Solving the Quantum Many-Body Problem with Bohmian Trajectories

Tarek A. Elsayed,† Klaus Mølmer,‡ and Lars Bojer Madsen†

1Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark

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Bohmian mechanics is an interpretation of quantum mechanics that describes the motion of quantum particles with an ensemble of deterministic trajectories. Several attempts have been made to utilize Bohmian trajectories as a computational tool to simulate quantum systems consisting of many particles, a very demanding computational task. In this paper, we present a novel ab-initio approach to solve the many-body problem for bosonic systems by evolving a system of one-particle wavefunctions representing pilot waves that guide the Bohmian trajectories of the quantum particles. The method is used to study the breathing dynamics and ground state properties in a system of several interacting bosons. The precision of our method is benchmarked against the numerically exact multiconfigurational time-dependent Hartree method for bosons.

Numerical simulation of the quantum dynamics of many-body systems is plagued by the dimension of the Hilbert space which increases exponentially with the number of particles. Much of the progress in theoretical condensed matter, atomic and molecular physics in the past few decades has been achieved by finding new ways to circumvent this problem. Some of the most powerful approaches are density functional theory [1], quantum Monte Carlo [2], density matrix renormalization group [3] and the multi-configuration time-dependent Hartree method [4]. Recently, nonconventional approaches based on artificial intelligence [5], Bohmian mechanics [6–9] and wavelet transforms [10] have been proposed as well. Several methods aim to reduce the complexity of the numerical simulation of many-body systems by resorting to low-dimensional objects such as density functions [1, 11] and natural orbitals [12] or by using mixed classical-quantum dynamics such as the Ehrenfest approach [13] and the surface hopping method [14, 15]. In this paper, we use another class of low-dimensional objects, namely single-particle pilot waves evolved concurrently with Bohmian trajectories to extract all the physical information about the system.

Within the de Broglie–Bohm interpretation of quantum mechanics [16–18], the quantum mechanical wavefunction is a pilot wave that guides the motion of the particle in the physical space. While this interpretation does not alleviate the need for dealing with many-dimensional functions, the prospect of replacing the full many-particle wavefunction by single-particle wavefunctions that guide the Bohmian particles in the physical space was recently explored [19]. However, this idea was only explored when the entanglement between the particles could be neglected [19, 20], thus ruling out its application to strongly correlated systems. Other approaches to treat many-body wavefunctions with trajectories involve other approximations such as the mean-field approximation or assume a certain form for the wavefunction [21, 22].

Here, we introduce a novel approach that simulates multi-particle quantum dynamics in a non-perturbative manner using pilot waves without neglecting the entanglement or relying on particular assumptions about the underlying quantum state. We apply our approach to study the breathing dynamics of many-boson systems in a trap with long- and short-range interactions. We use the same method to compute the ground state energies for an exactly solvable system. We compare our results with the multiconfigurational time-dependent Hartree method for bosons (MCTDHB), which has become a standard method to analyze systems of many interacting bosons beyond the mean-field method [23, 24].

Entangled quantum dynamics using Bohmian trajectories

Let us illustrate the usage of pilot waves in a 1D system consisting of 2 particles. The coordinates are denoted by \(x_1\) and \(x_2\), the potential by \(V(x_1, x_2)\) and the wavefunction describing the full system is \(\Psi(x_1, x_2, t)\). In order to evolve the Bohmian trajectories \(X_1(t)\) and \(X_2(t)\) for the two particles (we denote the Bohmian trajectories throughout this paper by uppercase letters), we need to evaluate the pilot waves \(\psi_i(x_i, t)\). The pilot waves are the full wavefunction projected on the coordinates of all the particles except one, i.e., \(\psi_i(x_i, t) \equiv \Psi(x_1, x_2, t)|_{x_j=X_j(t), j\neq i}\); hence, they are also called conditional wavefunctions (CWs) [25]. In the absence of gauge fields, the Bohmian velocities are computed in terms of the pilot waves as

\[
\frac{dX_i}{dt} = \frac{\hbar}{m_i} \text{Im} \left\{ \frac{\partial_{x_i} \psi_i(x_i, t)}{\psi_i(x_i, t)} \right\} \bigg|_{x_i=X_i(t)}, \tag{1}
\]

where \(m_i\) is the mass of particle \(i\).

It is guaranteed that the density of the Bohmian particles evolved by Eq. (1) follows the evolution of the density function as computed by Schrödinger’s equation [8]. In order to evolve the CWs without having to solve the time-dependent Schrödinger equation (TDSE) for \(\Psi(x_1, x_2, t)\), we introduce a generalized set of conditional...
wavefunctions $\psi_i^n(x_i,t)$ defined as

$$\psi_i^n(x_i,t) \equiv \frac{\partial^n \Psi(x_1,x_2,t)}{\partial x_j^n} \bigg|_{x_j=X_j(t), \ j \neq i} \tag{2}$$

where the pilot waves correspond to $\psi^0_i$. It can be easily proved (see Methods) that the equation of motion for $\psi_i^n(x_i,t)$ is

$$i\hbar \frac{\partial \psi_i^n(x_i,t)}{\partial t} = -\frac{\hbar^2}{2m_i} \frac{\partial^2 \psi_i^n(x_i,t)}{\partial x_i^2} + \sum_{k=0}^{n} \binom{n}{k} \psi_{i}^{n-k}(x_i,t) \frac{\partial^k V(x_i,x_j)}{\partial x_j^k} \bigg|_{x_j=X_j(t), \ j \neq i} - \frac{\hbar^2}{2m_j} \psi_{i}^{n+2}(x_i,t) + i\hbar \frac{dX_j(t)}{dt} \psi_{i}^{n+1}(x_i,t) \tag{3}$$

We see from this equation that the pilot waves corresponding to different particles interact indirectly through the last three terms of Eq. (3). In [19], a similar equation of motion is derived in terms of nonlocal potentials.

The price to be paid in order to evolve the interacting pilot waves using Eq. (3) in an exact manner instead of evolving the multi-dimensional full wavefunction is that we need to evolve the whole hierarchy of $\{\psi_i^n\}$. One can truncate the hierarchy at a finite order $N$. The higher the value of $N$, the longer it takes till the truncation error propagates from $\psi_i^N$ down to $\psi_i^0$ and affects the evolution of $X_i(t)$ and the precision of the results. Since the errors afflict the pilot waves through the last two terms in Eq. (3), this method of evolving the pilot waves is most suitable when we are interested in the dynamics of a very light particle interacting with a much heavier one over a very short time scale. In this case, we can omit the last two terms for the heavy particle while retaining them for the light particle.

To illustrate this method, we consider the entangled dynamics of two particles of masses $m_1 = 1$ and $m_2 = 100$ subject to the harmonic potential $V(x_1,x_2) = \frac{1}{2}kx_1^2 + \frac{1}{2}kx_2^2$ with $k = 0.1$ (atomic units are used in the rest of this paper). Let us take an initial entangled state (see Methods) and evolve the Bohmian trajectories for the initial conditions $X_1 = 1$, $X_2 = 2$. We first truncate the hierarchy at $N = 0$, thus making Eq. (3) unitary. This case corresponds to the small entanglement approximation, i.e., noninteracting pilot waves. Fig. 1 shows that the Bohmian trajectory evolved by the corresponding pilot wave deviates from the trajectory computed from the exact pilot wave already at half a cycle of the oscillatory motion. Increasing the depth of the hierarchy to $N = 7$ only extends the range of accurate dynamics for another cycle.

In this example, we see clearly that although the particles are non-interacting, we need to account for the interaction between the pilot waves of the two particles correctly through the higher order CWs even when the ratio of the particles’ masses is 1:100. Otherwise, the
errors originating from truncating the hierarchy of \( \{ \psi^n \} \) propagate very fast to \( \psi^n \). Increasing \( N \) beyond \( N \approx 10 \) will not help in prolonging the range of accuracy because of the numerical errors in the calculation of the higher-order derivatives of the wavefunction. Is there a more accurate way to propagate the pilot waves to avoid the errors originating from the truncated orders? It turns out, as we will show shortly, that the answer is yes! To this end, we assume an ansatz for the full wavefunction that allows the calculation of the first and second \( \psi^1 \) and \( \psi^2 \) which we subsequently use to evolve the interacting pilot waves \( \psi^0 \) and \( \psi^n \). In the rest of the paper, we consider only identical particles.

**A novel approach to propagate the pilot waves**

The most general form for the wavefunction of a 2-particle system is

\[
\Psi(x, y, t) = \sum_{i, j} c_{ij}(t) \phi_i(x) \phi_j(y),
\]

where \( \{ \phi_i \} \) is a complete basis for the one-body Hilbert space. The conditional wavefunctions of the first particle conditioned on the second particle located at \( y = Y \) are expressed as (the time variable and the particle index are dropped to simplify the notation)

\[
\psi^0(x) \equiv \Psi(x, y = Y) = \sum_i a_i \phi_i(x),
\]

\[
\psi^1(x) \equiv \frac{\partial \Psi(x, y = Y)}{\partial y} \bigg|_{y = Y} = \sum_i b_i \phi_i(x),
\]

\[
\psi^2(x) \equiv \frac{\partial^2 \Psi(x, y = Y)}{\partial y^2} \bigg|_{y = Y} = \sum_i c_i \phi_i(x),
\]

where \( a_i = \sum_j c_{ij} \phi_j(Y), \ b_i = \sum_j c_{ij} \frac{\partial \phi_j(y)}{\partial y} \bigg|_{y = Y} \) and \( c_i = \sum_j c_{ij} \frac{\partial^2 \phi_j(y)}{\partial y^2} \bigg|_{y = Y} \). These relations can be written in vector form as:

\[
\vec{a} = C \vec{\phi}(Y), \ \vec{b} = C \vec{\phi}'(Y) \quad \text{and} \quad \vec{c} = C \vec{\phi}''(Y).
\]

The problem of finding \( \psi^1 \) and \( \psi^2 \) boils down to finding the coefficients \( b_i \) and \( c_i \) constituting the vectors \( \vec{b} \) and \( \vec{c} \). This is accomplished by making use of an ensemble of Bohmian pairs of coordinates \( \{ X, Y \} \) which are selected initially from the one-particle density function \( \rho(x) \) at \( t = 0 \). Each of these pairs is called a configuration. If we can represent both \( \vec{\phi}' \) and \( \vec{\phi}'' \) for a certain value of \( Y \) as a linear superposition of all \( \{ \vec{\phi} \} \) corresponding to all members of the ensemble, i.e., if \( \vec{\phi}' = \sum_k \alpha_k \vec{\phi}_k \) and \( \vec{\phi}'' = \sum_k \beta_k \vec{\phi}_k \) then it follows from the linearity in Eq. (5) that \( \vec{b} = \sum_k \alpha_k \vec{a}_k \) and \( \vec{c} = \sum_k \beta_k \vec{a}_k \). Finding the values of \( \alpha_k \) and \( \beta_k \) is equivalent to solving a system of linear equations. In this way, we can predict \( \psi^1 \) and \( \psi^2 \) without ever constructing the coefficient matrix \( C \).

It should be noted that \( \psi^1 \) and \( \psi^2 \) can be obtained without expressing \( \psi^0 \) in terms of a basis at all, since \( \{ \alpha_k \} \) and \( \{ \beta_k \} \) depend only on the amplitudes of any complete basis at the location of the Bohmian particles. After \( \{ \alpha_k \} \) and \( \{ \beta_k \} \) are obtained, we can express \( \psi^1 \) and \( \psi^2 \) as

\[
\psi^1(x) = \sum_k \alpha_k \psi^0_k(x; Y_k),
\]

\[
\psi^2(x) = \sum_k \beta_k \psi^0_k(x; Y_k).
\]

With the CWs at our disposal, we use the equation of motion (3) for \( n = 0 \) to evolve the ensemble of CWs for all Bohmian particles as described in the Methods Section. We call this scheme Interacting Pilot Waves (IPW).

Some observables can be computed by averaging over the ensemble of Bohmian configurations \( \{ X, Y \} \) such as \( \langle x^2 \rangle \). Since we have access to the CWs, we can devise a more accurate method that approximates the exact expression of the expectation value of an operator \( \hat{A} \),

\[
\langle \hat{A} \rangle = \int \Psi^*(x, y) \hat{A} \Psi(x, y) dx dy
\]

by performing the integral over one variable as a Riemann sum over its Bohmian coordinates, i.e.,

\[
\langle \hat{A} \rangle \approx \sum_w \Delta_w \int w^* \hat{A} w w(x) dx,
\]

where \( w^* \) is the conditional wavefunction of the first particle conditioned on the coordinate of the second particle belonging to the \( w^{th} \) configuration of the ensemble, \( \Delta_w \) is the distance between adjacent values of \( Y \) at the \( w^{th} \) configuration and \( A_w \) is the operator \( \hat{A} \) conditioned on \( X_{2w} \). Similarly, the reduced one-body density can be approximated as \( \rho(x) \approx \sum_w \Delta_w \psi^0_w(x) \psi^0_w(x) \).

Let us apply this method to study the breathing dynamics of two bosons in a harmonic trap, \( V(x) = \frac{1}{2} k_x x^2 \). The bosons are initially condensed in the ground state of the trap, and start a breathing motion when a harmonic interaction \( V(x, y) = \frac{1}{2} k_{xy}(x-y)^2 \) is suddenly switched on.

A finite fixed set of orbitals are taken to be the lowest set of eigenfunctions of the one-body problem with the effective potential felt by one particle due to the other one, namely \( V_{eff}(x) = \frac{1}{2} k_x x^2 + \int \rho(y) V(x, y) dy \). We illustrate in Fig. 2 the behavior of \( \rho(0) \) for \( k_i = k_i = 1 \) computed by the IPW method with 6 orbitals compared with the exact dynamics (i.e., from the exact pilot waves obtained by solving the TDSE exactly).

**Generalization to many-particle systems**

Generalizing our algorithm to a many-particle problem consisting of \( N_B \) bosons is straightforward. Let us denote the coordinates of the particles by \( x, y, z, \cdots \) etc., while, as before, we denote the Bohmian coordinates by upper case letters. A single configuration of Bohmian walkers is denoted by \( \{ X, Y, Z, \cdots \} \).

Let us denote the conditional wavefunctions by
The generalization of Eq. (3) for the case of many particles:

\[ \psi^0(x; Y, Z, \cdots) \equiv \Psi(x, y, z, \cdots) \big|_{y=z=\cdots} \]

\[ \psi^1(x; Y', Z, \cdots) \equiv \frac{\partial \Psi(x, y, z, \cdots)}{\partial y} \big|_{y=z=\cdots} \]

\[ \psi^1(z; X, Y', \cdots) \equiv \frac{\partial \Psi(x, y, z, \cdots)}{\partial y} \big|_{x=X,y=Y,\cdots} \]

and so on.

The equation of motion for \( \psi^0(x; Y, Z, \cdots) \) is a simple generalization of Eq. (3) for the case of many particles:

\[ i\hbar \partial_t \psi^0(x; Y, Z, \cdots; t) = \left( -\frac{\hbar^2}{2m} \nabla_x^2 + V(x; Y, Z, \cdots) \right) \psi^0(x; Y, Z, \cdots; t) \]

\[ + \frac{i\hbar}{m} \frac{dY}{dt} \psi^1(x; Y', Z, \cdots; t) - \frac{\hbar^2}{2m} \psi^2(x; Y'', Z, \cdots; t) \]

\[ + \frac{i\hbar}{m} \frac{dZ}{dt} \psi^1(x; Y, Z', \cdots; t) - \frac{\hbar^2}{2m} \psi^2(x; Y, Z'', \cdots; t) + \cdots \text{etc.} \]

Similar equations can be written for all the CWs corresponding to all particles in every configuration. A generic ansatz for the many-body wavefunction similar to Eq. (4) reads

\[ \Psi(x, y, z, ..., t) = \sum_{i,j,k,...} c_{ijk...}(t) \phi_i(x) \phi_j(y) \phi_k(z) \cdots \]

In order to compute \( \psi^1(x; Y', Z, \cdots; t) \) from the \( \psi^0_w(x; Y_w, Z_w, \cdots; t) \) belonging to all configurations, we need to express the tensor \( \left[ \phi'_j(Y) \phi_k(Z) \cdots \right] \) as a linear superposition of all the \( \left[ \phi'_j(Y_w) \phi_k(Z_w) \cdots \right] \) tensors belonging to all configurations; i.e.,

\[ \left[ \phi'_j(Y) \phi_k(Z) \cdots \right] = \sum_{w} \alpha_w \left[ \phi'_j(Y_w) \phi_k(Z_w) \cdots \right] \]

This can be done with the existing numerical techniques by rearranging all the \( MN^{-1} \) terms of the tensors, where \( M \) is the number of orbitals, in vector forms and solving a linear system of equations.

In order to compute the expectation value of an operator, we can treat the collection of CWs belonging to all the particles as if they describe normal single particle wavefunctions (after renormalizing them). \( \langle A \rangle \) can then be computed as

\[ \langle A \rangle \approx \frac{1}{N_w} \sum_{w} \int \psi^*_w(x) A \psi_w(x) dx \]

where \( \psi_w(x) \) is the normalized CW of particle \( x \) belonging to the \( w \)-th configuration. If \( A \) is a two-body operator such as the interaction potential between two particles, we first compute a mean-field operator, and then treat it as a one-body operator. For example, the mean-field interaction potential felt by one particle is computed as

\[ V(x) \approx \frac{1}{N_w} \sum_{w} \int \psi^*_w(y) V(x-y) \psi_w(y) dy \]

The expectation value of \( V(x) \) is then computed as a one-body operator.

From the normalized collection of all the CWs, we can also compute the reduced density matrix of one particle \( \rho(x', x) \approx \frac{1}{N_w} \sum_{w} \psi^*_w(x') \psi_w(x) \). This matrix can be used to compute a set of natural orbitals in terms of the finite basis set used in the postulated ansatz as the eigenstates of \( \rho(x', x) \).

Many particles in a harmonic trap

We apply this generalization to the dynamics of 3 bosons and 5 bosons in a harmonic trap \( V(x) = \frac{1}{2}x^2 \) for two cases of interparticle interactions: long-range attractive harmonic interaction and short-range repulsive interaction. As in the two-particle case, all the bosons...
initially reside in the ground state of the harmonic trap before the interaction is suddenly switched on at $t = 0$. We study the breathing dynamics by computing $\langle x^2 \rangle$ as a function of time.

For a harmonic interaction of the form $V(x, y) = \frac{1}{2}k_i(x - y)^2$ we consider two cases of 5 bosons with weak interactions ($k_i = 0.1$) and 3 bosons with strong interaction ($k_i = 1$) and we use 3 and 4 orbitals in the two cases, respectively. In both cases we compare the results with the numerically exact simulation using MCTDHB [23, 26–29] and with the Hermitian limit (HL) of Eq. (7) where all the non-hermitian terms in Eq. (7) are dropped out. The Hermitian limit is equivalent to the time-dependent quantum Monte-Carlo (TDQMC) of Ref. [22] which does not take entanglement into consideration.

In Fig. 3, we show the results of computing $\langle x^2 \rangle$ by averaging over the Bohmian coordinates of all the particles using a single ensemble containing 1000 configurations. We notice that the IPW method is more accurate in the weak interaction regime than in the strong interaction regime. The Bohmian trajectories of the first particle in all configurations are shown in Fig. 3(c) for $k_i = 0.1$ while the Bohmian trajectories for all the 5 particles in a single configuration are shown in Fig. 3(d). The few constant trajectories appearing in Fig. 3(c) correspond to the cases where we manually set the Bohmian velocities to be zero when the denominator is Eq. (1) is below a certain threshold.

In Fig. 4, we plot $\langle x^2 \rangle$ after switching on a gaussian interaction $V(x - y) = k_i/\sqrt{2\pi\sigma^2} \times e^{-\frac{(x-y)^2}{2\sigma^2}}$ with $k_i = 0.1$, $\sigma = 0.25$ and compare the results with MCTDHB simulation and the HL of Eq. (7). In this calculation, we
In the ground state of the instantaneous Hamiltonian.

According to the adiabatic theory [30], the system remains, we switch on the interaction adiabatically. After-wards, we switch on the interaction adiabatically. Ac-

ground state of the noninteracting Hamiltonian. After-

initialize the CWs and the Bohmian trajectories in the

trajectories.

conditional wavefunctions rather than from the Bohmian

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compute \( \langle x^2 \rangle \) from the expectation value of \( x^2 \) using the conditional wavefunctions rather than from the Bohmian trajectories.

In order to compute the ground state energy for an inter-

acting system of particles using the IPW scheme, we ini-

tialize the CWs and the Bohmian trajectories in the

ground state of the noninteracting Hamiltonian. After-

wards, we switch on the interaction adiabatically. Ac-

cording to the adiabatic theory [30], the system remains

in the ground state of the instantaneous Hamiltonian.

In Fig. 5, we plot the evolution of the energy of the

instantaneous Hamiltonian of a 5-particle system as we

switch on the harmonic interaction \( V(x, y) = \frac{1}{2}k_1(x - y)^2 \)

adibatically and compare it with the exact ground state

energy \( E_0 = \frac{N_B - 1}{2}\sqrt{1 + k_1N_B + 0.5} [31] \) for \( k_1 = 0.1 \). The

ground state energy computed by MCTDHB [32] is more

accurate than the IPW calculation for the same number

of orbitals by several significant digits. Perhaps a better

method to compute ground state energy is to propagate

Eq. (7) in complex time, while evolving the Bohmian

trajectories in real time [22]. The optimal relation be-

tween the real and complex time evolution constitutes

an interesting topic of research.

Conclusion and discussion

We have presented a promising approach to analyze

the dynamic and static properties of systems consisting of

several bosons by evolving a system of nonunitary equa-

tions that goes beyond the small entanglement approxi-

mation and the mean-field approximation.

The accuracy of this new approach is outperformed by

the state-of-the-art MCTDHB algorithm. In the MCT-

DHB method, increasing the number of orbitals (\( M \))

is confronted with the exponentially large number of

configurations of permanents that needs to be taken into

account. We have a similar scaling problem in our ap-

proach; the number of configurations of Bohmian par-

icles has to be larger than \( M^{N_B-1} \) in order to avoid

having an undetermined linear system of equations when

solving for \( \alpha_w \). So, the complexity of our approach still

increases exponentially with the number of particles but

with a much smaller base for the exponent than the bare-

bones TDSE approach which scales as \( L^{N_B} \), where \( L \)

is the number of grid points per dimension.

It is still an open question whether the non-Hermitian

terms in the equations of motion can be replaced by an

effective entanglement potential that makes the equations

unitary and at the same time captures the entanglement

in the system. For systems consisting of many particles,

i.e., \( N_B > 20 \), the entanglement of the ground state is

so small [33] that even the Hermitian limit [22] can be

efficient for simulating the dynamics involving a small

number of excited states.

In principle, generalizing the IPW approach to

fermionic systems is straightforward, as long as we choose

the initial state with the proper symmetry requirements.

However, for fermions two problems arise. First, due to

the Pauli exclusion principle, we need a large number of

orbitals to describe a fermionic state and therefore, the

number of fermions that can be analyzed is small com-

pared to bosons. Second, the conditional wavefunctions

for fermions will have nodes, that complicate computing

the velocity of the Bohmian walkers around those nodes.

Since the node problem is a well known problem for simu-

lating quantum dynamics with Bohmian trajectories [6],

the methods developed in this regard in the literature

[34, 35] may benefit the solution of this problem.

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**Competing financial interests** The authors declare no competing financial interests.
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Methods

Derivation of Equation (3)

Let us derive Eq. (3) with respect to $\psi^n_1(x_1,t)$. Since $\psi^n_1(x_1,t) \equiv \frac{\partial^n \Psi(x_1,x_2)}{\partial x_2^n} \mid_{x_2=X_2(t)}$, we find by the chain rule that

$$\frac{\partial \psi^n_1(x_1,t)}{\partial t} = \frac{\partial}{\partial t} \frac{\partial^n \Psi(x_1,x_2)}{\partial x_2^n} \mid_{x_2=X_2(t)} + \frac{dX_2(t)}{dt} \frac{\partial^n \Psi(x_1,x_2)}{\partial x_2^n} \mid_{x_2=X_2(t)}. \quad (9)$$

By exchanging the time and spatial derivatives in the first term on the R.H.S. and using the TDSE:

$$i\hbar \frac{\partial \Psi(x_1,x_2)}{\partial t} = \left( -\frac{\hbar^2 \nabla^2_1}{2m_1} - \frac{\hbar^2 \nabla^2_2}{2m_2} + V(x_1,x_2) \right) \Psi(x_1,x_2),$$

we obtain after substituting back in Eq. (9)

$$i\hbar \frac{\partial \psi^n_1(x_1,t)}{\partial t} = -\frac{\hbar^2}{2m_1} \frac{\partial^2 \psi^n_1(x_1,t)}{\partial x_1^2} + \frac{\partial^n}{\partial x_2^n} \left( V(x_1,x_2) \Psi(x_1,x_2) \right) \mid_{x_2=X_2(t)} - \frac{\hbar^2}{2m_2} \psi^{n+2}_1(x_1,t) + i\hbar \frac{dX_2(t)}{dt} \psi^{n+1}_1(x_1,t). \quad (10)$$

By applying the chain rule to the second term on the R.H.S. we obtain $\frac{\partial^n}{\partial x_2^n} \left( V(x_1,x_2) \Psi(x_1,x_2) \right) \mid_{x_2=X_2(t)} = \sum_{k=0}^{n} \binom{n}{k} \psi^{n-k}_1(x_1,t) \frac{\partial^k V(x_1,x_2)}{\partial x_2^k} \mid_{x_2=X_2(t)}$ which after substituting in Eq. (10) recovers Eq. (3).

Initial entangled state

We take the initial entangled state in Fig. 1 for a two-particle system as the ground state of the Hamiltonian with the potential function $V(x_1,x_2) = \frac{1}{2} k_1 x_1^2 + \frac{1}{2} k_2 x_2^2 + \frac{1}{2} k_3 (x_1 - x_2)^2$ with $k_1 = k_2 = 0.1$, $k_3 = 1.0$ and the masses of the particle $m_1 = 1$ and $m_2 = 2$.

Interacting Pilot Waves for two particles

For the two-particle IPW simulations in Fig. 2 we express all the CWs in terms of the basis set $\{ \phi_i \}$, and evolve the expansion coefficients $\{a_i\}$. Equation 3 is then expressed as

$$i \sum_i \hat{a}_i(t) \phi_i(x) = -\frac{\hbar^2}{2m} \sum_i a_i(t) \frac{\partial^2 \phi_i(x)}{\partial x^2} + V(x,Y) \sum_i a_i(t) \phi_i(x) - \frac{\hbar^2}{2m} \sum_i c_i(t) \phi_i(x) + i\hbar \frac{dY}{dt} \sum_i b_i(t) \phi_i(x). \quad (11)$$

By taking the inner product with each of the orbitals $\{ \phi_i(x) \}$ we obtain the time derivative of the expansion coefficients $\{ \dot{a}_i \}$. This system of equations is then solved using a fourth-order Runge-Kutta method.

Propagating the conditional wavefunctions

Equations (3) and (7) represent a system of coupled nonlinear and nonunitary differential equations that needs to be solved together. Each of these equations can be cast in the form

$$i \frac{\partial \psi(x,t)}{\partial t} = H \psi(x,t) + W(x,t), \quad (12)$$

where the first term on the RHS represents the unitary part of the equation and $W(x,t)$ represents the nonunitary part which is a function of all other CWs. If, e.g., $H$ is a constant Hamiltonian, a general solution for this equation takes the form:

$$\psi(x,t) = e^{-iHt} \left[ \int_0^t e^{iHt'} W(x,t')dt' + \psi(x,t_0) \right]$$

In order to propagate $\psi(x,t)$ for a single time step from $t = 0$ to $t = \delta t$ using this solution, both the operator $e^{-iH\delta t}$ and $e^{-iHt'}$ are performed using a split-operator method [36]. The integral is performed using the trapezoidal rule

$$\int_0^{\delta t} e^{iHt'} W(x,t')dt' \sim \frac{1}{2} \left[ e^{iH}\delta t W(x,\delta t) + W(x,0) \right].$$

Miscellaneous numerical techniques

- The evaluation of the conditional wavefunctions at the position of the Bohmian particles was performed by FFT-based interpolation.
- Solving the linear system of equations in Eq. (5) was performed by the LAPACK routine gelsd() which uses singular value decomposition and a divide and conquer method to compute the minimum-norm solution to a linear least squares problem [37].
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