BOHMIAN MECHANICS:
a complementary computational tool to describe molecular dynamics

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Outline:

1. Motivation: A wave equation for a classical single particle

2. A short overview of Bohmian Mechanics:
   - ❑ Analytic Bohmian Mechanics
   - ❑ Synthetic Bohmian Mechanics

3. The Conditional wavefunction

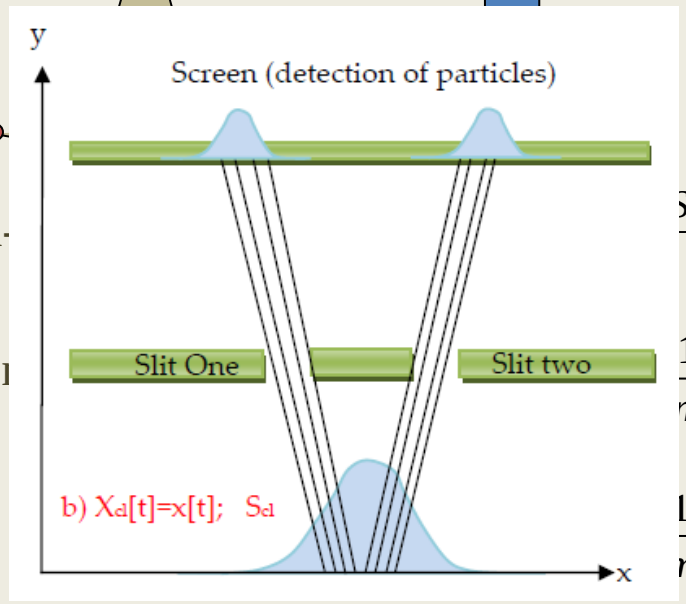
4. The use of Bohmian Mechanics in Molecular Dynamics

5. Conclusions and Future Work

❑ Classical wave equation for a single particle: [N. Rosen, Found. Phys. 16, 687 (1968)]

$$i\alpha\frac{\partial\psi_{cl}(x,t)}{\partial t}=-\frac{\alpha^2}{2m}\frac{\partial^2\psi_{cl}(x,t)}{\partial x^2}+V(x,t)\psi_{cl}(x,t)+\frac{\alpha^2}{2m}\frac{\partial^2\left|\psi_{cl}(x,t)\right|/\partial x^2}{\left|\psi_{cl}(x,t)\right|}\psi_{cl}(x,t)$$

"Extrinsic " uncertainty



Polar form of the wavefunction

$$\psi_{cl}(x,t)=R(x,t)\exp\left(iS(x,t)/\alpha\right)$$

Hamilton-

$$\left(\frac{\partial S(x,t)}{\partial x}\right)^2+V(x,t)=0$$

Local Cor

$$\frac{1}{m}\frac{\partial S(x,t)}{\partial x}R^2(x,t)=0$$

$$\frac{1}{m}\frac{\partial S(x,t)}{\partial x}$$

Can we do something similar with quantum mechanics?

Since S(x,t) does not depend on R(x,t), v(x,t) is independent of the shape of ψ_{cl}

Initial distribution of trajectories: $\left|\psi_{cl}(x,t_0)\right|^2=\lim_{M\to\infty}\frac{1}{M}\sum_{j=1}^{M}\delta\left(x-x^j[t_0]\right)$ $\quad x^j[t]=x^j[t_0]+\int_{t_0}^{t}v^j[t']dt'$

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❑ Quantum wave equation for a single particle: [D. Bohm, Phys. Rev. 85, 166 & 180 (1952)]

$$i\hbar\frac{\partial\psi_Q(x,t)}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi_Q(x,t)}{\partial x^2}+V(x,t)\psi_Q(x,t)$$

"Intrinsic "
uncertainty

Polar form of the wavefunction

$$t)=R(x,t)\exp(iS(x,t)/\hbar)$$

$$\equiv Q(x,t)$$

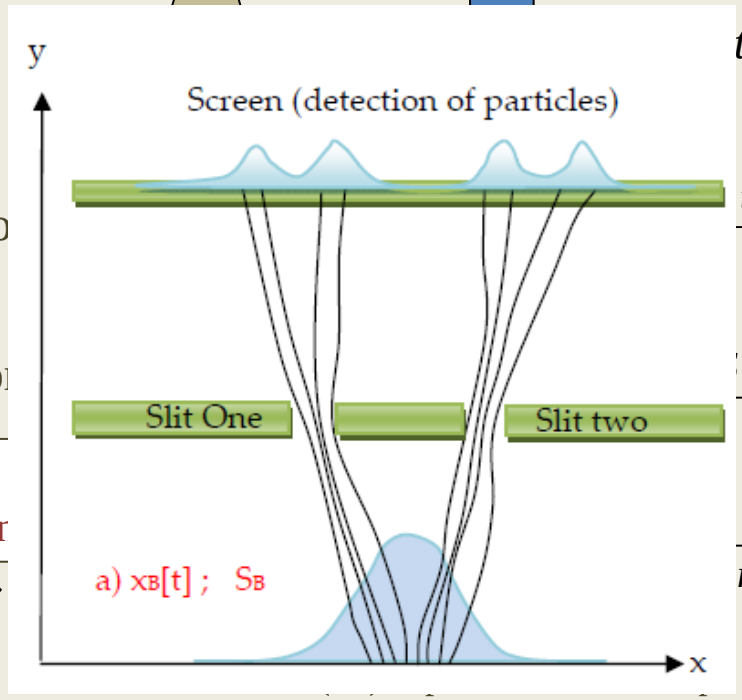
Q. Hamilto

$$\frac{t)}{}\Big)^2+V(x,t)-\frac{\hbar^2}{2m}\frac{\partial^2R(x,t)/\partial x^2}{R(x,t)}=0$$

Local Co

$$\frac{(x,t)}{\partial x}R^2(x,t)\Big)=0$$

Pilot-wave mechanics



"Analytic"
Bohmian Mechar

$$\frac{1}{m}\frac{\partial S(x,t)}{\partial x}$$

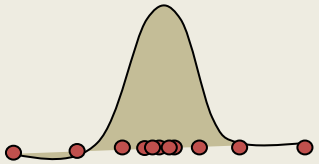
R(x,t),
of ψ_Q

"Synthetic"
Bohmian Mechanics

Initial distribution of trajectories $\left|\psi(x,t_0)\right|^2=\lim_{M\to\infty}\frac{1}{M}\sum_{j=1}^{M}\delta\left(x-x^j[t_0]\right)$ $x^j[t]=x^j[t_0]+\int_{t_0}^{t}v^j[t']dt'$

❑ Quantum wave equation for N many particles: [D. Bohm, Phys. Rev. 85, 166 & 180 (1952)]

$$i\hbar\frac{\partial\psi_Q(\vec{x},t)}{\partial t}=\sum_{k=1}^{N}-\frac{\hbar^2}{2m}\frac{\partial^2\psi_Q(\vec{x},t)}{\partial x_k^2}+V(\vec{x},t)\psi_Q(\vec{x},t)$$



Polar form of the wavefunction:

$$\psi(\vec{x},t)=R(\vec{x},t)\exp\left(iS(\vec{x},t)/\hbar\right)$$

Hamilton-Jacobi Equation:

$$\frac{\partial S(\vec{x},t)}{\partial t}+\sum_{k=1}^{N}\frac{1}{2m}\left(\frac{\partial S(\vec{x},t)}{\partial x_k}\right)^2+V(\vec{x},t)\underbrace{-\sum_{k=1}^{N}\frac{\hbar^2}{2m}\frac{\partial^2 R(\vec{x},t)/\partial x_k^2}{R(\vec{x},t)}}_{\equiv\sum_{k=1}^{N}Q_k(\vec{x},t)}=0$$

Local Continuity Equation:

$$\frac{\partial R^2(\vec{x},t)}{\partial t}+\sum_{k=1}^{N}\frac{\partial}{\partial x_k}\left(\frac{1}{m}\frac{\partial S(\vec{x},t)}{\partial x_k}R^2(\vec{x},t)\right)=0$$

Velocity field: $v_k(\vec{x},t)=\frac{1}{m}\frac{\partial S(\vec{x},t)}{\partial x_k}$

Since $S(\vec{x},t)$ does depend on $R(\vec{x},t)$, each $v_k(\vec{x},t)$ dependent of the shape of the whole wavefunction ψ_Q

Initial distribution of trajectories $\left|\psi(\vec{x},t_0)\right|^2=\lim_{M\to\infty}\frac{1}{M}\sum_{j=1}^{M}\prod_{k=1}^{N}\delta\left(x-x_k^j[t_0]\right)$ $\quad x_k^j[t]=x_k^j[t_0]+\int_{t_0}^{t}v_k^j[t']dt'$

❑ Evaluation of Observables

Expectation values:

$$\left\langle \hat{\mathrm{A}} \right\rangle = \left\langle \varphi \middle| \hat{\mathrm{A}} \middle| \varphi \right\rangle$$

$$= \int_{-\infty}^{+\infty} \mathrm{Re}\left\{ \varphi^*(\vec{x},t) \left[\hat{A}\left(x, -i\hbar\nabla_x\right)\varphi \right](\vec{x},t) \right\} d\vec{x}$$

where $\hat{\mathrm{A}}\varphi(\vec{x},t) = \int_{-\infty}^{+\infty} \hat{A}(\vec{x},\vec{x}')\varphi(\vec{x}',t)\, d\vec{x}'$

"Local expectation value":

$$\mathrm{A}_B(\vec{x},t) = \mathrm{Re}\left\{ \frac{\varphi^*(\vec{x},t)\left[\hat{A}\left(x,-i\hbar\nabla_x\right)\varphi \right](\vec{x},t)}{\varphi^*(\vec{x},t)\varphi(\vec{x},t)} \right\}$$

$$\left\langle \hat{\mathrm{A}} \right\rangle = \int_{-\infty}^{+\infty} \mathrm{R}^2(\vec{x},t)\,\mathrm{A}_B(\vec{x},t)\, d\vec{x}$$

$$= \lim_{M\to\infty} \frac{1}{M} \sum_{j=1}^{M} \mathrm{A}_B\left(\vec{x}^{\,j}[t],t\right)$$

Examples for common observables:

$$x_B(x) = x \qquad p_B(x,t) = \partial S(x,t)/\partial x$$

$$K_B(x,t) = \frac{1}{2m}\left(\frac{\partial S(x,t)}{\partial x}\right)^2 + Q(x,t) \qquad J_B(x,t) = v(x,t)$$

Main criticism against Bohmian Mechanics formalism:

"…In any case, the basic reason for not paying attention to the Bohm approach is not some sort of ideological rigidity, but much simpler…It is just that we are all too busy with our own work to spend time on something that doesn't seem likely to help us make progress with our real problems".

Steven Weinberg (private comunication with Shelly Goldstein)

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❑ The Conditional wave equation:

[X. Oriols, Phys. Rev. Lett. 98, 066803 (2007)]

$$\psi\left(\vec{x},t_0\right)$$

Initial Trajectory's Positions obey:

$$\left|\psi\left(\vec{x},t_0\right)\right|^2 = \lim_{M\to\infty}\frac{1}{M}\sum_{j=1}^{M}\prod_{k=1}^{N}\delta\left(x-x_k^j\left[t_0\right]\right)$$

Initial Trajectory's Velocity obey:

$$\vec{v}^{\,j}\left[t_o\right]=\left(\frac{1}{m_1}\frac{\partial S\left(\vec{x},t_0\right)}{\partial x_1}\bigg|_{\vec{x}=\vec{x}^{\,j}\left[t_0\right]},\ldots,\frac{1}{m_N}\frac{\partial S\left(\vec{x},t_0\right)}{\partial x_N}\bigg|_{\vec{x}=\vec{x}^{\,j}\left[t_0\right]}\right)$$

$$i\hbar\frac{\partial\psi\left(\vec{x},t\right)}{\partial t}=\left(\sum_{k=1}^{N}-\frac{\hbar^2}{2m}\nabla_k^2+V\left(\vec{x},t\right)\right)\psi\left(\vec{x},t\right)$$

$$\vec{x}^{\,j}\left[t\right]=\vec{x}^{\,j}\left[t_0\right]+\int_{t_0}^{t}\vec{v}^{\,j}\left[t'\right]dt$$

M grid points

$M^{\,N}$ **configuration points**

$$\vec{v}^{\,j}\left[t\right]=\left(\frac{1}{m_1}\frac{\partial S\left(\vec{x},t\right)}{\partial x_1}\bigg|_{\vec{x}=\vec{x}^{\,j}\left[t_0\right]},\ldots,\frac{1}{m_N}\frac{\partial S\left(\vec{x},t\right)}{\partial x_N}\bigg|_{\vec{x}=\vec{x}^{\,j}\left[t\right]}\right)$$

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Initial Trajectory's Positions obey:

$$\left|\psi\left(\vec{x},t_0\right)\right|^2=\lim_{M\to\infty}\frac{1}{M}\sum_{j=1}^{M}\prod_{k=1}^{N}\delta\left(x-x_k^j\left[t_0\right]\right)$$

Initial Trajectory's Velocity obey:

$$\vec{v}^{\,j}\left[t_o\right]=\left(\frac{1}{m_1}\frac{\partial S\left(\vec{x},t_0\right)}{\partial x_1}\bigg|_{\vec{x}=\vec{x}^{\,j}\left[t_0\right]},\ldots,\frac{1}{m_N}\frac{\partial S\left(\vec{x},t_0\right)}{\partial x_N}\bigg|_{\vec{x}=\vec{x}^{\,j}\left[t_0\right]}\right)$$

$$i\hbar\frac{\partial\psi\left(\vec{x},t\right)}{\partial t}=\left(\sum_{k=1}^{N}-\frac{\hbar^2}{2m}\nabla_k^2+V\left(\vec{x},t\right)\right)\psi\left(\vec{x},t\right)$$

$$\vec{x}^{\,j}\left[t\right]=\vec{x}^{\,j}\left[t_0\right]+\int_{t_0}^{t}\vec{v}^{\,j}\left[t'\right]dt$$

M grid p…

M^N configu…nts

$$\vec{v}^{\,j}\left[t\right]=\left(\frac{1}{m_1}\frac{\partial S\left(\vec{x},t\right)}{\partial x_1}\bigg|_{\vec{x}=\vec{x}^{\,j}\left[t_0\right]},\ldots,\frac{1}{m_N}\frac{\partial S\left(\vec{x},t\right)}{\partial x_N}\bigg|_{\vec{x}=\vec{x}^{\,j}\left[t\right]}\right)$$

$$\boxed{i\hbar\frac{\partial\varphi_k\left(x_k,t\right)}{\partial t}=\left(-\frac{\hbar^2}{2m}\nabla_k^2+V_{eff}\left(x_k,t\right)\right)\varphi_k\left(x_k,t\right)}$$

$$\vec{x}^{\,j}\left[t\right]=\vec{x}^{\,j}\left[t_0\right]+\int_{t_0}^{t}\vec{v}^{\,j}\left[t'\right]dt$$

M grid points

$M\cdot N$ **configuration points**

$$\vec{v}^{\,j}\left[t\right]=\left(\frac{1}{m_1}\frac{\partial S_1\left(x_1,t\right)}{\partial x_1}\bigg|_{x_1=x_1^j\left[t_0\right]},\ldots,\frac{1}{m_N}\frac{\partial S_N\left(x_N,t\right)}{\partial x_N}\bigg|_{x_N=x_N^j\left[t\right]}\right)$$

3. The Conditional wave function

$$i\hbar\frac{\partial\varphi_a(x_a,t)}{\partial t}=\left\{-\frac{\hbar^2}{2m_a}\frac{\partial^2}{\partial x_a^2}+V_a(x_a,\vec{x}_b[t],t)+G(x_a,\vec{x}_b[t],t)+i\cdot J(x_a,\vec{x}_b[t],t)\right\}\varphi_a(x_a,t)$$

- $G_a\left(x_a,\vec{x}_b,t\right)=V_b\left(\vec{x}_b,t\right)+\sum_{\substack{k=1\\k\neq a}}^{N}\left\{K_k\left(\vec{x},t\right)+Q_k\left(\vec{x},t\right)-\frac{\partial S\left(\vec{x},t\right)}{\partial x_k}v_k\left(\vec{x}[t],t\right)\right\}$
- $J_a\left(x_a,\vec{x}_b,t\right)=\sum_{\substack{k=1\\k\neq a}}^{N}\left\{\frac{\partial R^2\left(\vec{x},t\right)}{\partial x_k}v_k\left(\vec{x}[t],t\right)-\frac{\partial}{\partial x_k}\left(\frac{R^2\left(\vec{x},t\right)}{m_k}\frac{\partial S\left(\vec{x},t\right)}{\partial x_k}\right)\right\}$

[X. Oriols, Phys. Rev. Lett. 98, 066803 (2007)]

Good points :

An exact procedure for computing many-particle Bohmian trajectories where the correlations are introduced into time-dependent potentials:

- The interacting potential from (classical-like) Bohmian trajectories
- There is a real potential to account for “non-classical” correlations
- There is a imaginary potential to account for non-conserving norms

Bad points :

The terms G and J depend on the many-particle wave-function

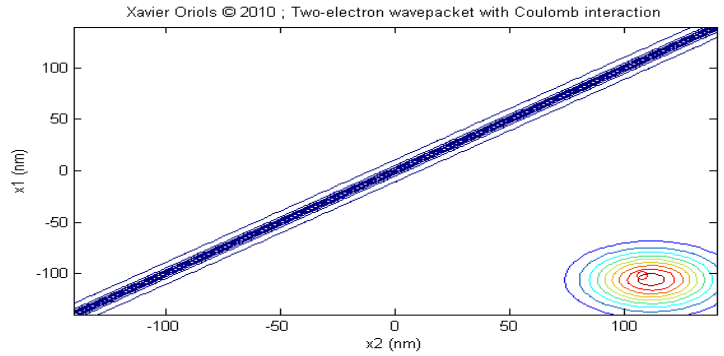
- This difficulty reminds the one it is found in the DFT (or TD-DFT)

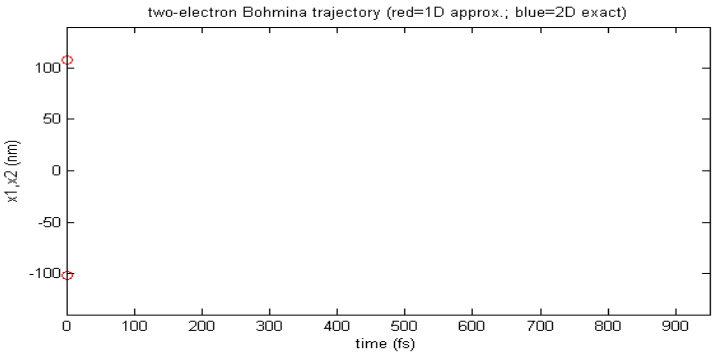
3. The Conditional wave function

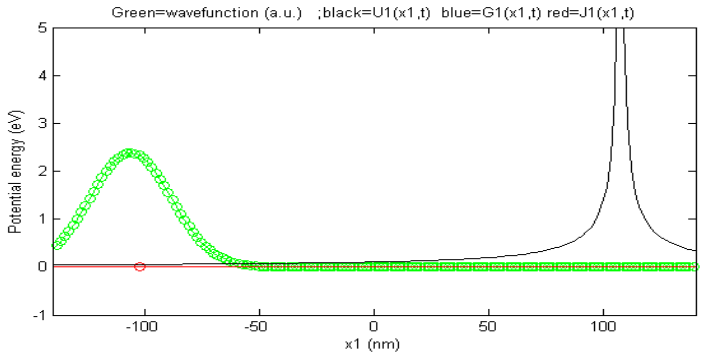
A simple case example: two Coulomb interacting electrons

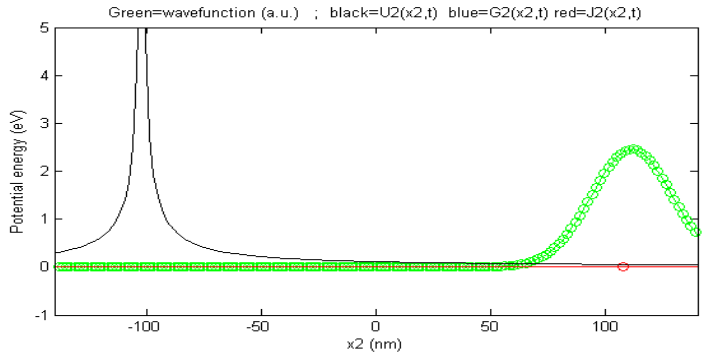
$$i\hbar\frac{\partial\Psi_1(\vec{r}_1,t)}{\partial t}=\left\{-\frac{\hbar^2}{2m^*}\nabla_1^2+\frac{q^2}{4\pi\varepsilon\varepsilon_0\left|\vec{r}_1-\vec{r}_2[t]\right|}\right\}\Psi_1(\vec{r}_1,t) \quad ; \quad \vec{r}_1[t]=\vec{r}_1[t_o]+\int_{t_o}^{t}dt\,\frac{J_1(\vec{r}_1,t)}{|\Psi_1(\vec{r}_1,t)|^2}\Bigg|_{\vec{r}_1=\vec{r}_1[t]}$$

$$i\hbar\frac{\partial\Psi_2(\vec{r}_2,t)}{\partial t}=\left\{-\frac{\hbar^2}{2m^*}\nabla_2^2+\frac{q^2}{4\pi\varepsilon\varepsilon_0\left|\vec{r}_1[t]-\vec{r}_2\right|}\right\}\Psi_2(\vec{r}_2,t) \quad ; \quad \vec{r}_2[t]=\vec{r}_2[t_o]+\int_{t_o}^{t}dt\,\frac{J_2(\vec{r}_2,t)}{|\Psi_2(\vec{r}_2,t)|^2}\Bigg|_{\vec{r}_2=\vec{r}_2[t]}$$





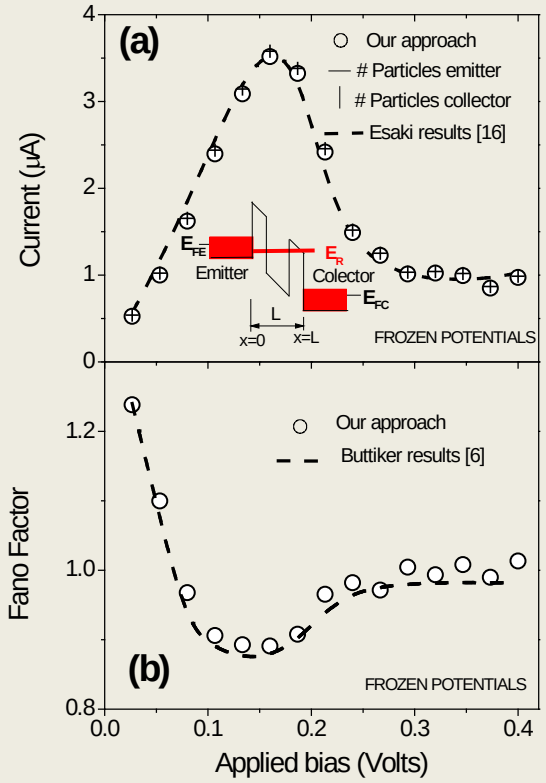


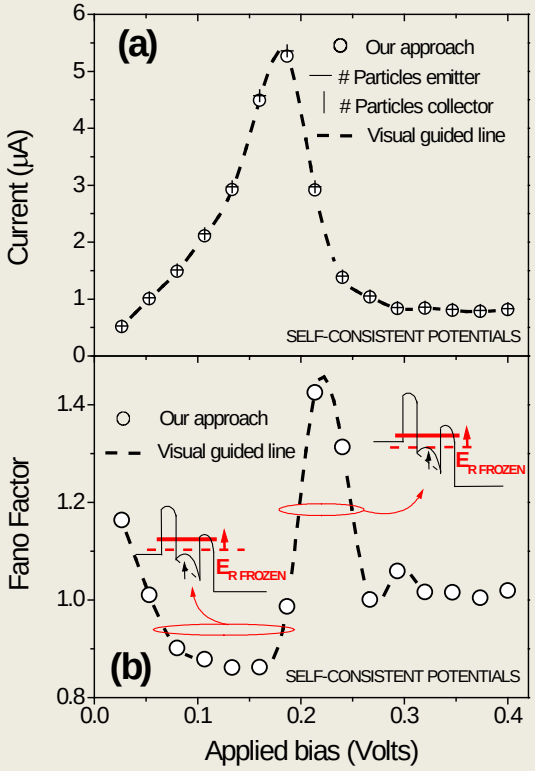


❑ Application to nanoelectronic device simulation:

BITLLES: Bohmian **I**nteracting **T**ransport in non-equi**L**ibrium e**LE**ctronic **S**tructures

$$i\hbar\frac{\partial\varphi_a(x_a,t)}{\partial t}=\left\{-\frac{\hbar^2}{2m_a}\frac{\partial^2}{\partial x_a^2}+V_a(x_a,\vec{x}_b[t],t)+G(x_a,\vec{x}_b[t],t)+i\cdot J(x_a,\vec{x}_b[t],t)\right\}\varphi_a(x_a,t)$$





Bowling pins

G. Albareda et al., Phys. Rev. B 79, 075315 (2009).

G. Albareda et al., Phys. Rev. B 82, 085301 (2010).

F.L.Traversa et al., IEEE Trans. Elect. Dev. 58, 2104 (2011).

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$$i\hbar\frac{\partial\psi\left(\vec{x},\vec{X},t\right)}{\partial t}=\hat{H}_{mol}\psi\left(\vec{x},\vec{X},t\right)$$ where $$\hat{H}_{mol}=\hat{K}_{el}+\hat{K}_{nuc}+V_{el-el}+V_{el-nuc}+V_{nuc-nuc}$$

- Conditional wavefunction of the electrons:

$$i\hbar\frac{\partial\varphi_{el}\left(\vec{x},t\right)}{\partial t}=\left\{\hat{H}_{el}\left(\vec{x},\vec{X}\left[t\right],t\right)+G_{el}\left(\vec{x},\vec{X}\left[t\right],t\right)+iJ_{el}\left(\vec{x},\vec{X}\left[t\right],t\right)\right\}\varphi_{el}\left(\vec{x},t\right)$$

Non-classical correlations between electrons and nuclei:

- $$G_{el}\left(\vec{x},\vec{X},t\right)=\sum_{n=1}^{N_{nuc}}\left\{\frac{1}{2M}\left(\frac{\partial S\left(\vec{x},\vec{X},t\right)}{\partial X_n}\right)^2-\frac{\hbar^2}{2M}\frac{\partial^2 R\left(\vec{x},\vec{X},t\right)/\partial X_n^2}{R\left(\vec{x},\vec{X},t\right)}-\frac{\partial S\left(\vec{x},\vec{X},t\right)}{\partial X_n}v_n\left[t\right]\right\}$$

Transmission of probability density between electrons and nuclei:

- $$J_{el}\left(\vec{x},\vec{X},t\right)=\sum_{n=1}^{N_{nuc}}\frac{\hbar}{2R^2\left(\vec{x},\vec{X},t\right)}\left\{\frac{\partial R^2\left(\vec{x},\vec{X},t\right)}{\partial X_n}v_n\left[t\right]-\frac{\partial}{\partial X_n}\left(\frac{R^2\left(\vec{x},\vec{X},t\right)}{M}\frac{\partial S\left(\vec{x},\vec{X},t\right)}{\partial X_n}\right)\right\}$$

- MQCB & Ehrenfest dynamics for the electronic part:

[E. Gindensperger J. Chem. Phys. 113, 1 (2000)]

$$i\hbar\frac{d\varphi_{el}\left(\vec{x},t\right)}{dt}=\hat{H}_{el}\left(\vec{x},\vec{X}\left[t\right],t\right)\varphi_{el}\left(\vec{x},t\right)$$

[E. J. Heller J. Chem. Phys. 62, 1544 (1975)]

$$i\hbar\frac{\partial\varphi_{el}\left(\vec{x},t\right)}{\partial t}=\hat{H}_{el}\left(\vec{x},\vec{X}\left[t\right],t\right)\varphi_{el}\left(\vec{x},t\right)$$

❑ Conditional wavefunction of the nuclei *a*:

$$i\hbar\frac{\partial\Omega_a\left(X_a,t\right)}{\partial t}=\left\{\hat{H}_a\left(\vec{x}\left[t\right],X_a,\vec{X}_b\left[t\right],t\right)+G_a\left(\vec{x}\left[t\right],X_a,\vec{X}_b\left[t\right],t\right)+iJ_a\left(\vec{x}\left[t\right],X_a,\vec{X}_b\left[t\right],t\right)\right\}\Omega_a\left(\vec{x},t\right)$$

where $\hat{H}_a=\hat{K}_a+V_{el-el}+V_{el-a}+V_{nuc-a}$

Non-classical correlations between the nuclei *a* and all the other particles:

❑ $$G_a\left(\vec{x},\vec{X},t\right)=\sum_{j=1}^{N_{el}}\left\{\frac{1}{2m}\left(\frac{\partial S\left(\vec{x},\vec{X},t\right)}{\partial x_j}\right)^2-\frac{\hbar^2}{2m}\frac{\partial^2R\left(\vec{x},\vec{X},t\right)/\partial x_j^2}{R\left(\vec{x},\vec{X},t\right)}-\frac{\partial S\left(\vec{x},\vec{X},t\right)}{\partial x_j}v_j\left[t\right]\right\}$$

$$+\sum_{\substack{n=1\\n\neq a}}^{N_{nuc}}\left\{\frac{1}{2M}\left(\frac{\partial S\left(\vec{x},\vec{X},t\right)}{\partial X_n}\right)^2-\frac{\hbar^2}{2m}\frac{\partial^2R\left(\vec{x},\vec{X},t\right)/\partial X_n^2}{R\left(\vec{x},\vec{X},t\right)}-\frac{\partial S\left(\vec{x},\vec{X},t\right)}{\partial X_n}v_n\left[t\right]\right\}$$

Transmission of probability density from the nuclei *a* to all the other particles:

❑ $$J_a\left(\vec{x},\vec{X},t\right)=\sum_{j=1}^{N_{el}}\frac{\hbar}{2R^2\left(\vec{x},\vec{X},t\right)}\left\{\frac{\partial S\left(\vec{x},\vec{X},t\right)}{\partial x_j}v_j\left[t\right]-\frac{\partial}{\partial x_j}\left(\frac{R^2\left(\vec{x},\vec{X},t\right)}{m}\frac{\partial S\left(\vec{x},\vec{X},t\right)}{\partial x_j}\right)\right\}$$

$$+\sum_{\substack{n=1\\n\neq a}}^{N_{nuc}}\frac{\hbar}{2R^2\left(\vec{x},\vec{X},t\right)}\left\{\frac{\partial S\left(\vec{x},\vec{X},t\right)}{\partial X_n}v_n\left[t\right]-\frac{\partial}{\partial X_n}\left(\frac{R^2\left(\vec{x},\vec{X},t\right)}{M}\frac{\partial S\left(\vec{x},\vec{X},t\right)}{\partial X_n}\right)\right\}$$

- Conditional wavefunction of the nuclei *a*:

$$i\hbar\frac{\partial\Omega_a\left(X_a,t\right)}{\partial t}=\left\{\hat{H}_a\left(\vec{x}\left[t\right],X_a,\vec{X}_b\left[t\right],t\right)+G_a\left(\vec{x}\left[t\right],X_a,\vec{X}_b\left[t\right],t\right)+iJ_a\left(\vec{x}\left[t\right],X_a,\vec{X}_b\left[t\right],t\right)\right\}\Omega_a\left(\vec{x},t\right)$$

$$\times\nabla_a \quad \Rightarrow \quad \Omega_a\left(X_a,t\right)=r_a\left(X_a,t\right)\exp\left(is_a\left(X_a,t\right)/\hbar\right)$$

$$M\cdot\ddot{r}_a\left(X_a,t\right)=-\nabla_a\left\{V_{el-a}\left(X_a,t\right)+V_{nuc-a}\left(X_a,t\right)+Q_a\left(X_a,t\right)+G_{nuc}\left(X_a,t\right)\right\}$$

- MQCB dynamics for the nuclei:

[E. Gindensperger J. Chem. Phys. 113, 1 (2000)]

$$\boxed{M\cdot\ddot{r}_a\left(X_a,t\right)=-\nabla_a\left[V_{el-a}\left(X_a,t\right)+V_{nuc-a}\left(X_a,t\right)\right]}$$

- Ehrenfest dynamics for the nuclei:

[E. J. Heller J. Chem. Phys. 62, 1544 (1975)]

$$\boxed{M\cdot\ddot{r}_a\left(X_a,t\right)=-\nabla_a\left[\left\langle\varphi_{el}\left(\vec{x},t\right)\middle|V_{el-a}\left(X_a,t\right)\middle|\varphi_{el}\left(\vec{x},t\right)\right\rangle+V_{nuc-a}\left(X_a,t\right)\right]}$$

Outline:

1. Motivation: A wave equation for classical single particles

2. A short overview of Bohmian Mechanics:
   - ❑ Analytic Bohmian Mechanics
   - ❑ Synthetic Bohmian Mechanics

3. The Conditional wavefunction

4. The use of Bohmian Mechanics in Molecular Dynamics

5. Conclusions and Future Work

- The exact splitting of electronic and nuclear degrees of freedom in terms of the Conditional wavefunction leads to a rigorous starting point for making approximations, specially for mixed quantum-classical approaches.

- In particular, Bohmian Mechanics together with the concept of Conditional wavefunction allows a rigorous derivation of the MQCB and Ehrenfest approaches to molecular dynamics.

- Coherence in the SSH model Hamiltonian:

$$H_{SSH} = H_{el} + H_{el-ph} + H_{ph}$$

$$H_{el} = \sum_{n=1}^{N-1} \sum_{s=\pm 1} -t_0 \times \left(c_{n+1,s}^{\dagger} c_{n,s} + c_{n,s}^{\dagger} c_{n+1,s} \right)$$

$$H_{el-ph} = \sum_{n=1}^{N-1} \sum_{s=\pm 1} \alpha \left(u_{n+1} - u_n \right) \times \left(c_{n+1,s}^{\dagger} c_{n,s} + c_{n,s}^{\dagger} c_{n+1,s} \right)$$

$$H_{ph} = \sum_{n=1}^{N} \frac{p_n^2}{2M} + \frac{k}{2} \sum_{n=1}^{N-1} \left(u_{n+1} - u_n \right)^2$$

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