Wave functions and Bohmian trajectories in interference phenomena

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Abstract

In the last few years the hydrodynamic formulation of quantum mechanics, equivalent to the Bohmian equations of motion, has been used to obtain numerical solutions of the Schrödinger equation. Problems, however, have been experienced near wave function nodes (or low probability regions). Here we attempt to compute wave functions and Bohmian trajectories for the interference of one particle or of two identical particles. It turns out that the large number of nodes (i.e. interference minima) makes the hydrodynamic equations impractical, whereas a more straightforward solution of the Schrödinger equation gives very good results.

Key words: Hydrodynamic equations, Bohmian trajectories, Schrödinger equation, Interference
PACS: 02.60.Cb, 03.65.-w

1 Introduction

Bohmian trajectories were first proposed in an attempt to restore determinism in quantum mechanics [1]. In Bohm’s view, quantum particles have at every instant well-defined positions which, however, can only be known probabilistically. The particles follow deterministic trajectories governed by equations of motion similar to Newton’s, except that a specific quantum contribution

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must be added to the classical potential. This *quantum potential* explicitly depends on the particles' total wave function and is responsible for characteristic quantum-mechanical effects like barrier penetration. All statistical predictions of quantum mechanics can be obtained through averages over trajectories [2,3].

One of the first numerical computations of Bohmian trajectories was carried out in the context of two-slit interference [4]. It showed vividly how one-particle interference effects can be understood in terms of particle dynamics. Trajectories associated with two-particle interference were also shown explicitly to reproduce standard quantum-mechanical results [5].

Bohmian trajectories can usually be computed rather straightforwardly if the particles' wave function is known analytically. Computation can also be carried out from a numerical approximation to the exact wave function. But this, it turns out, can be viewed from a different perspective. In the past few years, the computation of Bohmian trajectories has led to a powerful way of numerically integrating the Schrödinger equation.

The method is closely connected with the *hydrodynamic formulation* of the Schrödinger equation, which goes back to the early years of quantum mechanics [6,7]. In this formulation, the evolution of the wave function is associated with that of a fluid whose motion can be obtained through the trajectories of its elements. Among the quantum-mechanical problems that have been addressed in this way are photodissociation [8,9], reactive scattering with the Eckart barrier [10,11], the quartic double-well potential [12], and the harmonic oscillator with quartic anharmonicity [13]. The method has a number of advantages, in particular the use of a relatively small number of grid points and its applicability to higher-dimensional problems. It does, however, have difficulties in dealing with regions where the wave function vanishes or nearly vanishes.

The purpose of this paper is to investigate the numerical computation of wave functions and Bohmian trajectories in the context of particle interference [14]. This specifically quantum-mechanical phenomenon illustrates perhaps more than any other the properties of quantum superpositions. Moreover, interference minima correspond to zeros or near-zeros of the wave function, and therefore make severe tests on numerical methods. The hydrodynamic method and algorithms for its numerical solution will be reviewed side by side with the method based upon separating the Schrödinger equation into its real and imaginary parts. Both will be used to make detailed computations of the wave functions and Bohmian trajectories associated with the interference of one particle or two identical particles. Comparison with results obtained through an exact solution of the Schrödinger equation will show that zeros (or nodes) of the wave function make the hydrodynamic computation prohibitive in computer resources, whereas the approach using the real and imaginary parts of
the wave function yields accurate results in reasonable time.

2 Wave functions and trajectories

The Schrödinger equation for a system of \( n \) particles interacting through a potential \( V \) is given by

\[
i\hbar \frac{\partial \psi}{\partial t} = - \sum_{i=1}^{n} \frac{\hbar^2}{2m_i} \nabla_i^2 \psi + V(\vec{r}_1, \ldots, \vec{r}_n)\psi, \quad (1)
\]

where \( m_i \) is the mass of particle \( i \) and \( \nabla_i^2 \) the Laplacian operator with respect to that particle’s coordinates. We will focus here on the interference of one particle or of two identical particles. There is then only one mass and, in dimensionless units, Eq. (1) can be written as

\[
i \frac{\partial \psi}{\partial t} = - \frac{1}{2} \nabla^2 \psi + V(\vec{r})\psi. \quad (2)
\]

The vector \( \vec{r} \) now stands for the position in configuration space, and the operator \( \nabla^2 \) for the Laplacian in that space.

2.1 Hydrodynamic equations

The hydrodynamic equations follow from the Schrödinger equation when the wave function is written in polar form. They were first used as a basis for the numerical solution of Eq. (1) a number of years ago [15], but the method has been substantially improved recently.

To get the hydrodynamic equations we substitute \( \psi = \sqrt{P} \exp(iS) \) in Eq. (2), where \( S \) and \( \sqrt{P} \) are real dimensionless functions and \( \sqrt{P} \) is nonnegative. Equating separately the real and imaginary parts of (2), we obtain

\[
\frac{\partial P}{\partial t} = -\nabla \cdot (P \nabla S), \quad (3)
\]

\[
\frac{\partial S}{\partial t} = -\frac{1}{2}(\nabla S)^2 - Q - V(\vec{r}), \quad (4)
\]

where \( Q \), the quantum potential, is given by

\[
Q \equiv -\frac{1}{2} \frac{\nabla^2 \sqrt{P}}{\sqrt{P}}. \quad (5)
\]
The Bohmian trajectories of the particles are defined by writing the following equation for the velocity in configuration space:
\[ \vec{v} = \vec{\nabla} S. \] (6)

We now substitute (6) in (3) and (4). Noting that \( \nabla_a v_b = \nabla_b v_a \) (\( a \) and \( b \) are coordinate indices), we find
\[ \frac{DP}{Dt} = -P(t) \vec{\nabla} \cdot \vec{v}(t), \] (7)
\[ \frac{D\vec{v}}{Dt} = -\vec{\nabla}(Q + V), \] (8)

where the Lagrangian derivative is defined as
\[ \frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{v}(t) \cdot \vec{\nabla}. \] (9)

Eqs. (7) and (8), together with
\[ \frac{D\vec{r}}{Dt} = \vec{v}(t), \] (10)

must be solved to get the Bohmian trajectories and, eventually, the wave function.

The numerical solution of Eqs. (7), (8), and (10) can be carried out in two different ways. The first one, called Lagrange’s viewpoint, uses the fact that the Lagrangian derivative represents the total time derivative with respect to a moving coordinate system. Grid points are then defined which move with the particles according to Eq. (10). This method has a number of advantages. First, the Bohmian trajectories are automatically calculated. Secondly, as grid points follow Bohmian trajectories, they remain concentrated in regions of high probability. As a consequence, fewer points are needed since the grid adapts itself throughout time evolution. Finally, use of the Lagrangian derivative gives differential equations with very few terms.

Euler’s viewpoint, in contrast with Lagrange’s, uses a fixed grid. Eqs. (7) and (8) are solved with (9) substituted into them. That method may be more flexible for the purpose of computing spatial derivatives.

2.2 Schrödinger equation

Several methods for the numerical solution of the Schrödinger equation in its original form were developed over the years [16,17,18,19]. Heller’s approach [18], in particular, was used for the analysis of atom diffraction by
surfaces through computation of Bohmian trajectories [20,21]. Here we shall separate the Schrödinger equation into its real and imaginary parts [16] by substituting $\psi = \psi_R + i\psi_I$ in (2). We get

$$\frac{\partial \psi_R}{\partial t} = -\frac{1}{2} \nabla^2 \psi_I + V\psi_I,$$  \hfill (11)  
$$\frac{\partial \psi_I}{\partial t} = \frac{1}{2} \nabla^2 \psi_R - V\psi_R.$$  \hfill (12)

Starting with the value of $\psi$ at a given time, these equations are to be solved over an interval of time. Bohmian trajectories are then computed using (6) or, explicitly,

$$\frac{d\vec{r}(t)}{dt} = \vec{v}(t) = \vec{\nabla} \left\{ \arctan \left( \frac{\psi_I}{\psi_R} \right) \right\}.$$

3 Numerical methods

In this section, we address the problems of appropriately evaluating spatial derivatives and carrying out time integrations, in each of the two schemes considered.

3.1 Hydrodynamic equations

In the Lagrangian viewpoint, one needs to compute spatial derivatives on a grid that changes at each time step. We use the moving weighted least squares method proposed in Ref. [10]. It consists in fitting a series of polynomials to values of functions in a neighborhood of the point were the derivative is to be evaluated. Provided that the neighborhood is small enough, the function to be differentiated should be well represented by low-order polynomials. Function derivatives will then be given by the coefficients of the polynomials. This method can be adapted to almost any point distribution.

To be more specific, suppose we want to evaluate derivatives of a function $f$ at a point $\vec{r}_0$. We first write $f$ as a finite series of polynomials around $\vec{r}_0$, that is,

$$f(\vec{r}) = \sum_{s=1}^{M} a_s p_s(\vec{r} - \vec{r}_0).$$  \hfill (14)

We now use the values of $f$ at $N_b$ neighboring points $\vec{r}_n$ of $\vec{r}_0$, and find the coefficients $a_s$ by minimizing the following expression:

$$\chi^2 = \sum_{n=1}^{N_b} \left[ \frac{f(\vec{r}_n) - \sum_{s=1}^{M} a_s p_s(\vec{r}_n - \vec{r}_0)}{\sigma_n} \right]^2.$$  \hfill (15)
Introducing the rectangular matrix

\[ A_{ns} = \frac{p_s(\vec{r}_n - \vec{r}_0)}{\sigma_n} \]  

(16)

and the vector

\[ b_n = \frac{f(\vec{r}_n)}{\sigma_n}, \]  

(17)

we find that \( \chi^2 \) is minimized if

\[ \mathbf{A}^T \cdot \vec{b} = \mathbf{A}^T \cdot \mathbf{A} \cdot \vec{a}. \]  

(18)

This is called the *normal equation* [22]. The weighted least squares approximation is implemented by solving (18) for the unknown \( \vec{a} \). Note that \( \mathbf{A}^T \cdot \mathbf{A} \) is a square matrix. Once the \( a_s \) are known, derivatives of \( f \) can be evaluated from Eq. (14). The standard error \( \sigma_n \) is determined by assigning larger weights to closer points, using for instance a Gaussian distribution around \( \vec{r}_0 \). Further details on the use of the weighted least square method in connection with the hydrodynamic equations can be found in Refs. [11,12].

Time integration in Lagrange’s viewpoint is based on the following discretization of the Lagrangian derivative:

\[ \frac{Df(t)}{Dt} \rightarrow \frac{f(t + \Delta t) - f(t)}{\Delta t}. \]  

(19)

Here \( f \) is evaluated on the moving grid, whose points follow particle trajectories. In Euler’s viewpoint we have

\[ \frac{\partial f(t)}{\partial t} \rightarrow \frac{f(t + \Delta t) - f(t)}{\Delta t}, \]  

(20)

where \( f \) is now evaluated on a fixed grid.

The spatial derivatives turn out to be smoother if we make the transformation \( P = \exp(2g) \). Making use of Eqs. (7), (8), and (10), we find in Lagrange’s viewpoint

\[ \vec{r}_n(t + \Delta t) = \vec{r}_n(t) + \Delta t \vec{v}_n(t), \]  

(21)

\[ \vec{v}_n(t + \Delta t) = \vec{v}_n(t) - \Delta t \vec{\nabla} (Q_n + V_n), \]  

(22)

\[ g_n(t + \Delta t) = g_n(t) - \frac{1}{2} \Delta t \vec{\nabla} \cdot \vec{v}_n, \]  

(23)

where

\[ Q_n = -\frac{1}{2} \frac{\nabla^2 \sqrt{P_n}}{\sqrt{P_n}} = -\frac{1}{2} \left\{ \left( \vec{\nabla} g_n \right)^2 + \nabla^2 g_n \right\}. \]  

(24)

Here \( f_n(t) \), for instance, stands for the value of the function \( f \) at the grid point \( n \) at time \( t \), and \( \vec{\nabla} g_n \equiv (\vec{\nabla} g)_n \).
In Euler’s viewpoint, the following equations have to be solved, together with (24):

\[
\vec{v}_n(t + \Delta t) = \vec{v}_n(t) - \Delta t \vec{\nabla}(Q_n + V_n) - \Delta t \{\vec{v}_n(t) \cdot \vec{\nabla}\} \vec{v}_n(t), \tag{25}
\]

\[
g_n(t + \Delta t) = g_n(t) - \frac{1}{2} \Delta t \vec{\nabla} \cdot \vec{v}_n - \Delta t \vec{v}_n \cdot \vec{\nabla}g_n. \tag{26}
\]

It should be pointed out that a higher-order scheme like the conventional Runge-Kutta method cannot be used for time integration with the weighted least squares method, since the functional form of the spatial derivatives changes at each time step.

3.2 Schrödinger equation

The numerical solution of Eqs. (11) and (12) requires discrete approximations to the second-order spatial derivatives of $\psi_R$ and $\psi_I$. Let $\Delta$ denote the grid spacing. We use the following approximation, which neglects terms of order $\Delta^4$ and higher:

\[
\frac{\partial^2 f}{\partial x^2} = \frac{1}{12\Delta^2} \left[ -30f(x) + 16\{f(x + \Delta) + f(x - \Delta)\} \right.
- \left. \{f(x + 2\Delta) + f(x - 2\Delta)\} \right]. \tag{27}
\]

This formula cannot be used near the grid boundaries, where $f(x \pm \Delta)$ and $f(x \pm 2\Delta)$ may not be defined. In this case we write, for instance,

\[
\frac{\partial^2 f}{\partial x^2} = \frac{1}{12\Delta^2} \left[ 45f(x) - 154f(x + \Delta) + 214f(x + 2\Delta) - 156f(x + 3\Delta) + 61f(x + 4\Delta) - 10f(x + 5\Delta) \right], \tag{28}
\]

\[
\frac{\partial^2 f}{\partial x^2} = \frac{1}{12\Delta^2} \left[ -15f(x) + 10f(x - \Delta) - 4f(x + \Delta) + 14f(x + 2\Delta) - 6f(x + 3\Delta) + f(x + 4\Delta) \right], \tag{29}
\]

with similar expressions on the other side of the grid.

A fourth-order expression for first derivatives is also used for the computation of Bohmian trajectories.

Once the spatial discretization is done, Eqs. (11) and (12) read as

\[
\frac{\partial}{\partial t}\psi_{Rn} = -\frac{1}{2}F_n(\psi_{In}), \tag{30}
\]

\[
\frac{\partial}{\partial t}\psi_{In} = \frac{1}{2}F_n(\psi_{Rn}). \tag{31}
\]
For a grid with \( N \) points, this makes up a system of \( 2N \) coupled first-order differential equations. From Eqs. (27)–(29), one can see that for a given value of \( n \), the index \( m \) assumes up to six different values.

Since oscillations of the real and imaginary parts of the wave function may be important, the numerical integration of \( \psi_R \) and \( \psi_I \) requires an accurate and stable scheme. We use the fourth-order Runge-Kutta method. Note that we improve on Ref. [16] in both the spatial and the time discretization.

4 One- and two-particle interference

An idealized interference setup is shown in Fig. 1, where parameters later to be used in wave functions are indicated. The source \( S \) either emits one particle at a time, which may go through one of the slits and be detected on the screen. Or it emits two identical correlated particles, with identical \( x \) momenta and opposite \( y \) momenta, so that if one particle goes through slit \( A \) the other goes through slit \( B \).

Let \( \psi_A(\vec{r}_i, t) \) and \( \psi_B(\vec{r}_i, t) \) be the partial wave functions for particle \( i \) going through slit \( A \) or \( B \). Just like the symmetry of the setup, we assume that \( \psi_A \) and \( \psi_B \) transform into each other under reflection through the \( x \) axis, that is,

\[
\psi_A(x_i, y_i, t) = \psi_B(x_i, -y_i, t). \quad (32)
\]

The \( z \) coordinate is omitted throughout.

For one-particle interference, the global wave function is given by

\[
\Psi_{\text{one}}(\vec{r}, t) = N \left[ \psi_A(\vec{r}_1, t) + \psi_B(\vec{r}_1, t) \right], \quad (33)
\]

where the configuration space coordinate \( \vec{r} \) corresponds to the one-particle coordinate \( \vec{r}_1 \). Here \( N \) is a normalization constant. For two-particle interference, \( \vec{r} = (\vec{r}_1, \vec{r}_2) \) and we can write

\[
\Psi_{\text{two}}(\vec{r}, t) = N \left[ \psi_A(\vec{r}_1, t)\psi_B(\vec{r}_2, t) \pm \psi_B(\vec{r}_1, t)\psi_A(\vec{r}_2, t) \right]. \quad (34)
\]

The + sign corresponds to bosons, for which the global wave function is symmetric under particle exchange, while the − sign corresponds to fermions, for which the wave function is antisymmetric. In the one-particle case the interference pattern shows up on the screen, whereas in the two-particle case it is a property of configuration space.

At \( t = 0 \), the partial wave functions are picked as plane waves in the \( x \)-direction, and Gaussian wave packets in the \( y \)-direction, centered on the ap-
appropriate slit. Explicitly,
\[ \psi_A(\vec{r_i}, t = 0) = \left(2\pi\sigma_0^2\right)^{-1/4} \exp\left\{-\frac{(y_i - Y)^2}{4\sigma_0^2} + i k_x x_i\right\}, \tag{35} \]
with \(\psi_B\) given through (32). The time evolution of such wave functions in free space (where \(V = 0\)) is known exactly. It is given by
\[ \psi_A(\vec{r_i}, t) = \left(2\pi\sigma_t^2\right)^{-1/4} \exp\left\{-\frac{(y_i - Y)^2}{4\sigma_0\sigma_t} + i \left[k_x x_i - \frac{k_x^2 t}{2}\right]\right\}, \tag{36} \]
where
\[ \sigma_t = \sigma_0 \left(1 + \frac{2\sigma_0^2}{\sigma_t^2}\right). \tag{37} \]
For plane waves along \(x\), one can show [5] that the \(x\)-coordinate Bohmian trajectory is simply given by \(x(t) = x(0) + k_x t\). In the numerical implementation, we therefore concentrate only on the \(y\)-coordinates. One-particle interference thus reduces to a one-dimensional problem, whereas two-particle interference is a two-dimensional problem.

We recall that Bohmian trajectories have been obtained, from exact wave functions, for one-particle interference in [4] and for two-particle interference in [5]. In the numerical computations of wave functions and trajectories that follow, we let throughout \(Y = 1\), \(\sigma_0 = 0.2\), and \(k_x = 0.1\).

5 Results and discussion

5.1 Hydrodynamic equations

One of the main advantages of the Lagrangian viewpoint is the possibility of concentrating grid points in regions of high probability. Accordingly, our first attempts at solving the hydrodynamic equations for one-particle interference used grid points in the immediate neighborhood of the slits only. The numerical results obtained with such initial conditions were very different from what should be expected. Instead of building up an interference pattern, they represented essentially independent Gaussian wave packets emerging from each slit. Clearly then, grid points are needed in the whole region between the slits, even where the probability of finding a particle is very low. This is related to the fact that the development of plateaux and troughs in the quantum potential responsible for the formation of fringes really begins around \(y = 0\) [4]. These remarks point to one of the main problems encountered with the hydrodynamic equations: wave function nodes [12,13,23,24].
The reason why nodes or quasinodes of the wave function are apt to cause problems in the hydrodynamic approach is apparent from Eq. (5). While the denominator of the quantum potential then nearly vanishes, the numerator normally does not. The quantum potential may thus experience rapid and important variations which challenge approximation procedures. Moreover, in the Lagrangian approach the trajectories tend to group in regions of higher probability, thereby going away from nodes. Thus precision is lacking just where the most important variations of the quantum potential occur. The problem is especially acute in our case of one-particle interference. Nodes then correspond to some of the most interesting parts of the wave function, namely interference minima.

Since the wave function (33) for one-particle interference nearly vanishes initially at the point \( y = 0 \), it should help to understand the node problem. With grid points in the neighborhood of slits only, no interference pattern is formed and trajectories go through the node just as if it were absent. But Bohmian trajectories should never cross, hence in this case the quantum potential is not properly calculated. When points are added near the node, the quantum potential can be calculated better. Fig. 2 shows that getting an accurate approximation is no easy matter. As expected, the approximation tends to get better as points are added and more polynomials are used. In the Lagrangian approach, however, the matrix \( A^T \cdot A \) has to be inverted at every point and every time step. Since the dimension of the matrix is equal to the number of polynomials, computation time increases quickly, which makes the method inefficient.

Moreover, small inaccuracies in the initial quantum potential cause important effects in later times, as can be seen in Fig. 3. Although a good approximation is found for the quantum potential with 801 grid points between \(-4\) and 4 and fifth-order polynomials, oscillations appear in the quantum potential and in the velocity as early as \( t = 0.01 \) (1000 time steps). These oscillations can be caused by instabilities in the time integration or by small errors in the approximation of the spatial derivatives, or both.

The grid used for these tests was uniform. Although the weighted least square method allows for nonuniform grids, it would not really help concentrating points around the initial node. Other nodes would develop as the interference pattern builds up, which would also require additional points.

Several solutions have been proposed in connection with the node problem, for example grid adaptation [25] and a hybrid method consisting of solving the Schrödinger equation near nodes and the hydrodynamic equations elsewhere [24,26]. In the case of interference, however, nodes are permanent in time as well as moving in space, so that adaptation is too expensive. As far as the Schrödinger equation goes, we shall show in the next section that it is in
fact more efficient than the hydrodynamic equations, and therefore does not need to be coupled with it.

Instead of using Lagrange’s approach, we may try Euler’s. Since grid points are then fixed, precision can be controlled easily. Because matrix inversion is carried out only at the first time step, computation times are somewhat shorter. Yet use of the weighted least square method still makes this approach inefficient. As a matter of fact, the behavior of the quantum potential and velocity is roughly similar in the Eulerian approach as in Figs. 2 and 3, since almost no dispersion of the wave packet has yet occurred at \( t = 0.01 \). In addition, numerical instabilities arise due to the terms in Eqs. (25) and (26) that are absent in the Lagrangian approach. This suggests that a higher-order scheme is probably needed for time propagation.

Other ways of approximating derivatives can be used with Euler’s approach and give good results in reasonable time. The approximations described in Sect. 3.2, for example, give very good results for the initial node. However, they require more points than needed in connection with the Schrödinger equation, and the time integration is highly unstable. In this case the fourth-order Runge-Kutta scheme could be used. But again the Schrödinger equation looks more promising, since it involves at most second-order (instead of third-order) derivatives.

There is no point here to look at two-particle interference, since the behavior of \( \vec{v}, Q, \) and \( P \) is similar to what was found for one particle, and the two-particle problem requires a much larger number of points.

5.2 Schrödinger equation

Figs. 4 and 5 show the real and imaginary parts of the wave function for one-particle interference. Excellent agreement is found between the numerical solution of the Schrödinger equation (dots) and the exact value (solid lines). The grid spans \( y \)-values between \(-13\) and \(13\) with spacing \( \Delta \) equal to 0.1, for a total of 261 points. 5000 steps were used to go from \( t = 0 \) to \( t = 1 \).

With the real and imaginary parts of the wave function in hand, Bohmian trajectories can be obtained through Eq. (13). Some of these trajectories are shown in dotted lines in Fig. 6, solid lines representing trajectories obtained from the exact wave functions. Again the agreement is excellent. In general the grid should cover enough space to avoid boundary effects. But with the scheme of Sect. 3.2, second-order derivatives are computed quickly and, even with 5000 times steps, the overall computation time (for the wave function and trajectories) is a few minutes on a 1.8 GHz Pentium 4 processor. For comparison, the computation time of wave functions in the Lagrangian approach is
between one and two orders of magnitude higher [27].

As mentioned earlier, two-particle interference here is a two-dimensional problem, and therefore the grid must be much larger. We have used a square grid with $261 \times 261$ points, both $y$-coordinates going from $-13$ to $13$. The computation time is therefore much longer. Bosons wave functions (the $+$ sign in Eq. (34)) were used throughout.

Once again results obtained for the real and imaginary parts of the wave function are in very good agreement with exact values. Some Bohmian trajectories, obtained with 15,000 time steps, are shown in Fig. 7 as dotted lines. Solid lines represent trajectories computed with exact wave functions. The agreement is usually very good, with just a small difference showing up in the upper curve in Fig. 7a. The main reason for this is here again that the trajectory goes through a node of the wave function, where the velocity varies quickly. The complete numerical solution for the wave function and trajectories is then more demanding. Similar behavior was observed for one-particle interference, but in both cases differences are small, in sharp contrast with results from the hydrodynamic equations.

6 Conclusion

To our knowledge, Bohmian trajectories in the context of interference through wave packet spreading have hitherto been calculated only from exact wave functions. In this paper, we have investigated two different methods for the numerical computation of wave functions. The hydrodynamic equations, written either in Lagrange’s or Euler’s viewpoint, are sensitive to the evaluation of derivatives of the quantum potential. This is especially delicate near wave function nodes, inevitable in interference problems. Lagrange’s viewpoint is usually attractive because the grid automatically adapts to regions of high probability, and because it addresses higher-dimensional problems with relative ease. Yet here proper evaluation of derivatives with the weighted least squares method requires a large number of points and high-order polynomials, and time propagation tends to be unstable. In Euler’s viewpoint, derivatives can be computed more efficiently, and higher-order schemes can be used for time propagation. But then it is simpler and more accurate to use the Schrödinger equation directly, which involves at most second-order derivatives (instead of the gradient of the quantum potential). In both one- and two-particle interference problems, the direct numerical solution of the Schrödinger equation thus provides an accurate and relatively quick way of obtaining wave functions and Bohmian trajectories.
Acknowledgment

One of us (EG) would like to thank the Natural Sciences and Engineering Research Council of Canada for the award of a postgraduate scholarship.

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Our code implementing the Lagrangian approach can probably be improved for speed. Yet with the problem at hand, and for a given number of points and time steps, the Lagrangian approach is much slower than the two others considered.
Figure captions

Figure 1. Two-slit interferometer.

Figure 2. Initial quantum potential. (a) 12 neighbors, 401 points, order of polynomials varied; (b) 12 neighbors, fifth-order polynomials, number of points varied.

Figure 3. Velocity at $t = 0.01$. Other conditions same as in Fig. 2.

Figure 4. Real part of the wave function at $t = 1$.

Figure 5. Imaginary part of the wave function at $t = 1$.

Figure 6. Bohmian trajectories in one-particle interference. The $x$-coordinate is proportional to the $t$-coordinate, since $x(t) = k_x t$.

Figure 7. Bohmian trajectories associated with pairs of particles. (a) $y_1(0) = 1$, $y_2(0) = -0.6$; (b) $y_1(0) = 1$, $y_2(0) = -1.4$. 
Figure 3

(a) Velocity

(b) Velocity

- 2nd degree
- 3rd degree
- 5th degree
- Exact value

(y)
Figure 7