Università degli studi di Genova 21 June 2012

NUMERICAL SOLUTION OF

QUANTUM PROBLEMS

VIA BOHMIAN TRAJECTORIES

Outline of the talk

- Time Dependent Schroedinger Equation

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

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    - Quantum Trajectory Method
    - Single Trajectory
  - Many Particle
- 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

$$i\hbar\frac{\partial\psi}{\partial t} = (-\frac{\hbar^2}{2m}\nabla^2 + V)\psi$$

$$\psi = \psi(x, t)$$

Reference: C. L. Lopreore and R. E. Wyatt: *Quantum Wavepacket Dynamics with Trajectories*, Phys. Rev. Lett. 82, 5190-5193 (1999).

Many Particle

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

$$\psi = \psi(x_1, x_2, ..., x_N, t)$$

Reference: X. Oriols: *Quantum-trajectory approach to time-dependent transport in mesoscopic systems with electron-electron interactions*, Phys. Rev. Lett. 98, 066803 (2007).

Bohmian Mechanics

We can use the trajectories X_t of Bohmian Mechanics

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

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Schroedinger equation

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

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

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Equation of motion

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

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

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

Single Particle

Quantum Trajectory Method

Solve the hydrodynamic equations in the lagrangian frame for a time interval δt.

$$\Downarrow$$

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

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Single Trajectory

We solve the Schoredinger equation along a single trajectory.

$\Downarrow$

Sampling we can obtain the entire wave function.

Reference : J. O. Taylor: *Connection with Bohmian Mechanics*, Ph.D. Thesis (2003).

Quantum Trajectory Method

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

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

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

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The Propagation at discret time is

$$\begin{aligned}
\rho(\vec{x}_i(t_{n+1}), t_{n+1}) &= \rho(\vec{x}_i(t_n), t_n)e^{-\vec{\nabla}\cdot\vec{v}(\vec{x}_i(t_n),t_n)\delta t} \\
\vec{v}(\vec{x}_i(t_{n+1}), t_{n+1}) &= \vec{v}(\vec{x}_i(t_n), t_n) - \frac{\delta t}{m}\vec{\nabla}[V(\vec{x}_i(t_n), t_n) + U(\vec{x}_i(t_n), t_n] \\
\vec{x}_i(t_{n+1}) &= \vec{x}_i(t_n) + \vec{v}(\vec{x}_i(t_n), t_n)\delta t.
\end{aligned}$$

The TDSE is solved along the trajectories and step by step.

Single Trajectory

The idea of the algorithm

$$Q_0 \to \psi_0 \to Q_1 \to \psi_1 \to \cdots \to Q_n \to \psi_n$$

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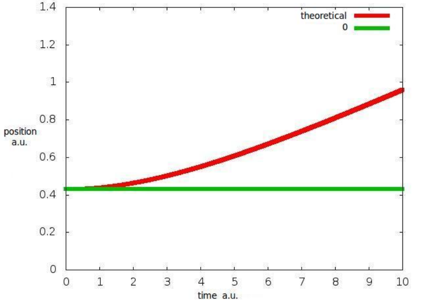
Single trajectory: x_0 on $|\psi_0|^2$



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

- $\dot{Q}_n = \frac{\nabla S_{n-1}}{m}$
- $R_n = R_{n-1}(x_0, 0)|J_{n-1}|^{\frac{1}{2}}$
- $S_n = S_{n-1}(x_0, 0) +$
  $+ \int_0^{t} \frac{1}{2} m \dot{Q}_{n-1}^2 - V_{n-1} - U_{n-1}$

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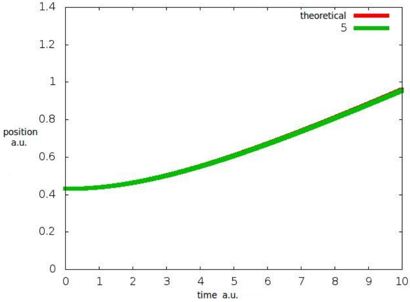

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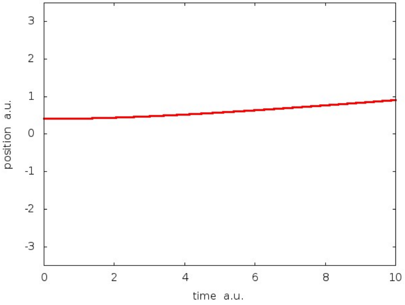
Single Trajectory

Sampling new initial position



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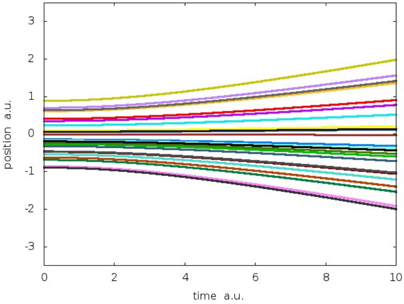
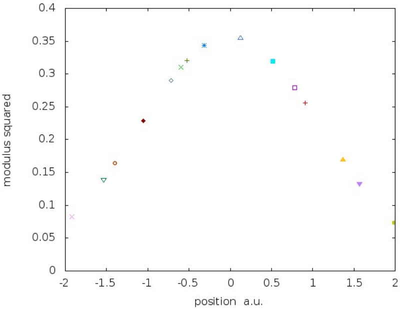


We obtain the wave function



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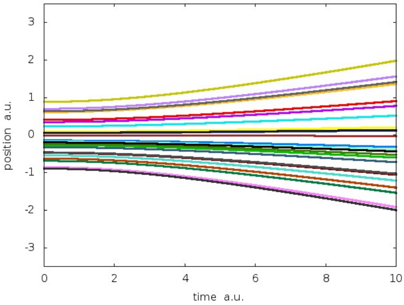

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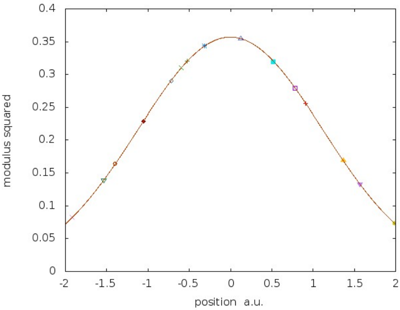

Interpolation gives ψ_t at every x

Many Particle - *TDSE*

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

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

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

$$\left\{\begin{array}{c} \dots \\ \frac{d^2x_i}{dt^2}=-\nabla_i[V(x_1,x_2,...,x_N,t)+U(x_1,x_2,...,x_N,t)]|_{x_1=x_1(t),...,x_N=x_N(t)} \\ \dots \end{array}\right.$$

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$$\Downarrow$$

At this point we have to know Ψ
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We need a new approach!

Many Particle - *Trajectory*

Theorem: Many-particle Bohm trajectory

$x_a(t)$ solution of many particle Schroedinger equation $\Psi(x_a, \vec{x}, t)$

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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

$$\begin{aligned} i\hbar\frac{\partial\psi_a(x_a,t)}{\partial t} &= [-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_a^2} + V_a(x_a, \vec{x}(t), t) + \\ &+ G_a(x_a, \vec{x}(t), t) + iJ_a(x_a, \vec{x}(t), t)]\psi_a(x_a, t) \end{aligned}$$

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with a suitable approximation for

$$G_a(x_a, \vec{x}(t), t) \ \ and \ \ iJ_a(x_a, \vec{x}(t), t)$$

we can solve many particle problems.

X. Oriols: *Quantum-trajectory approach to time-dependent transport in mesoscopic systems with electron-electron interactions*, Phys. Rev. Lett. 98, 066803 (2007).

Applications

- Quantum Trajectory Method
  Kinetic chemistry, dissociation problems.
  eg. E. R. Bittner: *Quantum Tunneling Dynamics using Hydrodynamic Trajectories*, J. Chem. Phys. **112**, 9703-9710 (2000).

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- Single Trajectory

- Many Particle
  Problems of transport in nanoelectric devices.
  eg. G. Albareda et al. : *Many-particle Hamiltonian for open systems with full Coulomb interaction: Application to classical and quantum time-dependent simulations of nanoscale electron devices*, Phys. Rev. B **79**, 075315 (2009)

Measurement issue

Von Neumann Model

Interaction between system and apparatus

x e $X \rightarrow$ system $\quad y$ e $Y \rightarrow$ apparatus

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x e $X \rightarrow$ system $\quad y$ e $Y \rightarrow$ apparatus

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

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

$$\text{where } A\psi_\alpha = a_\alpha \psi_\alpha$$

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$$H_{meas} = H_0^{syst} + H_0^{app} + H_{VN} \quad \text{where} \quad A(x) = \chi_{[0,+\infty)} - \chi_{(-\infty,0]}$$

We assume that $M \gg m$

Hydrodynamic equations

$$\begin{aligned}\frac{\partial S}{\partial t} &= -\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 - \frac{1}{2M}\left(\frac{\partial S}{\partial y}\right)^2 + \\ &+ \lambda A(x)\frac{\partial S}{\partial y} + \frac{\hbar^2}{2mR}\frac{\partial^2 R}{\partial x^2} + \frac{\hbar^2}{2MR}\frac{\partial^2 R}{\partial y^2}\end{aligned}$$

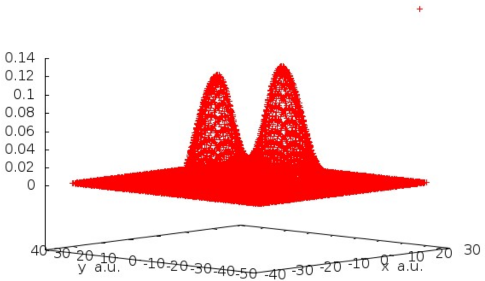
$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x}\left(\rho\frac{1}{m}\frac{\partial S}{\partial x}\right) - \frac{\partial}{\partial y}\left[\rho\left(\frac{1}{M}\frac{\partial S}{\partial y} + \lambda A(x)\right)\right]$$

Guidance equations

$$v_x \equiv \frac{1}{m}\frac{\partial S}{\partial x} \qquad v_y \equiv \frac{1}{M}\frac{\partial S}{\partial y} + \lambda A(x)$$

Measurement issue

Evolution of the complete wave function *system* + *apparatus* (Ψ)



$$\Psi_0 = \psi_0(x)\phi_0(y)$$

where

$$\psi_0(x) = \psi_+(x) + \psi_-(x)$$

$$A\psi_+ = +1 \cdot \psi_+$$
$$A\psi_- = -1 \cdot \psi_-$$

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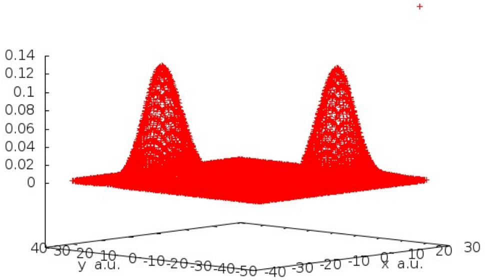

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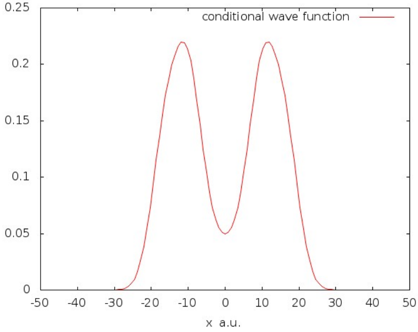
After the interaction we have

$$\Psi_t = \psi_+(x)\phi_+(y) + \psi_-(x)\phi_-(y)$$

Measurement issue

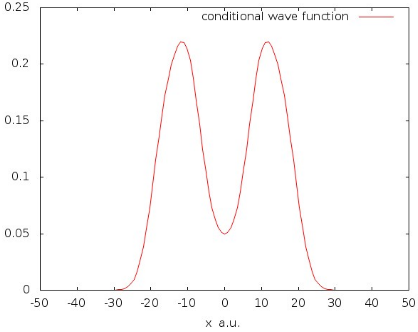
Wave Function of the Measured System $\psi_{\text{cond}} = \dfrac{\Psi_t(x, Y_t)}{||\Psi_t(x, Y_t)||}$

ψ_+



$X_0 = 6.6$ a.u. $Y_0 = 0.6$ a.u.

ψ_-



$X_0 = -5.2$ a.u. $Y_0 = 0.6$ a.u.

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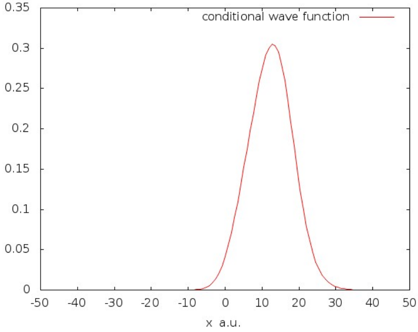

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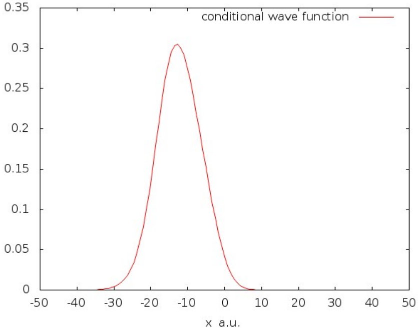

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Thank you for your attention!