eta, 0) = e^{-\eta^T \eta}.$$  

(35)

Recall that $C_I$ is symmetric and positive definite and so $B(0)$ is well defined. An important point should be made here: (35) is the initial condition for the $w$-equation for any Gaussian wave packet initial condition for the Schrödinger equation.

To summarize, we have shown that if we solve (29) with the initial conditions given by (35) and the system of o.d.e.s. given by (20)–(23) and (28) with initial conditions given by

$$q(0) = x_0, \quad p(0) = p_0, \quad \gamma_2(0) = \delta, \quad A(0) = C_R + iC_I, \quad \text{and} \quad B(0) = \sqrt{C_I},$$

then

$$\psi(x, t) = w(B\xi / \sqrt{\epsilon}, t) \exp\left[ (i / \sqrt{\epsilon}) \theta(x, t) \right],$$  

(36)

where $\psi$ is the solution of (7) with initial data given by (34), and

$$\xi = x - q(t) \quad \text{and} \quad \theta = \xi^T A_R \xi + \xi^T p(t) + \gamma_2(t).$$  

(37)

3.1.1. More general initial data

Even though we will only be considering Gaussian wave packet initial conditions in this paper, it is worth mentioning that our approach easily extends to initial conditions that are not necessarily Gaussian. In particular, we can consider initial conditions of the form

$$\psi(x, 0) = f(x - q_0) \exp\left( (i / \sqrt{\epsilon}) [g(x - q_0) + (x - q_0)^T p_0 + \delta] \right),$$  

(38)

where $f(x)$ and $g(x)$ are complex valued smooth functions with $g(0) = \nabla g(0) = 0$ and $\int_{-\infty}^{\infty} |\psi(x, 0)|^2 dx = 1$. It is convenient to define $C = C_R + iC_I = \frac{1}{2} \nabla \nabla g(0)$. We demand that $C_I$ is a symmetric positive definite matrix. The initial condition for (29) is then

\[ w(\eta, 0) = f(x - q_0) \exp\left[ \frac{i}{\varepsilon} \left( g(x - q_0) - (x - q_0)^T C_R(x - q_0) \right) \right], \tag{39} \]

where \( x - q_0 = \sqrt{\varepsilon} B^{-1} \eta \). The initial conditions for the system (20)–(23), (28) are

\[ q(0) = q_0, \quad p(0) = p_0, \quad \gamma_2(0) = \delta, \quad A(0) = C_R + i C_I \quad \text{and} \quad B(0) = \sqrt{C_I}. \]

This aspect was discussed in more detail in Part 1 [16].

3.2. Connection with Gaussian wave packets

In this part, we show that if the potential is harmonic and if the initial condition for Eq. (29) is a Gaussian then one recovers (8). Since \( V \) is harmonic, then (29) becomes

\[ w_t = \frac{i}{2} \text{Tr}(M^{-1} B^T \nabla_\eta \nabla_\eta wB) - 2i \eta^T BM^{-1} B^T \eta w. \tag{40} \]

Suppose now we take for initial data

\[ w(\eta, 0) = e^{-\eta^T \eta}. \tag{41} \]

Then it follows, from a direct calculation, that

\[ w(\eta, t) = w_{GB} \equiv \exp\left( -\eta^T \eta - i \int_0^t \text{Tr}(M^{-1} A_I(s)) \, ds \right) \tag{42} \]

takes (40). It follows from (31) and (32) that \( B^{-T} A_I B^{-1} = I \) so we can write

\[ -\eta^T \eta = -\eta^T B^{-T} A_I B^{-1} \eta = -\xi^T A_I \xi / \varepsilon. \]

So

\[ w(\eta, t) = W(\xi, t) = \exp\left( -\xi^T A_I \xi / \varepsilon - i \int_0^t \text{Tr}(M^{-1} A_I(s)) \, ds \right), \]

therefore

\[ \psi_W = \exp\left( \frac{i}{\varepsilon} \left[ \xi^T A_I \xi + \xi^T p + \gamma_2 - \varepsilon \int_0^t \text{Tr}(M^{-1} A_I(s)) \, ds \right] \right). \]

It follows from (11) and (22) that

\[ \frac{d}{dt}(\gamma - \gamma_2) = -\varepsilon \text{Tr}(M^{-1} A_I), \]

consequently we have

\[ \psi_W = \exp\left( \frac{i}{\varepsilon} \left[ \xi^T A_I \xi + \xi^T p + \gamma \right] \right), \]

which is the Gaussian wave packet given by (8).

3.3. Calculation of expectation values

An important aspect of this work is that expectation values can be computed directly from \( w \). Here we present the calculation of the expectation value of position and momentum. These quantities are defined as

\[ \langle x \rangle = \int x \psi^* \psi \, dx \quad \text{and} \quad \langle \hat{p} \rangle = -\int i \varepsilon \psi^* \partial_x \psi \, dx. \]

Next, one applies (26) and (36) to find

\[ \langle x \rangle = q(t) + z B^{-1} \int \eta w^* w \, d\eta, \tag{43} \]

where
\[ z = \frac{\xi^{n+1}}{|B|} e^{-2 \text{Im}(\gamma_2)/\varepsilon} \]

and \( |B| \) denotes the determinant of \( B \). One can also show

\[ \langle (x - q)(x - q)^T \rangle = z \sqrt{\varepsilon} B^{-1} \int |w|^2 \eta \eta^T d\eta B^{-T}. \]

The uncertainty, \( \Delta x \), is the symmetric \( N \times N \) matrix given by

\[ (\Delta x)^2 = \langle (x - \langle x \rangle)(x - \langle x \rangle)^T \rangle = \langle (x - q)(x - q)^T \rangle - \langle x - q \rangle \langle x - q \rangle^T, \]

which can be evaluated using the expressions immediately above. In a similar way one can show

\[ \langle \hat{p} \rangle = p(t) + 2z A_R B^{-1} \int \eta w^* w d\eta - i z B^T \int w^* w \eta d\eta. \]

One can use these formulas to compute the expectation values for the Gaussian wave packet solution by substituting (42) for \( w \). One finds

\[ \langle x \rangle_G = q(t), \quad \langle \hat{p} \rangle_G = p(t), \quad \text{and} \quad (\Delta x_G)^2 = \frac{1}{4} \xi A^{-1}. \]

4. Numerical implementation

In this section we describe the numerical implementation and error estimation. The computational complexity of our implementation can be understood from the discussion given in Part 1 [16]. The only difference is that now the \( w \)-equation is solved in \( N \) dimensions rather than in one dimension.

4.1. Transformed Schrödinger equation

The main issue of this formulation is the numerical solution of the \( w \)-equation (29). The algorithm we use is based on a fourth order operator splitting method proposed by Chin and Chen [1,2] for the Schrödinger equation with both stationary [1] and time dependent potentials [2]. Our choice is motivated by the excellent accuracy properties of these methods. Here we extend them to the case in which the kinetic energy is time dependent. For the convenience of the reader, we will briefly summarize their work.

4.1.1. 4th order scheme for time independent potential

We write (7) in the form

\[ \psi_t = (T + \mathcal{V}) \psi, \]

where \( T \psi = (i\varepsilon/2) \text{Tr}(M^{-1} \nabla \nabla \psi) \) and \( \mathcal{V} = -i V(x)/\varepsilon \).

Chin and Chen [1] introduce and analyze the following splitting scheme for (7).

\[ \psi^{n+1} = e^{\xi \Delta t \mathcal{V}} e^{\frac{\Delta t^2}{48} \nabla \nabla (V(x))} e^{\frac{\Delta t^2}{48} \nabla \nabla (V(x))} e^{\frac{\Delta t^2}{48} \nabla \nabla (V(x))} \psi^n, \]

where

\[ C = \frac{-i}{\varepsilon} \left( V(x) - \frac{\Delta t^2}{48} |\nabla \nabla (V(x))|^2 \right). \]

In Part 1 [16] we proved that the local truncation error of this method is \( O(\Delta t^5/\varepsilon) \).

4.1.2. A 4th order scheme for a time dependent potential

Chin and Chen [2] also show how to extend (47) to the case of time dependent potentials. In this case the operators \( \mathcal{V} \) and \( C \) depend on time, and the fourth order splitting scheme takes the form

\[ \psi^{n+1} = e^{\xi \Delta t \mathcal{V}(t_n+1)} e^{\frac{\Delta t^2}{48} \nabla \nabla (V(x))} e^{\frac{\Delta t^2}{48} \nabla \nabla (V(x))} e^{\frac{\Delta t^2}{48} \nabla \nabla (V(x))} \psi^n. \]
4.1.3. A 4th order scheme for Eq. (29)

For the \( w \)-equation the kinetic energy operator \( T \) depends on time, so the method developed in [2] cannot be directly applied. However, because of the particular structure of the time dependence of the operator \( T \), the method can be extended to this case. Consider the kinetic energy part of \( (29) \) with initial data specified at time \( t_0 \), namely,

\[
v_t = (i/2) \text{Tr} \left[ \begin{array}{c} M^{-1} B(t) \end{array} \right] v B(t) \quad \text{with} \quad v(t, t_0) = v_0(t).
\]

We write \( B(t) \) here instead of \( B \) to emphasize that the kinetic energy operator is time dependent because of this term. For our purposes it is useful to introduce the solution operator \( S \) associated to Eq. (49), defined through

\[
v(t, t_0) = S(t, t_0)v_0(t).
\]

We propose to modify scheme (48) for Eq. (29) as

\[
w_{n+1} = e^\Delta t \mathcal{V}(t_{n+1}) S(\Delta t/2, t_n + \Delta t/2) e^\Delta t \mathcal{C}(t_n + \Delta t/2) S(\Delta t/2, t_n) e^\Delta t \mathcal{V}(t_n) w_n,
\]

where \( \mathcal{V} \) is now \(-iU(\eta, t)/\varepsilon \) and

\[
C = -i \varepsilon \left( U - \frac{\Delta t^2}{48} B^T \nabla \eta U \cdot B^T \nabla \eta U \right).
\]

The operator \( S(t, t_0) \) can be easily and efficiently computed using Fourier transforms. In Fourier space Eq. (49) becomes

\[
\hat{v}_t = -\frac{i}{2} k^T B(t) M^{-1} B^T(t) k \hat{v},
\]

where \( k \in \mathbb{R}^N \) is the wave number. It is worth noticing that in \( k \)-space the factor multiplying \( \hat{v} \) is a scalar quantity which means

\[
\hat{v}(t + \Delta t) = \exp \left( -\frac{i}{2} \int_{t}^{t+\Delta t} k^T B(s) M^{-1} B^T(s) k ds \right) \hat{v}(t).
\]

One then applies the inverse Fourier transform to find \( S(\Delta t, t) v(\eta, t) \). The integrals contained in (51) are approximated by Simpson’s rule, which appears to be sufficiently accurate. Numerical experiments suggest that the method is 4th order in time, but we have no proof.

We solve (29) using the algorithm given by Eq. (50) with initial conditions given by (35) in the domain \( \eta \in [-\frac{\pi}{2}, \frac{\pi}{2}]^N \). We pick \( \sigma \) to be large enough so that the numerical support of the solution is well inside the computational domain, in this way the use of periodic boundary conditions incurs only a very small error. We use \( \tilde{m} \) grid points in each direction. This yields a solution for \( w \) at the points \( \eta_j = j \sigma / \tilde{m} \), denoted as \( w(\eta_j) \) where the multi-index \( j = (j_1, j_2, \ldots, j_N) \) with \( j_\ell = \left(-\frac{\tilde{m}}{2}, -\frac{\tilde{m}}{2}, \ldots, \frac{\tilde{m}}{2} - 1 \right) \) for \( \ell = 1, 2, \ldots, N \). We let \( \Delta t \) denote the time step.

The o.d.e. system given by (20)-(23), (28) is solved using a 4th order Runge-Kutta scheme with a time step \( \Delta t/40 \). We remark that due to the presence of the \( \varepsilon^{-1} \) terms in the expression given by (36) it is crucial to compute this o.d.e. system with a very small time step to achieve the necessary accuracy.

4.1.4. Verification of 4th order accuracy in time

To verify the accuracy of the algorithm given by Eq. (50) we will solve the \( w \)-equation in the case of a harmonic potential, since we know that \( w_{GB} \) in Eq. (42) is an exact solution in this case. We will consider an example in 4 dimensions with the potential

\[
V(x) = \frac{1}{2} x^T A_p x \quad \text{where} \quad A_p = \begin{pmatrix} 1.0 & 0.2 & 0.2 & 0.2 \\ 0.2 & 2.0 & 0.2 & 0.2 \\ 0.2 & 0.2 & 2.0 & 0.2 \\ 0.2 & 0.2 & 0.2 & 3.0 \end{pmatrix}.
\]

We take \( q(0) = (1.3, 0, -1.0)^T \), \( p(0) = (0, 1.3, 0, 1)^T \), and \( A(0) = A_R(0) + iA_I(0) \), where

\[
A_R = \begin{pmatrix} 0 & 0.2 & 0 & 0 \\ 0.2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad A_I = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1.2 & 0 & 0 \\ 0 & 0 & 0.8 & 0.3 \\ 0 & 0 & 0.3 & 1.1 \end{pmatrix}.
\]

The initial condition is given by (41) and the \( L^2 \) relative error, defined by

\[
\frac{\|w - w_{GB}\|_2}{\|w_{GB}\|_2}.
\]
is computed at $t = 4$ using $\bar{m} = 32$ and $\sigma = 10$. This choice of $\bar{m}$ ensures that the problem is sufficiently resolved in space so the main source of error is due to time discretization. These errors are tabulated in Table 1. The results clearly show 4th order convergence in time.

4.2. Reconstruction of $\psi$ from $w$

In this section, we describe how to reconstruct the wave function, $\psi$, at any point in space from the numerical values of $w$. To accomplish this task, one must be able to determine $w$ for any point in the $\eta$-space. Because of the smoothness of $w$, this can be easily accomplished with trigonometric interpolation as follows.

We use the Discrete Fourier Transform (DFT)

$$\hat{w}_k = \sum_{j_1 = -\bar{m}/2}^{\bar{m}/2 - 1} \cdots \sum_{j_N = -\bar{m}/2}^{\bar{m}/2 - 1} w(\eta_j) e^{-i2\pi k \eta_j/\sigma},$$

where $k$ is another multi-index defined the same way as $j$, and $w(\eta_j)$ are the computed values of $w$ on the $\eta$ grid. The inverse of the above formula suggests that we define

$$w_{\bar{m}}(\eta) = \frac{1}{m^N} \sum_{k_1 = -\bar{m}/2}^{\bar{m}/2 - 1} \cdots \sum_{k_N = -\bar{m}/2}^{\bar{m}/2 - 1} \hat{w}_k e^{i2\pi k \eta/\sigma}. \quad (52)$$

Indeed, $w_{\bar{m}}(\eta) = w(\eta_j)$. In this way, we can compute values of $w$ for any point $\eta$. To find $\psi$ at any point in physical space we use (36) where $w$ is replaced by $w_{\bar{m}}$. In other words, the wave function reconstructed from the numerical solution of (29) is given by

$$\psi_w(x) = w_{\bar{m}}(B(x - q)/\sqrt{\varepsilon}) e^{i\theta/\varepsilon}, \quad (53)$$

where $\theta$ is defined by Eq. (37).

4.3. “Exact” solution

Direct convergence checks are performed in two space dimensions, i.e. $N = 2$, by comparing the solution obtained from the $w$ equation with a reference solution which is obtained by solving the Schrödinger equation directly using the 4th order algorithm given by Eq. (47). The physical domain is $[-\pi, \pi]^2$ with periodic boundary conditions and we let $\bar{m}_E$ denote the number of grid points used, and so the grid spacing is $\Delta x = 2\pi/\bar{m}_E$. The value of $\bar{m}_E$ is selected large enough so that the highly oscillatory solution is fully resolved to spectral accuracy. The solution is numerically computed for points located in physical space at $x_J = \Delta x J$ where $J = (J_1, J_2, \ldots, J_N)$ is a multi-index with $J_\ell \in [-\bar{m}/2, -\bar{m}/2 + 1, \ldots, \bar{m}/2 - 1]$ for $\ell = 1, 2, \ldots, N$. The time step for the reference solution is chosen in such a way to fully resolve the oscillatory behavior. For example, for $\varepsilon = 10^{-3}$, we choose $\Delta t = 0.01$. We shall denote this benchmark solution as the “exact” solution.

4.4. Error evaluation

The locations in physical space corresponding to the computational points in $\eta$-space are given by

$$x_J = q(t) + \sqrt{\varepsilon} B^{-1} \eta_J.$$ 

Let $x^\text{max}$ and $x^\text{min}$ denote the maximum and minimum values of $x$ in the $\ell$th coordinate. We now take $\mu_\ell = \max(x^\text{min} / \Delta x)$ and $v_\ell = \int(x^\text{max} / \Delta x)$. The $L^2$ relative error is then defined as

$$\text{Error}^2 = \frac{\sum_{J_1 = \mu_1}^{v_1} \cdots \sum_{J_N = \mu_N}^{v_N} S(x_J) |\psi(x_J) - \psi_w(x_J)|^2}{\sum_{J_1 = \mu_1}^{v_1} \cdots \sum_{J_N = \mu_N}^{v_N} S(x_J) |\psi(x_J)|^2}, \quad (54)$$
Part 1 of this paper and can be attributed to phase error (see Fig. 6 of Ref. [54]). The error by increasing the number of grid points used. A significant feature demonstrated by these numerical results is that our method is able to provide accurate solutions with a small number of grid points. More importantly, we are able to reduce each test case both \( m_j \) and \( \sigma_j \) are varied allowing us to establish convergence of the numerical method. As we shall see, our method is able to provide accurate solutions with a small number of grid points. More importantly, we are able to reduce the error by increasing the number of grid points used. A significant feature demonstrated by these numerical results is that error (54) of the Gaussian wave packet grows quite rapidly. This behavior was also observed in one space dimension in Ref. [3]. In a similar way, we make a comparison with the Gaussian wave packet approximation, \( \psi_G \), obtained by solving the system (9)–(12) and using expression (8).

5. Numerical tests

In this section we shall evaluate the performance of our formulation. In the first part we will consider \( N = 2 \) and compare our results with a very accurate direct computation of the Schrödinger equation. Two examples from Ref. [3] are used. Finally, we consider an example with \( N = 4 \). Here it is not possible to compare with a direct simulation of the Schrödinger equation since this would require approximately \( 6 \times 10^{11} \) grid points for \( \varepsilon = 10^{-2} \). Instead we establish, by looking at moments of \( w \), that our method is converging. In the results below, we shall take mass \( m_j = 1 \) for all \( j \).

5.1. Direct comparison with Schrödinger equation

We consider a domain \(( x_1, x_2 ) \in [ -\pi, \pi ]^2 \) with periodic boundary conditions. We take the initial condition of the form

\[
\psi_0 = \exp\left[ (i(x - q_0)^T A (x - q_0) + ip_0^T (x - q_0) - \delta)/\varepsilon \right].
\]

(55)

where \( \delta \) is chosen so that initial conditions are properly normalized. We chose two tests from §5.1 of Faou et al. [3]. In each case below we plot the time evolution of the relative \( L^2 \) norm of the error for \( \varepsilon = 10^{-2} \) and \( \varepsilon = 10^{-3} \). For each test case both \( m \) and \( \sigma \) are varied allowing us to establish convergence of the numerical method. As we shall see, our method is able to provide accurate solutions with a small number of grid points. More importantly, we are able to reduce the error by increasing the number of grid points used. A significant feature demonstrated by these numerical results is that error (54) of the Gaussian wave packet grows quite rapidly. This behavior was also observed in one space dimension in Part 1 of this paper and can be attributed to phase error (see Fig. 6 of Ref. [16]).

5.1.1. Torsional potential

For the first test case, the potential is given by

\[
V(x_1, x_2) = 2 - \cos x_1 - \cos x_2.
\]

The initial condition is given by (55) with \( A = i \frac{1}{2} \text{diag}(1, 1), q_0 = (1, 0)^T \) and \( p_0 = (0, 0)^T \). The results for \( \varepsilon = 10^{-2} \) and \( \varepsilon = 10^{-3} \) are presented in Figs. 2 and 3 respectively.

5.1.2. Modified Henon–Heiles potential

For the second test case we consider the potential

\[
V(x_1, x_2) = \frac{1}{2}(x_1^2 + x_2^2) + \sigma_x \left( x_1 x_2 - \frac{1}{3} x_2^3 \right) + \frac{1}{16} \sigma_z^2 (x_1^2 + x_2^2)^2.
\]
Fig. 2. The relative $L^2$ error is plotted as function of time for the torsional potential. Here $\epsilon = 10^{-2}$, $\Delta t = 0.02$. The dashed line represents the error of the Gaussian beam. The two numbers in the legend represent the number of modes $\tilde{m}$ used for the $w$-equation and the size of the computational domain, $\sigma$. The "exact" solution used $\tilde{m}_E = 2^9$ modes in each direction.

Fig. 3. The relative $L^2$ error is plotted as function of time for the torsional potential. Here $\epsilon = 10^{-3}$, $\Delta t = 0.01$. The "exact" solution used $\tilde{m}_E = 2^{12}$ modes.

with $\sigma^* = 0.2$. The initial conditions are given by (55) where we take $A = i \text{diag}(0.4465, 1.0416)$, $q = (1.8, 0)^T$ and $p = (0, 1.2)^T$. The results for $\epsilon = 10^{-2}$ and $\epsilon = 10^{-3}$ are presented in Figs. 4 and 5 respectively.

5.2. Further convergence tests

In the section above, we demonstrated that our approach converges to an accurately computed solution of the Schrödinger equation. In higher dimensions this is not feasible, so one must rely on a self-consistent convergence check. In this section, we will fix $\sigma = 16$, increase $\tilde{m}$ and show that $w$ converges. As a measure of error we use the $L^2$ difference of $w$ computed on a grid with $\tilde{m}$ points in each direction and $w$ compared with the results obtained using a $2\tilde{m}$ grid points in each direction. This will be evaluated on a grid with $\tilde{m}$ points in each direction. We write:

$$\text{err}_{\tilde{m}} = \frac{\|w_{\tilde{m}} - w_{2\tilde{m}}\|_2}{\|w_{2\tilde{m}}\|_2}.$$

An example of this convergence check for the Henon–Heiles potential is shown in Table 2. In practice, this convergence test may not be particularly convenient since we have found that it is useful to vary both the number of grid points, $\tilde{m}$, and the size of the domain, $\sigma$. This makes it difficult to compare the computed values of $w$ since the grids for different $\tilde{m}$ are not commensurate. We have found that a useful convergence test is to consider the deviation between classical and quantum values of position and momentum. In particular we have...
Fig. 4. The relative $L^2$ error is plotted as function of time for the Henon–Heiles potential. Here $\varepsilon = 10^{-2}$, $\Delta t = 0.01$. The “exact” solution used $\tilde{m}_E = 2^{10}$ modes.

Fig. 5. The relative $L^2$ error is plotted as function of time for the Henon–Heiles potential. Here $\varepsilon = 10^{-3}$, $\Delta t = 0.01$. The “exact” solution used $\tilde{m}_E = 2^{12}$ modes.

Table 2
Spatial convergence check for the Henon–Heiles example for $\sigma = 16$, $\Delta t = 0.01$, and $\varepsilon = 10^{-2}$. The errors were evaluated at $t = 20$.

<table>
<thead>
<tr>
<th>$\tilde{m}$</th>
<th>$\text{err}_{\tilde{m}}$</th>
<th>Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>$6.202 \times 10^{-4}$</td>
<td>9.6</td>
</tr>
<tr>
<td>64</td>
<td>$8.264 \times 10^{-7}$</td>
<td>9.0</td>
</tr>
<tr>
<td>128</td>
<td>$1.686 \times 10^{-9}$</td>
<td></td>
</tr>
</tbody>
</table>

$$
D_x(t) = \| \langle x \rangle(t) - q(t) \|_2 \quad \text{and} \quad D_p(t) = \| \langle \hat{p} \rangle(t) - p(t) \|_2.
$$

These expressions can be evaluated using (43) and (45). Fig. 6 shows a convergence check for Henon–Heiles potential using these quantities; the results are consistent with those reported in Table 2.

5.3. An example in 4 dimensions

We consider two particles each moving in two dimensions. The position operator for particle 1 is $(x_1, x_2)^T$ whereas the position operator for particle 2 is $(x_3, x_4)^T$. The particles will move within a harmonic potential and interact with each other through a repulsive Gaussian potential. More specifically we take

Fig. 6. The deviation (56) between the classical and quantum position (upper panel) and momentum (lower panel) vs time for two one dimensional particles interacting by the Henon–Heiles potential. In the legend the first number is the value of $\tilde{m}$ while the second is the value of $\sigma$.

Fig. 7. Trajectories of two interacting particles in an external potential in two space dimensions. Red and black identify the two particles. Classical trajectories are represented by continuous line while the trajectories of the expectation values of the position is represented by a dashed line. The contour lines represent the uncertainties, i.e. they are ellipses whose half axis are equal to the square root of the inverse of the eigenvalues of the moment matrix. The right panel represents a zoom of the left panel, that emphasizes the difference between quantum and classical properties. The computation with $32^4$ modes has been used to produce the image. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

$$V(x) = \frac{1}{2}(x_1^2 + x_2^2 + x_3^2 + x_4^2) + K \exp\left[-((x_1 - x_3)^2 + (x_2 - x_4)^2)/2s^2\right],$$

where $K$ is the strength and $s$ is the length scale of the interaction; we have taken $K = 0.5$ and $s = 1$. For initial conditions we will use (55) with $A = i\text{diag}(1, 1, 1)/2, q_0 = (1.05, 0, -1, 0)^T$ and $p = (0, 1.05, 0, 1)^T$. Fig. 7 shows a plot of the trajectory of each particle by making a two dimensional plot of $(\langle x_1 \rangle, \langle x_2 \rangle)$ (particle 1) and $(\langle x_3 \rangle, \langle x_4 \rangle)$ (particle 2). This figure shows that particle 1 initially moves counter-clock-wise whereas particle 2 moves clock-wise. As they approach each other, the strength of the interaction increases and they deviate noticeably from their elliptical trajectory. The simulation continues until $t = 10$, during which time they will have interacted strongly a total of three times. Fig. 8 shows a plot of the magnitude of the deviation of the expectation of position from its classical value as function of time. This is quite interesting since the Gaussian wave packets are not able to compute deviations of the expectation values from classical dynamics, which is a genuine quantum effect. On the other hand, in the semi-classical limit such a deviation is quite small, and very hard to capture with other techniques. The figure also shows a convergence study, which suggests that for this problem 32 modes per direction are sufficient to obtain an accurate solution at least up to time $T = 10$.

6. Summary

In this paper, we have proposed an efficient approach for solving the Schrödinger equation in the semi-classical regime for an arbitrary number of degrees of freedom. The formulation is based on a transformation, inspired by Gaussian wave packets, that maps Schrödinger equation into another Schrödinger equation. This new Schrödinger equation now has both
Fig. 8. Convergence check for the 4 dimensional case of two interacting particles. The deviation of the classical position from the expectation value is plotted as function of time for different resolutions in the upper panel. The lower panel plots the deviation between the classical momentum and its expectation value. In the legend the first number indicates the number of modes per degree of freedom ($\tilde{m}$) while the second number is the size of the domain ($\sigma$) in each direction. The dotted vertical lines correspond to the times in Fig. 7 where the uncertainty is plotted.

a time dependent kinetic energy operator and potential. Nevertheless it proves to be much more amenable to numerical treatment in the semi-classical limit than the original Schrödinger equation, and offers a significant improvement over Gaussian wave packets.

We develop an extension of the 4th order splitting algorithm of Chin & Chen [2] that provides an accurate and efficient technique for the numerical solution of Eq. (29). The algorithm proposed in Ref. [2] allowed for a time dependent potential and our extension allows for a time dependent kinetic energy operator. We have shown that with a small number of modes (16–32) for each degree of freedom we can obtain a fully resolved solution of the Schrödinger equation that is orders of magnitude more accurate than the Gaussian wave packet approximation. Furthermore, we have provided evidence that this method is robust as $\epsilon \to 0$. Detailed comparisons with fully resolved computations of the Schrödinger equation in two dimensions were performed to verify the above assertions.

It has been demonstrated that the original wave function can be easily reconstructed from the transformed wave function. In addition, some expectations can be computed directly from the transformed wave function. The small number of modes needed by this approach means that computations for a moderate number of degrees of freedom are possible. To this end, we considered an example with 4 degrees of freedom, namely two distinguishable particles moving in two dimensions. It should be pointed out that to evolve a single wave packet that has an initial condition given by Eq. (5), it is much faster to compute the evolution with Gaussian wave packets or high order Gaussian wave packets than with the method we propose in this paper. However, it should also be pointed out that using Gaussian wave packets one incurs an uncontrollable error for a fixed value of $\epsilon$ because of the asymptotic nature of that approach. With the method outlined here, no such error exists since we are solving the Schrödinger equation (in a different form). These issues are discussed, in depth, in Part 1 [16].

Future work will involve the development and application of various approaches to further reduce the number of modes needed and thereby allowing one to study systems with more degrees of freedom. One possible line of attack is the application of basis thinning approaches such as the hyperbolic cross approximation.

In addition, the Schrödinger equation shares some similarities to the Helmholtz equation which has been tackled using Eulerian Gaussian beams [10]. It may be possible to apply our approach in that setting as well.

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