Chaotic Bohmian trajectories for the hydrogen atom

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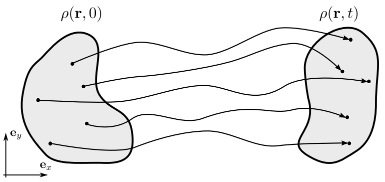
Introduction

In 1952, David Bohm proposed an alternative formulation of quantum mechanics which is deterministic and non local. More precisely, a single-particle quantum system is described in part by its wave function $\psi(\mathbf{r},t)$ and in part by the actual position $\mathbf{r}$ of the particle [1]

- Wave function evolves according to usual Schrödinger equation
- Deterministic trajectories satisfy the guiding equation

$$\frac{d\mathbf{r}}{dt} = \mathbf{v}_B(\mathbf{r},t) \equiv \frac{\hbar}{m}\mathrm{Im}\left(\frac{\nabla\psi(\mathbf{r},t)}{\psi(\mathbf{r},t)}\right)$$

- Unknown initial position $\Leftrightarrow$ probabilistic behaviour
  Initial positions distributed according to $\rho(\mathbf{r},0) = |\psi(\mathbf{r},0)|^2$
  $\Rightarrow$ Same results as standard quantum mechanics



Chaos and Bohmian mechanics

Relaxation [2] : $\rho(\mathbf{r},0) \neq |\psi(\mathbf{r},0)|^2$ + chaos $\Rightarrow \rho(\mathbf{r},t) \to |\psi(\mathbf{r},t)|^2$

Node of the wave function : $\psi(\mathbf{r}_{\text{node}},t) = 0$

$$\mathbf{v}_B(\mathbf{r},t) \to \infty \quad \text{if} \quad \mathbf{r} = \mathbf{r}_{\text{node}}$$

Questions addressed in this work

Moving nodes $\overset{?}{\Leftrightarrow}$ chaotic Bohmian trajectories [3]

Particle in 2d Coulomb potential $\overset{?}{\Rightarrow}$ chaotic Bohmian trajectories

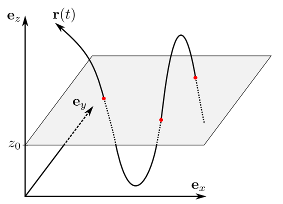
Probing chaotic behaviour

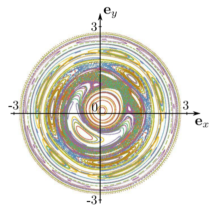
Trajectories in n-dimensional space

Explicit time dependence of $\mathbf{v}_B \Rightarrow n+1$ effective degrees of freedom

Chaos $\Rightarrow$ exponential sensitivity to initial conditions
$\Rightarrow n - c \geq 3$ with c the number of constants of motion

Poincaré section



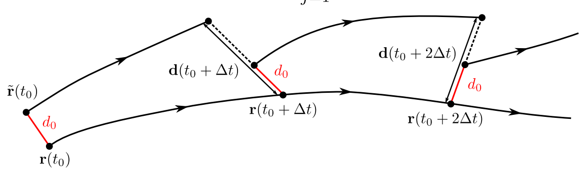


Periodicity : $\mathbf{v}_B(\mathbf{r},t+\tau) = \mathbf{v}_B(\mathbf{r},t) \Rightarrow$ stroboscopic view

Maximum Lyapunov exponent

Quantifying exponential divergence of nearby trajectories [4]

$$\lambda(\mathbf{r}_0) = \lim_{N\to\infty}\frac{1}{N\Delta t}\sum_{j=1}^{N}\ln\left(\frac{|\mathbf{d}(j\Delta t)|}{d_0}\right)$$



2d hydrogen atom

2d Coulomb potential $V(\mathbf{r}) = -e^2/r$

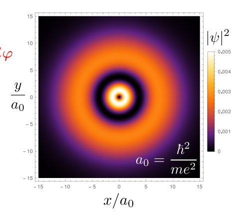
Eigenstates of $\hat{H}$ and $\hat{L}_z$

$$\phi_{n,l}(r,\varphi) = \mathcal{N}_{n,l}(\beta_n r)^{|l|}e^{-\frac{\beta_n r}{2}}L^{2|l|}_{n-|l|-1}(\beta_n r)e^{il\varphi}$$

with $\beta_n = (2me^2)/[\hbar^2(n-1/2)]$ and energy

$$E_n = \frac{me^4}{2\hbar^2(n-1/2)^2}$$

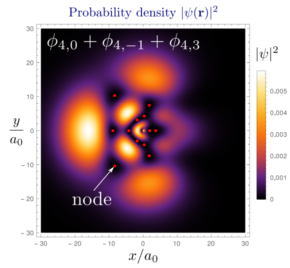
$n = 1, 2, \ldots$ and $|l| = 0, 1, \ldots, n-1$

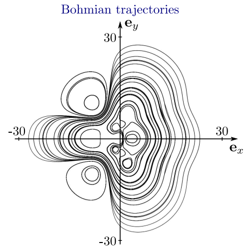


Results for 2d hydrogen atom

Stationary states

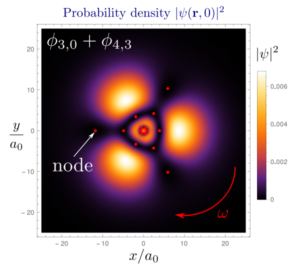
Wave function and Bohmian velocity field independent of time

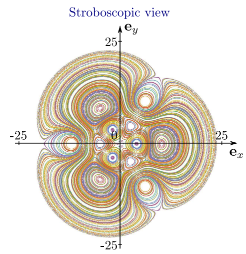




- Two degrees of freedom $\Rightarrow$ regular trajectories ($\lambda(\mathbf{r_0}) \leq 0$)

Two eigenstates of $\neq$ E : $\psi(\mathbf{r},t) = c_1\phi_{n_1,l_1}(\mathbf{r},t) + c_2\phi_{n_2,l_2}(\mathbf{r},t)$



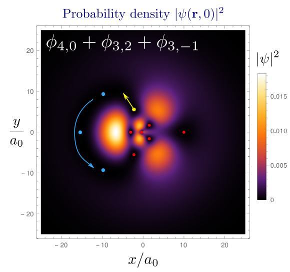


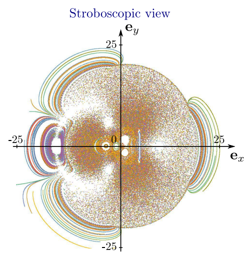
- Regular trajectories even with large number of moving nodes!
- Rigid rotation of $|\psi(\mathbf{r},t)|^2$ and $\mathbf{v}_B(\mathbf{r},t)$ with angular velocity

$$\omega = (E_a - E_b)/(\hbar(l_a - l_b))$$

Velocity field $\mathbf{v}_B(\mathbf{r})$ independent of time in a frame rotating at ω
$\Rightarrow$ only two degrees of freedom and thus no chaos ($\lambda(\mathbf{r_0}) \leq 0$)

Three eigenstates of $\neq$ E : $\psi(\mathbf{r},t) = \sum_{i=1}^{3} c_i\phi_{n_i,l_i}(\mathbf{r},t)$





- Nodes of ψ move with $\neq$ velocities but $\mathbf{v}_B$ periodic in time
- Both chaotic and regular trajectories
- Chaotic region : $\lambda(\mathbf{r_0}) \approx 0.1 > 0$

Conclusion and outlook

Particle in a 2d Coulomb potential

- Stationary states and superpositions of two eigenstates of $\neq E$
  $\Rightarrow$ regular trajectories even with many (moving) nodes
- More than two eigenstates of $\neq$ energies $\Rightarrow$ chaotic trajectories

Preliminary results : Particle in a 3d Coulomb potential

Stationary states $\Rightarrow$ chaotic Bohmian trajectories

Motion and number of nodes of the wave function
$\neq$ sufficient condition for emergence of chaos in Bohmian mechanics

To do : Relaxation computation
Bohmian trajectories for entangled states

References

[1] D. Bohm, Phys. Rev. **85**, 166 (1952).
[2] A. Valentini, and H. Westman, Proc. R. Soc. A **461**, 253 (2004).
[3] D. A. Wisniacki, and E. R. Pujals, Europhys. Lett. **7**, 159 (2005).
[4] G. Benettin, *et. al.*, Phys. Rev. A **14**, 2338 (1976).