NUMERICAL SOLUTION OF QUANTUM PROBLEMS VIA BOHMIAN TRAJECTORIES
Outline of the talk

- Time Dependent Schroedinger Equation
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- Numerical Methods via Bohmian Trajectories
  - Single Particle
    - Quantum Trajectory Method
    - Single Trajectory
  - Many Particle
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- Time Dependent Schroedinger Equation

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- Measurement issue
  - Theoretical Model
  - Numerical Simulation
Time Dependent Schroedinger Equation

\[ i\hbar \frac{\partial \psi}{\partial t} = \mathbf{H}\psi \]

Different numerical approaches for different problems

Single Particle

\[ i\hbar \frac{\partial \psi}{\partial t} = \left( -\frac{\hbar^2}{2m} \nabla^2 + V \right)\psi \]

\[ \psi = \psi(x, t) \]


Many Particle

\[ i\hbar \frac{\partial \psi}{\partial t} = \left( -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \nabla_i^2 + V \right)\psi \]

\[ \psi = \psi(x_1, x_2, \ldots, x_N, t) \]

We can use the trajectories $X_t$ of Bohmian Mechanics

$$\dot{X}_t = v \quad \text{where} \quad v = \frac{\hbar}{m} \text{Im} \frac{\nabla \psi}{\psi}$$
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Polar form

$$\psi = \text{Re} \frac{i}{\hbar} S \quad \rightarrow \quad v = \frac{\nabla S}{m}$$
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Polar form $\psi = \text{Re} \frac{i}{\hbar} S$ $\rightarrow$ $v = \frac{\nabla S}{m}$

Schroedinger equation

$$\frac{\partial S}{\partial t} = -\frac{\nabla^2 S}{2m} - V + \frac{\hbar^2}{2m} \frac{\nabla^2 R}{R}$$

$$\frac{\partial \rho}{\partial t} + \nabla \left( \rho \frac{\nabla S}{m} \right) = 0$$
Bohmian Mechanics

We can use the trajectories $X_t$ of Bohmian Mechanics

$$\dot{X}_t = v \quad \text{where} \quad v = \frac{\hbar}{m} \text{Im}\frac{\nabla \psi}{\psi}$$

Polar form

$$\psi = \text{Re}\left(\frac{i}{\hbar} S\right) \quad \rightarrow \quad \psi = m \frac{\nabla S}{m}$$

Schroedinger equation

$$\frac{\partial S}{\partial t} = -\frac{\nabla^2 S}{2m} - V + \frac{\hbar^2}{2m} \frac{\nabla^2 R}{R}$$

$$\frac{\partial \rho}{\partial t} + \nabla \left( \rho \frac{\nabla S}{m} \right) = 0$$

Equation of motion

$$m \frac{d^2 X_t}{dt^2} = F_{\text{class}} + F_{\text{quant}}$$

$$F_{\text{class}} = -\nabla V$$

$$F_{\text{quant}} = -\nabla \left( -\frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} \right)$$
Quantum Trajectory Method

Solve the hydrodynamic equations in the lagrangian frame for a time interval $\delta t$.

$\downarrow$

Reconstruct the wave function in the update positions of the particles by means of an interpolation method. (eg. MWLS, RBF, ...)

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Reconstruct the wave function in the update positions of the particles by means of an interpolation method. (eg. MWLS, RBF, ...)

Single Trajectory

We solve the Schrödinger equation along a single trajectory.

$\Downarrow$

Sampling we can obtain the entire wave function.

Quantum Trajectory Method

The method uses the Lagrangian formulation of the Hamilton-Jacobi and Continuity Equation

\[ m \frac{d \vec{v}(\vec{x}, t)}{dt} = - \vec{\nabla}[V(\vec{x}, t) + U(\vec{x}, t)] \]

\[ \frac{d \rho(\vec{x}, t)}{dt} = - \rho(\vec{x}, t) \frac{\vec{\nabla} \cdot \vec{v}(\vec{x}, t)}{m} \]
Quantum Trajectory Method

The method uses the Lagrangian formulation of the Hamilton-Jacobi and Continuity Equation

\[
m \frac{d\vec{v}(\vec{x}, t)}{dt} = -\vec{\nabla} [V(\vec{x}, t) + U(\vec{x}, t)]
\]

\[
d \rho(\vec{x}, t) \frac{dt}{dt} = -\rho(\vec{x}, t) \frac{\vec{\nabla} \cdot \vec{v}(\vec{x}, t)}{m}
\]

The Propagation at discrete time is

\[
\rho(\vec{x}_i(t_{n+1}), t_{n+1}) = \rho(\vec{x}_i(t_n), t_n) e^{-\vec{\nabla} \cdot \vec{v}(\vec{x}_i(t_n), t_n) \delta t}
\]

\[
\vec{v}(\vec{x}_i(t_{n+1}), t_{n+1}) = \vec{v}(\vec{x}_i(t_n), t_n) - \frac{\delta t}{m} \vec{\nabla} [V(\vec{x}_i(t_n), t_n) + U(\vec{x}_i(t_n), t_n)]
\]

\[
\vec{x}_i(t_{n+1}) = \vec{x}_i(t_n) + \vec{v}(\vec{x}_i(t_n), t_n) \delta t.
\]

The TDSE is solved along the trajectories and step by step.
The idea of the algorithm

\[ Q_0 \rightarrow \psi_0 \rightarrow Q_1 \rightarrow \psi_1 \rightarrow \cdots \rightarrow Q_n \rightarrow \psi_n \]
Single Trajectory

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we stop the iteration when

\[ \psi_n \approx \psi_{n-1} \text{ and } Q_n \approx Q_{n-1} \]
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Single trajectory: \( x_0 \) on \( |\psi_0|^2 \)

Known \( R_{n-1} \) and \( S_{n-1} \), we calculate

1. \( \dot{Q}_n = \frac{\nabla S_{n-1}}{m} \)
2. \( R_n = R_{n-1}(x_0, 0)|J_{n-1}|^{\frac{1}{2}} \)
3. \( S_n = S_{n-1}(x_0, 0) + \int_{0}^{t_1} m\dot{Q}_{n-1}^2 - V_{n-1} - U_{n-1} \)
Single Trajectory

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\[ R_n = R_{n-1}(x_0, 0)|J_{n-1}|^{1/2} \]

\[ S_n = S_{n-1}(x_0, 0) + \int_0^{t_1/2} m\dot{Q}_{n-1}^2 - V_{n-1} - U_{n-1} \]
Single Trajectory

Sampling new initial position

![Graph showing position vs. time for a single trajectory]

We obtain the wave function...
Single Trajectory

Sampling new initial position

We obtain the wave function
Single Trajectory

Sampling new initial position

We obtain the wave function

Interpolation gives $\psi_t$ at every $x$
Many Particle - TDSE

\[ i\hbar \frac{\partial \psi(x_1, x_2, \ldots, x_N, t)}{\partial t} = \left[ -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \nabla_i^2 + V(x_1, x_2, \ldots, x_N, t) \right] \psi(x_1, x_2, \ldots, x_N, t) \]

Impossibility to solve numerically the above equation with standard methods!!!
Many Particle - TDSE

\[ i\hbar \frac{\partial \Psi(x_1, x_2, \ldots, x_N, t)}{\partial t} = \left[ -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \nabla_i^2 + V(x_1, x_2, \ldots, x_N, t) \right] \Psi(x_1, x_2, \ldots, x_N, t) \]

Impossibility to solve numerically the above equation with standard methods!!!

***

Using the same Bohmian method for single particle equation we obtain a system of \(N\) coupled equations

\[
\begin{aligned}
\frac{d^2 x_i}{dt^2} = -\nabla_i [V(x_1, x_2, \ldots, x_N, t) + U(x_1, x_2, \ldots, x_N, t)] \bigg|_{x_1=x_1(t),\ldots,x_N=x_N(t)} \\
\end{aligned}
\]
Many Particle - *TDSE*

\[ i\hbar \frac{\partial \psi(x_1, x_2, \ldots, x_N, t)}{\partial t} = \left[ -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \nabla_i^2 + V(x_1, x_2, \ldots, x_N, t) \right] \psi(x_1, x_2, \ldots, x_N, t) \]

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&\vdots \\
&\text{At this point we have to know } \psi \\
&\text{Impossible to solve numerically the above system}
\end{aligned}
\]
Many Particle - TDSE

\[
\frac{i\hbar}{\partial t} \psi(x_1, x_2, \ldots, x_N, t) = \left[ -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \nabla_i^2 + V(x_1, x_2, \ldots, x_N, t) \right] \psi(x_1, x_2, \ldots, x_N, t)
\]

Impossibility to solve numerically the above equation with standard methods!!!

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\begin{align*}
\frac{d^2 x_i}{dt^2} = -\nabla_i [V(x_1, x_2, \ldots, x_N, t) + U(x_1, x_2, \ldots, x_N, t)] |_{x_1=x_1(t),\ldots,x_N=x_N(t)} \\
\vdots
\end{align*}
\]

At this point we have to know \( \Psi \)

Impossibility to solve numerically the above system

\[\Downarrow\]

We need a new approach!
Theorem: Many-particle Bohm trajectory

\[ x_a(t) \] solution of many particle Schroedinger equation \( \Psi(x_a, \vec{x}, t) \)
Many Particle - Trajectory

**Theorem:** Many-particle Bohm trajectory

\[ x_a(t) \text{ solution of many particle Schrödinger equation } \Psi(x_a, \vec{x}, t) \]

can be calculated from a single particle wave function

\[ \psi_a(x_a, t) = \Psi(x_a, \vec{x}(t), t) \text{ solution of the pseudo-Schrödinger equation} \]

\[
i\hbar \frac{\partial \psi_a(x_a, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_a^2} + V_a(x_a, \vec{x}(t), t) + G_a(x_a, \vec{x}(t), t) + iJ_a(x_a, \vec{x}(t), t) \right] \psi_a(x_a, t)
\]
Many Particle - *Trajectory*

**Theorem:** Many-particle Bohm trajectory

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can be calculated from a single particle wave function

\[ \psi_a(x_a, t) = \Psi(x_a, \vec{x}(t), t) \] solution of the pseudo-Schroedinger equation

\[
i\hbar \frac{\partial \psi_a(x_a, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_a^2} + V_a(x_a, \vec{x}(t), t) + G_a(x_a, \vec{x}(t), t) + iJ_a(x_a, \vec{x}(t), t) \right] \psi_a(x_a, t)
\]

with a suitable approximation for

\[ G_a(x_a, \vec{x}(t), t) \text{ and } iJ_a(x_a, \vec{x}(t), t) \]

we can solve many particle problems.

Applications

- Quantum Trajectory Method
  Kinetic chemistry, dissociation problems.
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- Single Trajectory
Applications

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- Single Trajectory

- Many Particle
  Problems of transport in nanoelectric devices.
Measurement issue

Von Neumann Model

Interaction between system and apparatus

$x \in X \rightarrow \text{system} \quad y \in Y \rightarrow \text{apparatus}$

\[ H_{VN} = -\lambda \hat{A} \otimes \hat{P}_y \]

Only

\[ H_{VN} \rightarrow \psi_\alpha(x) \phi_0(y - \lambda a_\alpha t) \]

where

\[ A_\psi_\alpha = a_\alpha \psi_\alpha \]

\[ H_{\text{meas}} = H_{\text{syst}} + H_{\text{app}} + H_{VN} \]

We assume that

\[ M \gg m \]
Measurement issue

Von Neumann Model

Interaction between system and apparatus
\[ x \in X \to \text{system} \quad y \in Y \to \text{apparatus} \]

\[ H_{VN} = -\lambda \hat{A} \otimes \hat{P}_y \quad \text{where} \quad \hat{P}_y \equiv i\hbar \partial/\partial y \]

Only \( H_{VN} \to \psi_\alpha(x)\phi_0(y - \lambda a_\alpha t) \)

where \( A\psi_\alpha = a_\alpha \psi_\alpha \)
**Von Neumann Model**

Interaction between system and apparatus

\[ x \in X \rightarrow \text{system} \quad y \in Y \rightarrow \text{apparatus} \]

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Only \( H_{VN} \rightarrow \psi_\alpha(x)\phi_0(y - \lambda a_\alpha t) \)

where \( A\psi_\alpha = a_\alpha \psi_\alpha \)

\[ H_{\text{meas}} = H_{0}^{\text{syst}} + H_{0}^{\text{app}} + H_{VN} \quad \text{where} \quad A(x) = \chi[0, +\infty) - \chi(-\infty, 0] \]

We assume that \( M \gg m \)
Measurement issue

Hydrodynamic equations

\[
\frac{\partial S}{\partial t} = -\frac{1}{2m} \left( \frac{\partial S}{\partial x} \right)^2 - \frac{1}{2M} \left( \frac{\partial S}{\partial y} \right)^2 + \\
+ \lambda A(x) \frac{\partial S}{\partial y} + \frac{\hbar^2}{2mR} \frac{\partial^2 R}{\partial x^2} + \frac{\hbar^2}{2MR} \frac{\partial^2 R}{\partial y^2}
\]

\[
\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x} \left( \rho \frac{1}{m} \frac{\partial S}{\partial x} \right) - \frac{\partial}{\partial y} \left[ \rho \left( \frac{1}{M} \frac{\partial S}{\partial y} + \lambda A(x) \right) \right]
\]

Guidance equations

\[
v_x \equiv \frac{1}{m} \frac{\partial S}{\partial x} \quad v_y \equiv \frac{1}{M} \frac{\partial S}{\partial y} + \lambda A(x)
\]
Evolution of the complete wave function system + apparatus ($\Psi$)

\[ \Psi_0 = \psi_0(x)\phi_0(y) \]

where

\[ \psi_0(x) = \psi_+^0(x) + \psi_-^0(x) \]

\[ A\psi_+ = +1 \cdot \psi_+ \]
\[ A\psi_- = -1 \cdot \psi_- \]
Evolution of the complete wave function system + apparatus ($\Psi$)

\[
\Psi_0 = \psi_0(x) \phi_0(y)
\]

where

\[
\psi_0(x) = \psi_+(x) + \psi_-(x)
\]

\[
A\psi_+ = +1 \cdot \psi_+ \\
A\psi_- = -1 \cdot \psi_-
\]

After the interaction we have

\[
\Psi_t = \psi_+(x) \phi_+(y) + \psi_-(x) \phi_-(y)
\]
Measurement issue

Wave Function of the Measured System \( \psi_{\text{cond}} = \frac{\psi_t(x, Y_t)}{||\psi_t(x, Y_t)||} \)

\[ \psi_+ \]

\[ \psi_- \]

\( X_0 = 6.6 \text{ a.u.} \quad Y_0 = 0.6 \text{ a.u.} \)

\( X_0 = -5.2 \text{ a.u.} \quad Y_0 = 0.6 \text{ a.u.} \)
Wave Function of the Measured System

\[ \psi_{\text{cond}} = \frac{\psi_t(x, Y_t)}{||\psi_t(x, Y_t)||} \]

\[ \psi_+ \]

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Thank you for your attention!