Quantum Dynamics with Bohmian Trajectories

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Short Introduction to Bohmian Mechanics

Ontology and Equations of Motion

- *Bohmian Mechanics* like Newtonian Mechanics is a *mechanical* theory describing the motion of N particles.
- This mechanical theory is of first order. Therefore the motion of the N-particles is governed by an equation of the type

$$\frac{dQ}{dt} = v(Q,t)$$

for particle positions $Q = (\mathbf{q}_1, \ldots \mathbf{q}_N)$ in *configuration space* $\mathbb{R}^{3N}$ and a time-dependent velocity field $v(Q,t)$.

- The Bohmian trajectory $t \mapsto Q(t)$ in configuration space is defined as the integral curve to the velocity field such that $Q(t)|_{t=0} = Q^0$ for some initial configuration Q^0.

- The velocity field is given by

$$v(Q,t) = \Im\mathfrak{m}\frac{\psi_t^* \nabla_Q \psi_t}{\psi_t^* \psi_t}(Q)$$

where ψ_t is the Schrödinger wave function which is a solution of

$$i\frac{\partial \psi_t}{\partial t}(X) = \underbrace{\left(-\nabla_X^2 + V(X) \right)}_{\text{Hamiltonian } H} \psi_t(X)$$

for some initial condition $\psi_t|_{t=0} = \psi^0$.

Formally ∇_X stands for $(\nabla_{\mathbf{x}_1}, \ldots, \nabla_{\mathbf{x}_N})$.
Moreover, $X = (\mathbf{x}_1, \ldots, \mathbf{x}_n) \in \mathbb{R}^{3N}$ and throughout the talk we shall use units of mass $m = \hbar = 1$.

Existence and Uniqueness

- For almost every Q^0 and under general conditions on the initial condition ψ^0 and the potential V one has *existence* and *uniqueness* of Bohmian trajectories

$$t \mapsto Q(t; Q^0, \psi^0) = Q(t)$$

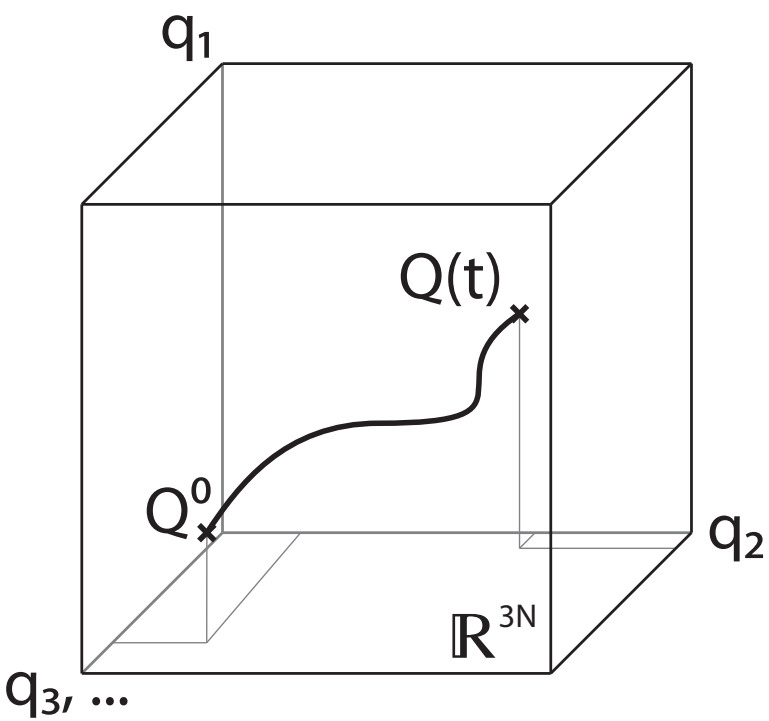
in Configuration space (!).

This means in particular that in configuration space:

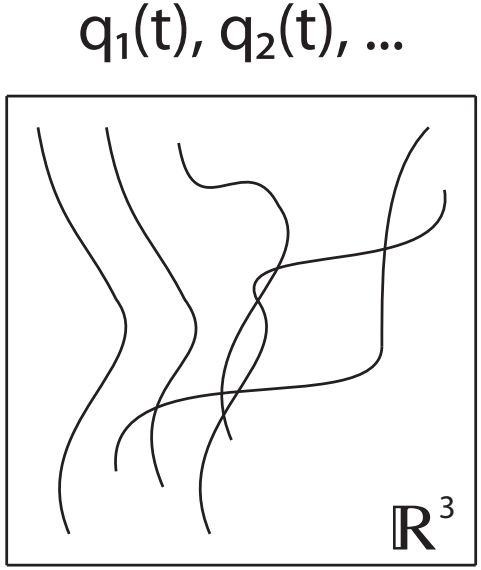
- Bohmian trajectories cannot run into nodes of the wave function where the velocity field is ill-defined.
- Bohmian trajectories cannot cross.

Configuration Space and Physical Space

configuration space:



physical space:



Equivariance and Agreement with QM

By virtue of the Bohmian velocity field the continuity equation for the Bohmian flow on configuration space is identically fulfilled by $\rho_t = |\psi_t|^2$:

$$\frac{\partial}{\partial t}|\psi_t(X)|^2 + \nabla_X \cdot \left(|\psi_t(X)|^2 \, v(X) \right) = 0.$$

Equivariance:

- So if the initial configuration of particles $Q^0 = (\mathbf{q}_i^0, \ldots, \mathbf{q}_N^0)$ is distributed according to $|\psi^0|^2$ at time $t = 0$ then the configuration $Q(t; Q^0, \psi^0)$ will be $|\psi_t|^2$ distributed for any time t.

- This is Born's law.

The Euler Form

- By expressing the wave function in its Euler form:

$$\psi_t(X) = R_t(X)e^{iS_t(X)}$$

we may rewrite the Bohmian velocity law as

$$\frac{dQ}{dt} = \nabla_Q S_t(Q)$$

and the Schrödinger equation as

$$\frac{\partial R_t(X)}{\partial t} = -\nabla_X \cdot \Big(R_t(X)\, \nabla_X S_t(X) \Big) - \frac{1}{2} R_t(X) \Big(\nabla_X^2 S_t(X) \Big)$$

$$\frac{\partial S_t(X)}{\partial t} = -\frac{1}{2} \left(\nabla_X S_t(X) \right)^2 - V(X) + \frac{1}{2} \frac{\nabla_X^2 R_t(X)}{R_t(X)}.$$

In the Reference Frame of a Bohmian Configuration

Substituting a X by a Bohmian trajectory $Q(t)$ and carrying out the t differentiation turns these equations into the form:

$$\frac{dQ}{dt} = \nabla_Q S_t(Q)$$
$$\frac{dR_t(Q)}{dt} = -\frac{1}{2} R_t(Q)\, \nabla_Q^2 S_t(Q)$$
$$\frac{dS_t(Q)}{dt} = \underbrace{\frac{1}{2}\left(\frac{dQ}{dt}\right)^2 - V(Q)}_{\text{classical Lagrangian}} + \underbrace{\frac{1}{2}\frac{\nabla_Q^2 R_t(Q)}{R_t(Q)}}_{\text{quantum potential}}$$

- These are the Bohmian equations of motion viewed from the reference frame of a moving Bohmian configuration.
- In contrast to the classical Hamilton-Jacobi equation an additional term, the *quantum potential*, shows up in Bohmian Mechanics.

Numerical Simulations using Bohmian Mechanics

The Goal

- The task of such numerical simulations is to integrate the Schrödinger equation

$$i\frac{\partial \psi_t}{\partial t}(X) = \underbrace{\left(-\nabla_X^2 + V(X) \right)}_{\text{Hamiltonian } H} \psi_t(X).$$

  Recall $X = (\mathbf{x}_1, \ldots, \mathbf{x}_N)$.

- More specifically, given an initial wave function ψ^0, known only on a grid of M grid points $Q_1, \ldots, Q_M$, and a time t, we want to find a numerical approximation ψ_t^{num} of the real solution

$$\psi_t = e^{-iHt}\psi^0.$$

- The sense of the approximation has to be physically meaningful.

- Recall Born's law:

$$|\psi_t(X)|^2 d^{3N}X$$

  is the probability of finding N particle configuration in the volume element $d^{3N}X$ at $X = (x_1, \ldots, x_N)$.
- Therefore a good approximation ψ_t^{num} is one for which the L^2 distance

$$\|\psi_t - \psi_t^{num}\|_{L^2} := \sqrt{\int d^{3N}X \, |\psi_t(X) - \psi_t^{num}(X)|^2}$$

  is small.
- While there are many methods for this task, here, we only want to discuss the one of Lopreore and Wyatt $\rightarrow$

The Method of Lopreore and Wyatt

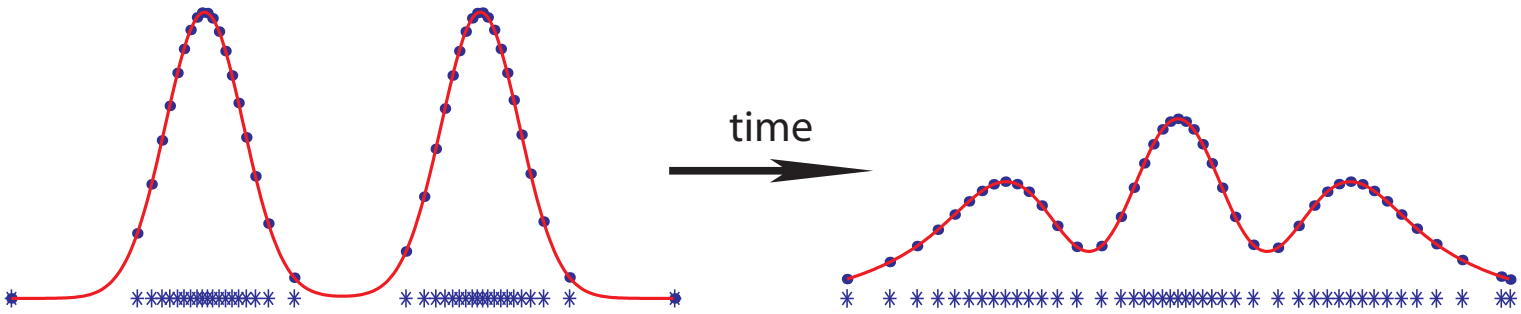
- Instead of integrating the Schrödinger equation alone we integrate the equations of Bohmian Mechanics in Euler form

$$\frac{dQ}{dt} = \nabla_Q S_t(Q)$$
$$\frac{dR_t(Q)}{dt} = -\frac{1}{2} R_t(Q)\, \nabla_Q^2 S_t(Q)$$
$$\frac{dS_t(Q)}{dt} = \frac{1}{2}\left(\frac{dQ}{dt}\right)^2 - V(Q) + \frac{1}{2}\frac{\nabla_Q^2 R_t(Q)}{R_t(Q)}$$

  simultaneously for M grid points $Q_1, \ldots, Q_M$ in configuration space.
- The grid points, however, are not fixed but move along their Bohmian trajectories $Q(t; Q_i, \psi^0)_{1 \le i \le M}$ in configuration space.

The Bohmian Grid and its Advantages

- Recall that initially $|\psi^0|^2$ distributed grid points $Q_1, \ldots, Q_M$ moving on their Bohmian trajectories $Q(t; Q_1; \psi^0), \ldots, Q(t; Q_M; \psi^0)$ will remain $|\psi_t|^2$ distributed for all times t by equivariance!



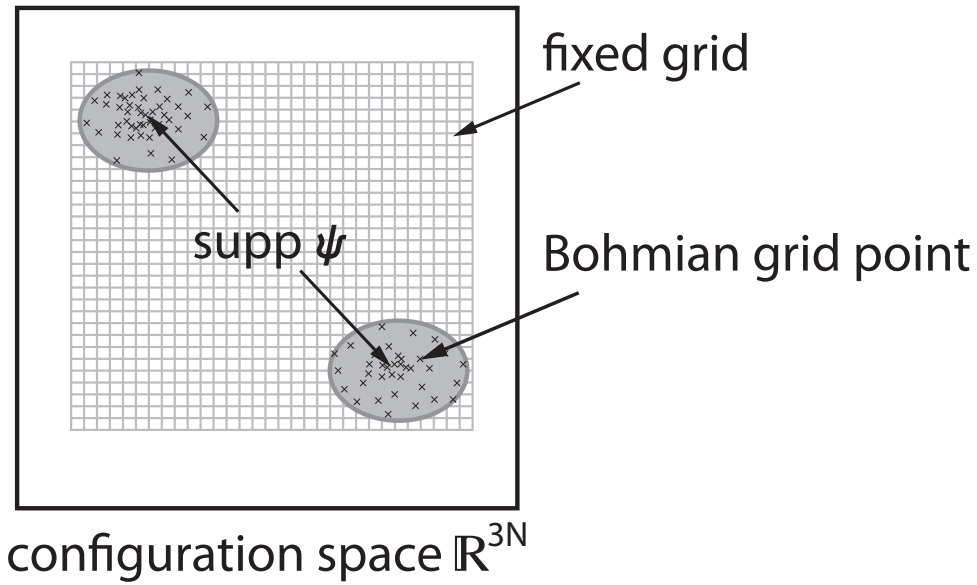
- Such grids shall be called Bohmian grids.

- Thus, grid points will typically stay in regions where $|\psi_t|^2 = R_t^2$ is large and avoid regions where $|\psi_t|^2$ is small. This distribution of grid points naturally respects the L^2-norm!
- Hence, numerically problematic cases where $R_t = |\psi_t|$ is near zero are typically excluded. Recall the form of the quantum potential:

$$\frac{1}{2}\frac{\nabla_Q^2 R_t(Q)}{R_t(Q)}.$$

- As the grid points move along with the support of ψ_t this method is particular interesting for long-time asymptotics.

- Considerably less grid points are needed than in methods using fixed grids. Consider a ψ_t with a support shown below:



- It is therefore expected that this algorithm scales considerably better with the number of degrees of freedom than any fixed grid method - which roughly scales like $const^{3N}$.
- The dynamical system is over-determined since the grid points are $|\psi_t|^2$ distributed by equivariance. This allows real-time error detection.

However, all of these advantages crucially depend on whether the grid points move along their Bohmian trajectories.

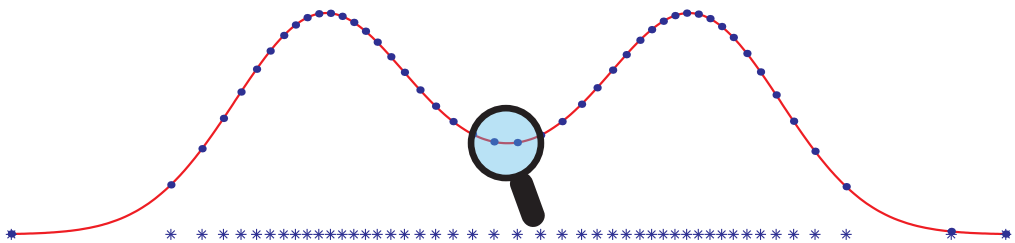
- Recall that by uniqueness of the Bohmian trajectory in configuration space, trajectories do not cross!
- Therefore, a simple criterion weather the numerically computed grid point trajectories behave at least "Bohmian-like" is to check if they stay apart from each other for all times.
- A trajectory crossing during a numerical simulation means that the simulated time-evolution is not Bohmian anymore, and thus not quantum mechanical, and therefore physically false.

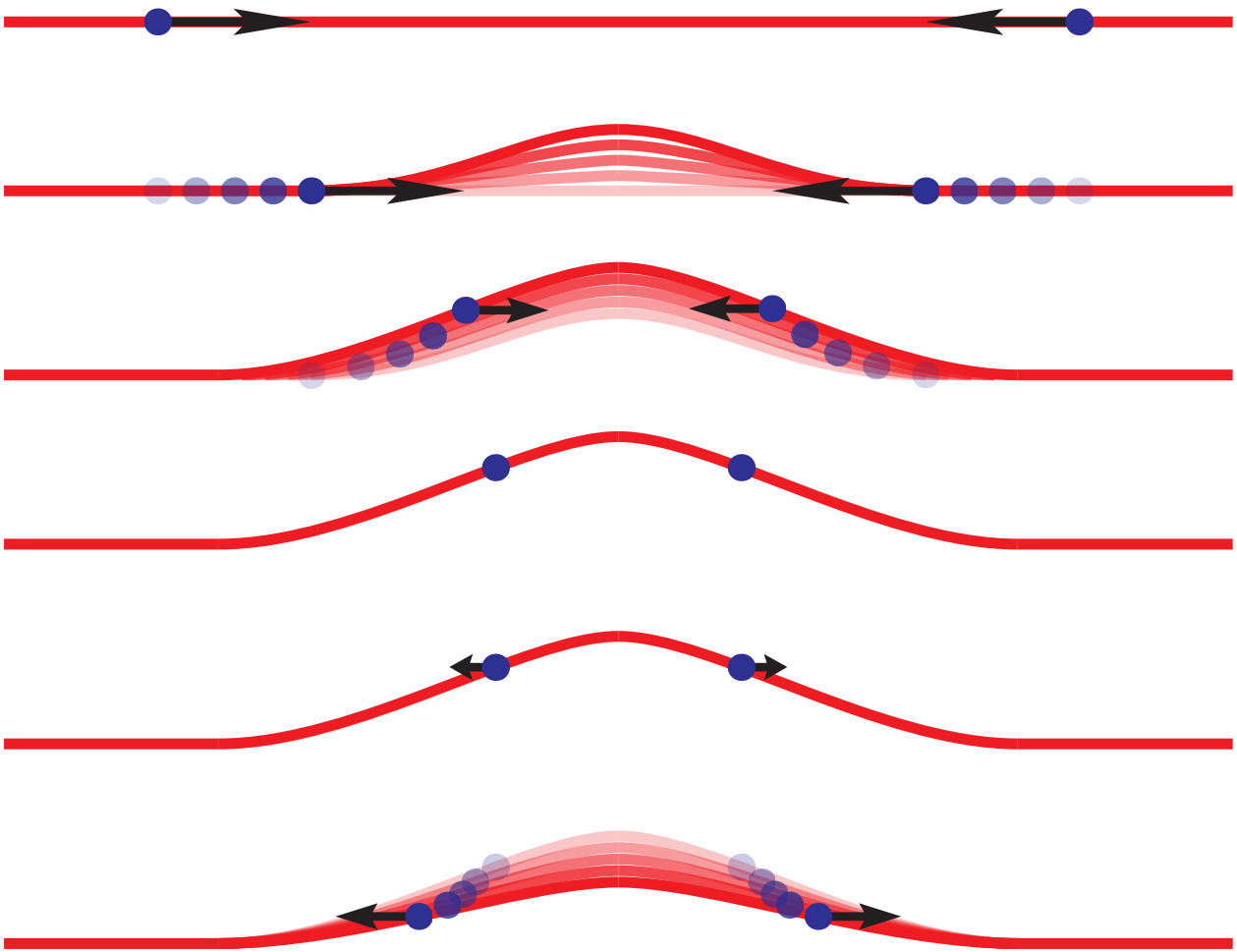
The Quantum Potential

- By its form the quantum potential

$$\frac{1}{2}\frac{\nabla_Q^2 R_t(Q)}{R_t(Q)}$$

  recognizes the curvature of $R_t = |\psi_t|$ in terms of the second derivative of R_t.
- In particular, it is responsible for the dispersion (spreading of the wave function).
- Let us see how the quantum potential keeps grid point apart by means of an example with two initially approaching particles, e.g.:





1. initially both particles approach each other

2. formation of a microscopic bump in $|\psi|$

3. the quantum potential recognizes this increase in curvature

4. the particles are decellerated

5. in an extreme case the particles may pick up velocities in opposite direction

6. the curvature of $|\psi|$ relaxes again

Fitting Algorithms

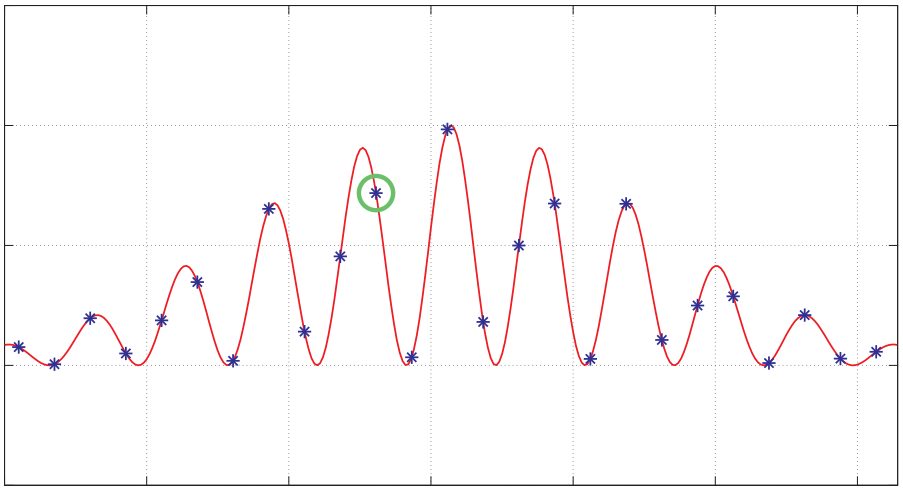
- The crucial part in the numerical simulation is to compute the derivatives involved in the Bohmian equations of motion.
- One commonly used idea is to use a fitting algorithm which finds polynomials in some sense locally close to the functions S_t and R_t. The derivative can then be computed by algebraic means.
- In order to reproduce the correct quantum potential we have to choose a fitting algorithm that computes a very good approximation of the second derivative of R_t!

First Assertion: Smoothing is bad!

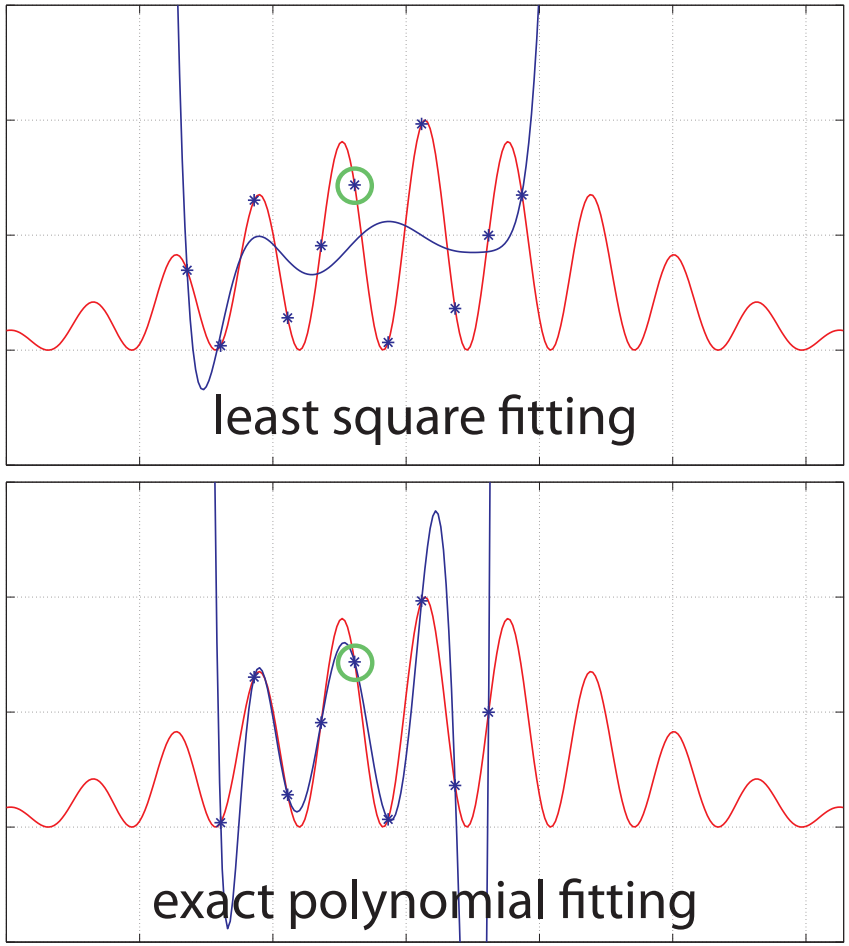
- Fitting algorithms with smoothing behavior like *least square fitting* do not have the chance to reproduce the quantum potential correctly because they cannot recognize these microscopic bumps of R_t, and hence not the true second derivative of R_t.
- Therefore the discussed mechanism which keeps the grid points apart is bound to fail.

- We need to apply a fitting algorithm which has no smoothing behavior.
- This is provided by what we shall call exact polynomial fitting, which for $n > 0$ distinct points, e.g. $(X_i, R_t(X_i))_{1 \leq i \leq n}$, finds a unique fitting polynomial of $(n-1)$-th order that goes exactly through the given points.
- Such fitting polynomials are forced to recognize the microscopic bumps of R_t.

Suppose we want to find a derivative at the marked grid point of the red function below which is known only at the displayed grid points:



- We compute two local fitting polynomials of 8-th order in the neighborhood of the marked grid point.
- The first time by least square minimization with 11 data points and the second time by exact polynomial fitting with 9 data points $\longrightarrow$

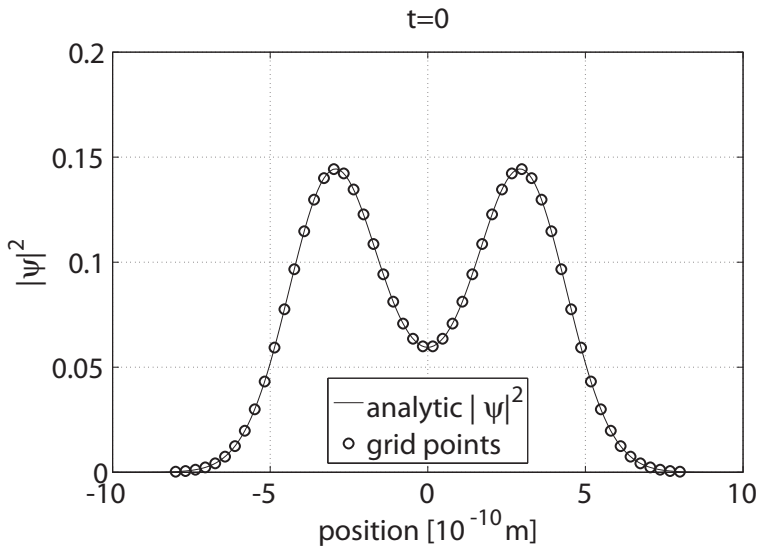

least square fitting
exact polynomial fitting

A Numerical Example

A Numerical Example

In [Dürr,Pickl,D.-A.D.] we gave an numerical example which implements the idea of Lopreore and Wyatt for one particle with the mass of an electron in one dimension:

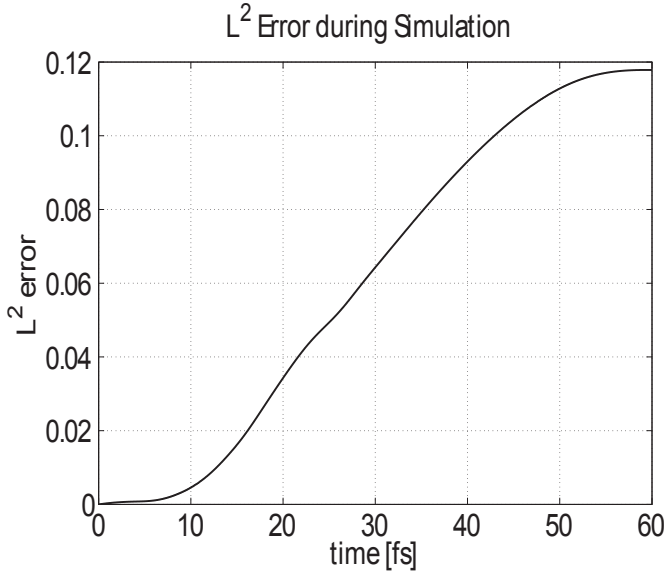
- We ran the numerical simulation twice. First with exact polynomial fitting and second with least square fitting.
- As initial conditions we took two superposed real gaussians as ψ^0 and uniformly distributed grid points $Q_1, \ldots, Q_M$ for $M = 51$.



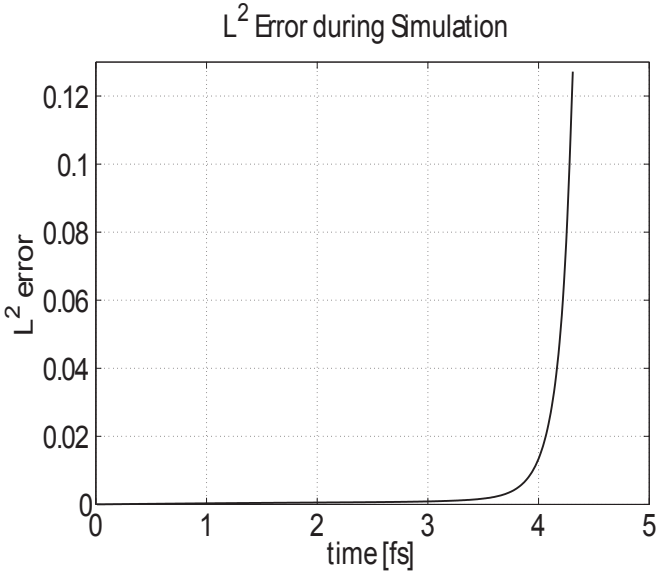
- As time step we took $10^{-2} fs$ which, in our case, is sufficiently small to give the quantum potential enough time-steps to prevent trajectory crossings.
- In both runs we used fitting polynomials of 6th order which provide sufficient information for the computation of the first three derivatives.
- In the first run exact polynomial fitting was applied using 7 grid points per local fit.
- In the second run least square fitting is applied using 9 grid points per local fit. Note that this induces only a very mild smoothing!

Results:

- The first run with exact polynomial fitting runs way beyond 5000 integration steps, i.e. $50fs$.
- In the second run a trajectory crossing is reported after 430 integration steps, i.e. $4.3fs$.



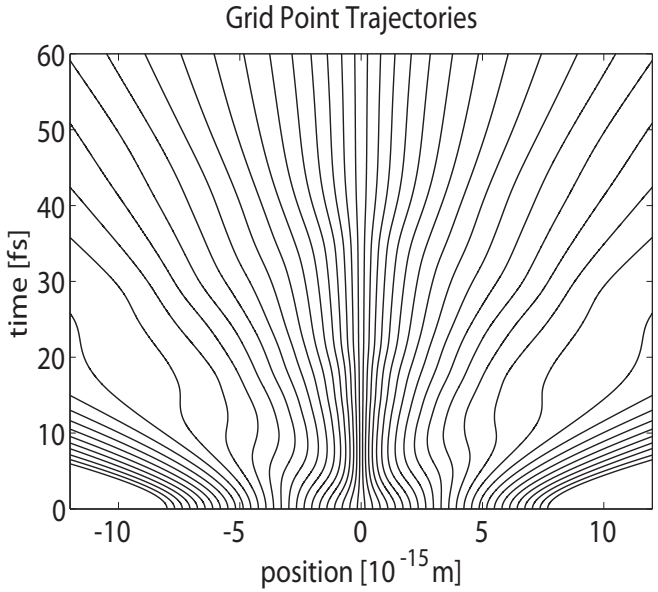
exact polynomial fitting



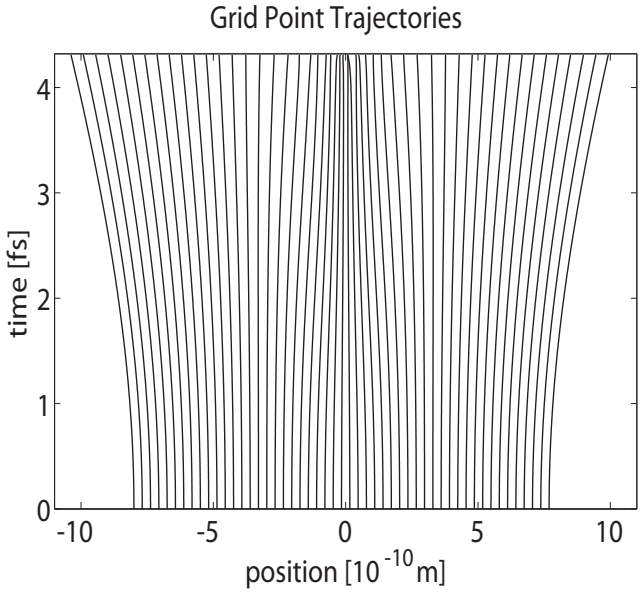
least square fitting

Trajectories

A look at the trajectories of both runs clearly shows where least square fitting fails:



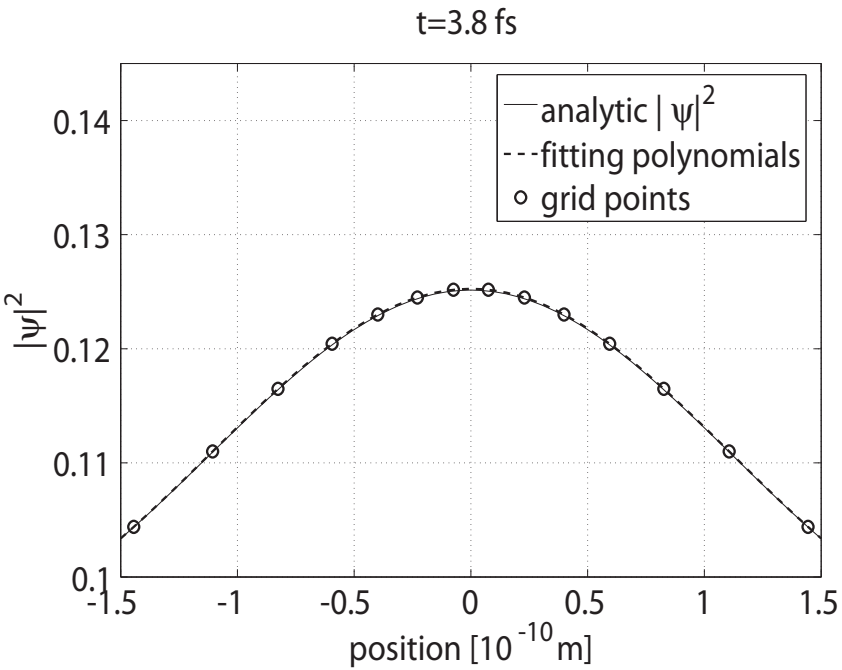
exact polynomial fitting



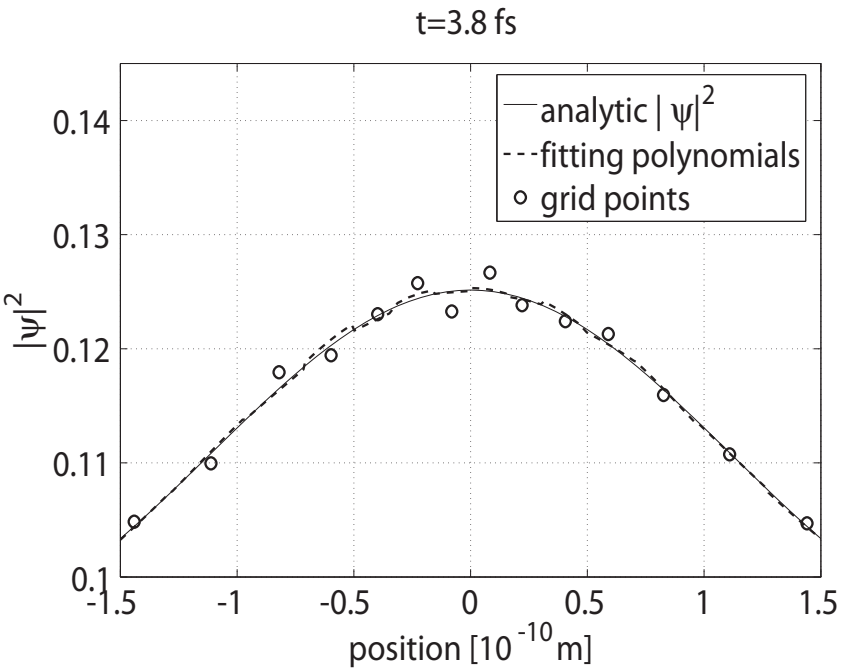
least square fitting

Fitting polynomials

A zoomed in view of the middle region where the tails of the gaussians meet and the particles move fastest towards each other shortly before the trajectory crossing:



exact polynomial fitting



least square fitting

Summary

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- Bohmian trajectories do not cross and do not run into nodes.
- If the initial configuration Q^0 is $|\psi^0|^2$ distributed, then the configuration at any time t: $Q(t; Q^0, \psi^0)$ transported by the Bohmian flow is again $|\psi_t|^2$ distributed.
- Bohmian Mechanics can be used to integrate the Schrödinger equation on a best-adapted grid, i.e the Bohmian grid.
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Appendix

Finding local fitting polynomials

We want to find an approximating by polynomials of degree $(m-1)$ to a function f, from which we only know n pairwise distinct points $(x_i, f(x_i))_{1\leq i\leq n}$ of its graph. Let

$$\begin{aligned} y &:= (f(x_i))_{1\leq i\leq n} \\ X &:= (x_i^{(j-1)})_{1\leq i\leq n, 1\leq j\leq m} \\ a &= (a_i)_{1\leq i\leq m} \in \mathbb{R}^m \\ \delta &= (\delta_i)_{1\leq i\leq n} \in \mathbb{R}^n \end{aligned}$$

Using this notation the problem of finding a fitting polynomial to f on the reduces to finding the coefficients of the vector a obeying the equation

$$y = X \cdot a + \delta$$

such that the error term δ is in some sense small. The fitting polynomial is then given by $p(x) = \sum_{j=1}^{m} a_j x^{j-1}$.

- In the case $n = m$. The fitting polynomial is uniquely defined by $a = X^{-1} \cdot y$. This is what we called exact polynomial fitting.
- For arbitrary $n > m$ there is in general no unique solution anymore. Therefore an additional principle to determine the fitting polynomial is needed. In the case of least square fitting it is minimization of the weighted error:

$$\triangle := \sum_{i=1}^{n} w(x - x_i)\delta_i^2$$

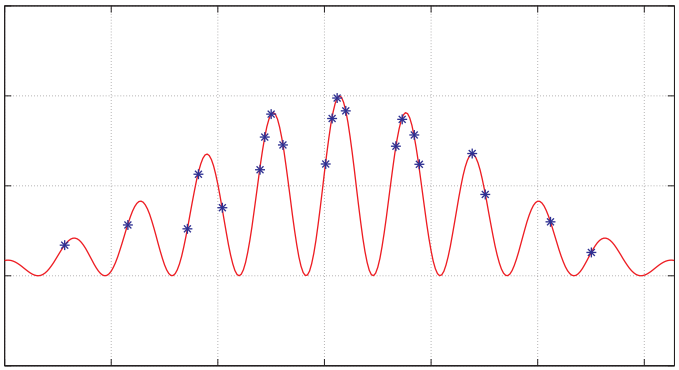
where w is a given weight function. The vector a is then determined by the equation:

$$\left(\frac{\partial \Delta(a)}{\partial a_j}\right)_{1 \leq j \leq m} = \left(-2 \sum_{i=1}^{n} w(x - x_i)(y - X \cdot a)_i x_i^{j-1}\right)_{1 \leq j \leq m} = 0$$

- Clearly, for any weight $w > 0$ and $m = n$ exact polynomial fitting and least square fitting produces the same a.

Disadvantages of Bohmian Grids

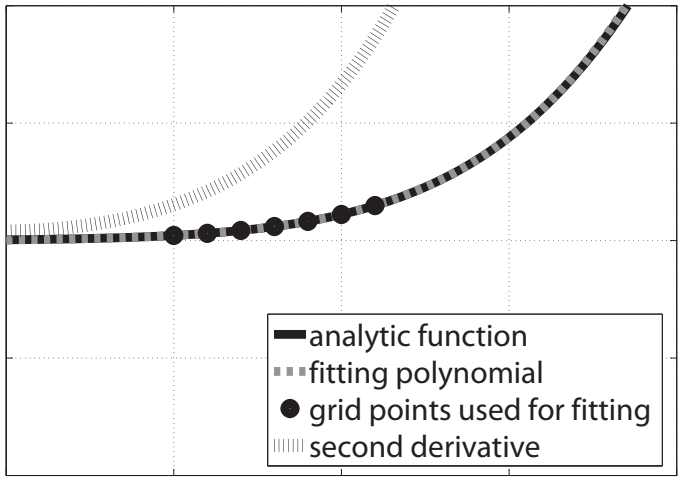
- As we have seen, on a Bohmian grid the grid points are typically where $|\psi_t|^2$ is large and avoid regions where it is small by equivariance.
- Bad situations may arise whenever $|\psi_t|^2$ is highly oscillatory since such a grid might not accurately detect the curvature of $|\psi_t|^2$. E.g.

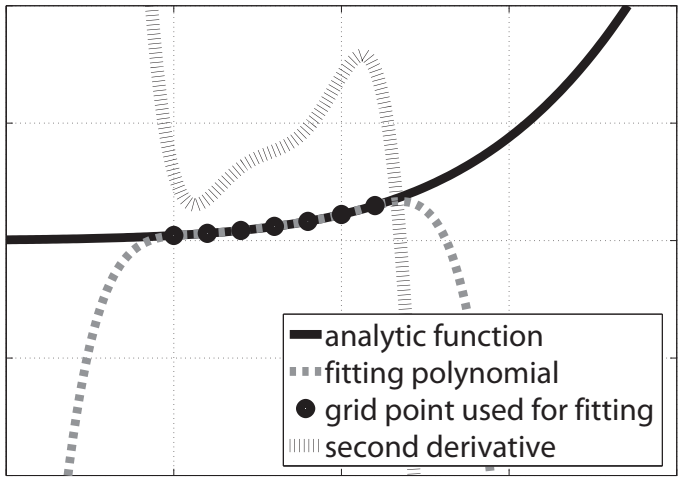


- One idea is to control such situations, which can be detected by measuring the increase in curvature of R_t, by adding an auxiliary grid which can be deleted when the situations improves.

Boundary Problem

- Exact polynomial fitting creates a more severe problem at the boundary of the supporting grid than e.g. least square fitting because the fitting polynomials are a lot more sensitive to numerical errors.
- This problem, however, is of conceptual kind because there is a generic lack of knowledge of how to continue the wave function beyond the boundary of the grid.
- That is why this problem will eventually show up also with least square fitting.
- One idea is to use the smoothness of the decay of the wave function near the boundary of the grid as a guide to solve this problem.





- Left: Exact polynomial fitting as well as least square fitting give the same fitting polynomial. The second derivative of the fitting polynomial decays.
- Right: The very left grid point is shifted by an (invisible) small amount to simulate a numerical error. While least square fitting (not shown) smoothes over the numerical error, exact polynomial fitting reacts severely and the second derivative strongly increases which will cause non-physically high velocities.