Interacting Quantum Trajectories and Dwell Times for Particles with Spin ½

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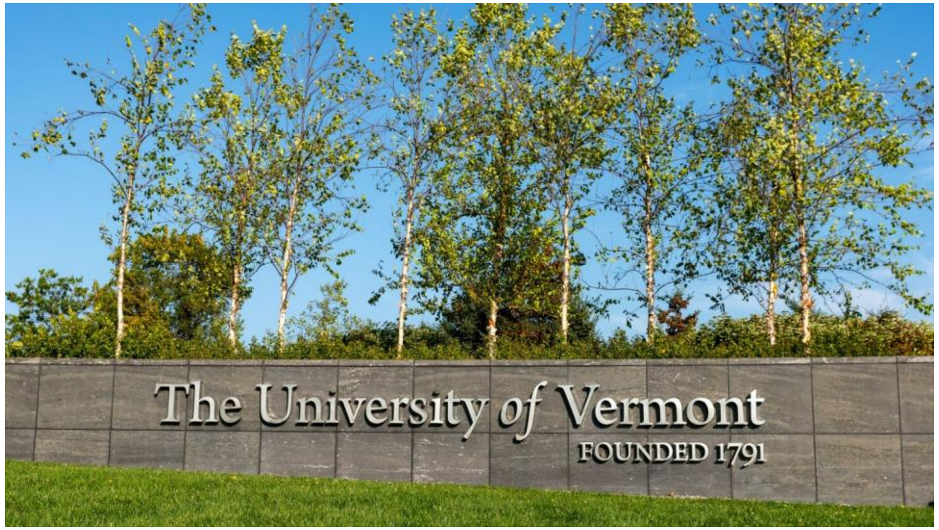
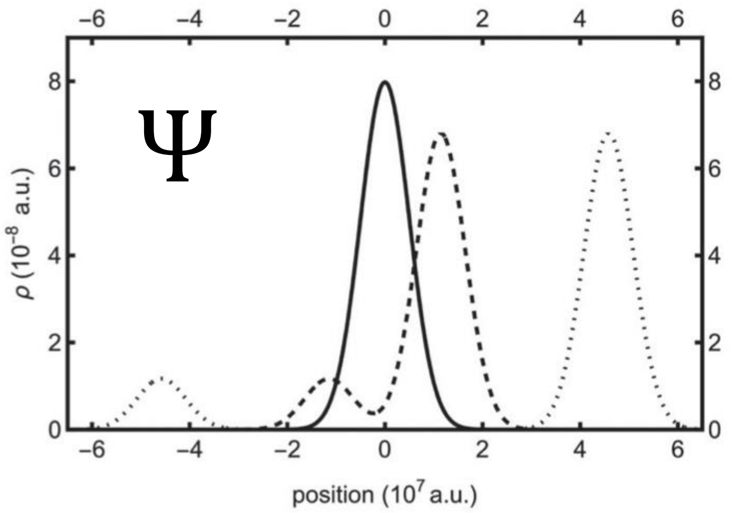
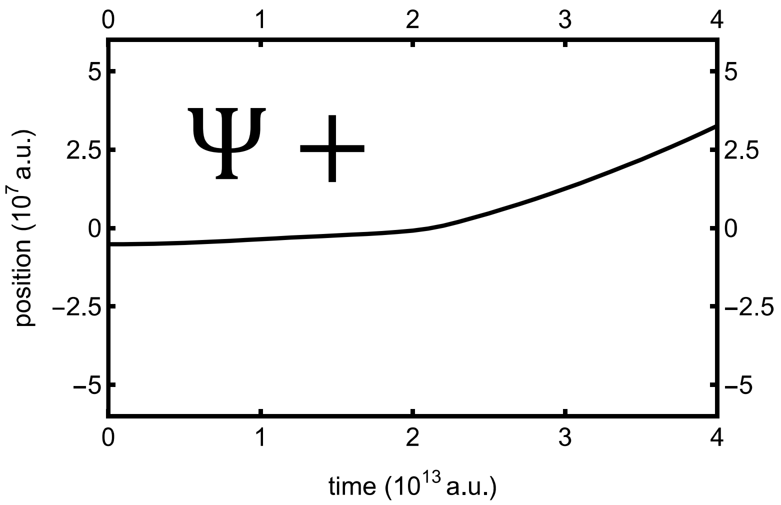


1. R. Lombardini and B. Poirier. Interacting quantum trajectories for particles with spin 1/2. [Molecular Physics **122**, e2334805 (2024)].
2. B. Poirier and R. Lombardini. Dwell times, wavepacket dynamics, and quantum trajectories with spin 1/2. [Entropy **26**, 336 (2024)].

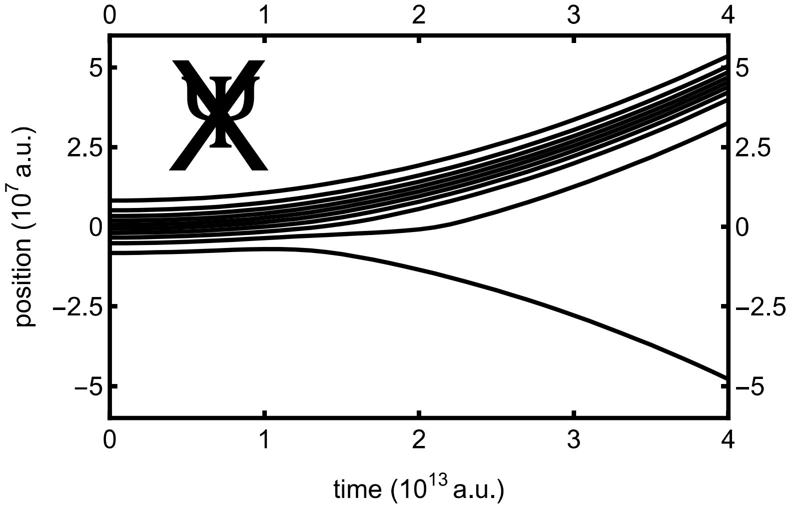
Introduction



Traditional Quantum Mechanics



De Broglie-Bohm (dBB)



Interacting Quantum Trajectories (IQT)

- In IQT, B. Poirier [Chem. Phys. **370**, 4-14 (2010)] found a way to treat "…the trajectory ensemble itself as the fundamental quantum entity" (pg. 5).

- Quantum effects manifest as interactions among trajectories.

Pauli Equation

- $i\hbar \frac{\partial \vec{\psi}}{\partial t} = \hat{H}\vec{\psi}$

  where $\hat{H} = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\mathbf{A}\right)^2 + qV - \frac{q\hbar}{2m}\mathbf{B}\cdot\boldsymbol{\sigma}$

- Probability flux

  $$\mathbf{j} = \frac{\hbar}{2mi}\left(\vec{\psi}^{\dagger}\nabla\vec{\psi} - \nabla\vec{\psi}^{\dagger}\vec{\psi}\right) - \frac{q}{m}\mathbf{A}\rho + \frac{1}{m}\nabla \times (\rho\mathbf{s})$$

  where $\rho = \vec{\psi}^{\dagger}\vec{\psi}$ and $\mathbf{s} = \frac{\hbar}{2\rho}\vec{\psi}^{\dagger}\boldsymbol{\sigma}\vec{\psi}$

- Flow velocity $\mathbf{v} = \mathbf{j}/\rho$

dBB Approach

- Developed in late 80s by C. Dewdney, P. R. Holland, A. Kyprianidis, and J. P. Vigier.

- Madelung-Bohm polar form ansatz combined with Bloch-like spinor $\vec{\chi}$ (single particle case)

$$\vec{\psi} = Re^{iS/\hbar}\vec{\chi} \text{ where } \vec{\chi} = \begin{pmatrix} \cos\frac{\theta}{2}e^{i\frac{\phi}{2}} \\ \sin\frac{\theta}{2}e^{-i\frac{\phi}{2}} \end{pmatrix}$$

- Four real functions of space and time: $R(\mathbf{r},t)$, $S(\mathbf{r},t)$, $\theta(\mathbf{r},t)$, and $\phi(\mathbf{r},t)$

- Move from Eulerian to Lagrangian picture: $\mathbf{v} = \frac{d\mathbf{r}}{dt} = \dot{\mathbf{r}}$

dBB Approach

- Four (coupled) time-evolution equations involving wavefunction
- For the free 1D case:

$$m\ddot{x} = F_Q + F_{Q_S}$$

where $F_Q = -Q'$ and $Q = -\frac{\hbar^2}{2m}\frac{R''}{R}$

$$F_{Q_S} = -\frac{\hbar^2}{4m\rho}\left(\rho\phi'^2 \sin^2\theta + \rho\theta'^2\right)'$$

IQT Approach

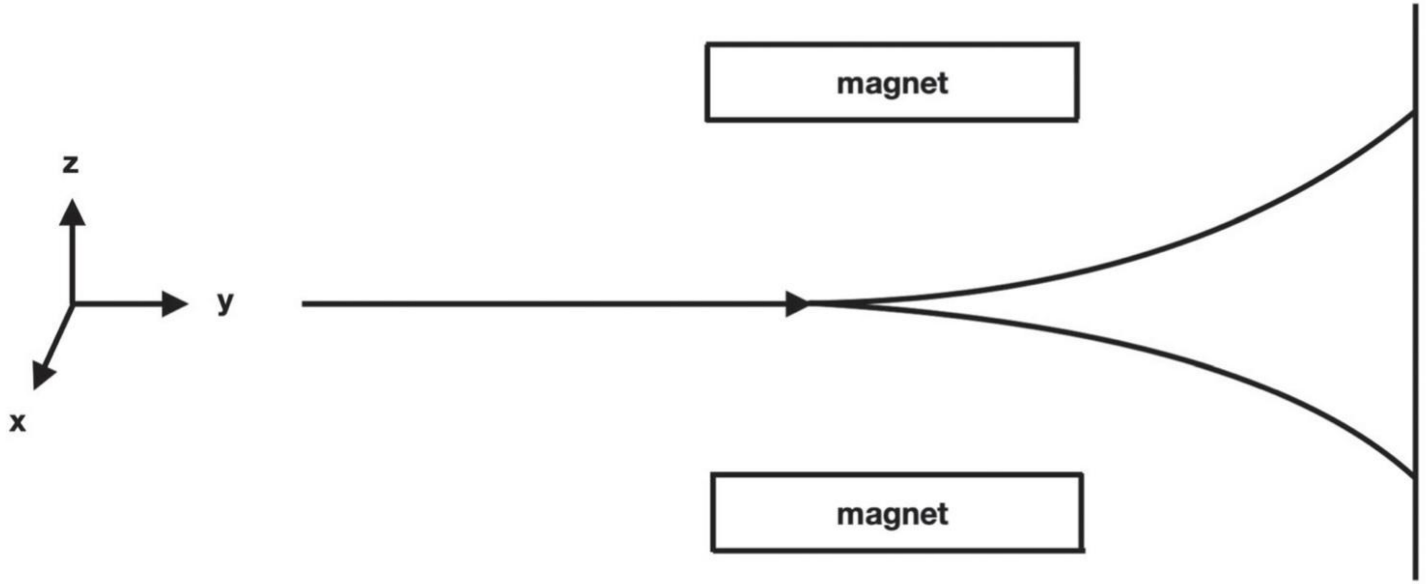
- Replace wavefunction $\vec{\psi}$ with ensemble of trajectories by introducing a new independent trajectory-labelling variable C.
    - $x(t) \rightarrow x(C,t),\ \theta(x,t) \rightarrow \theta(C,t)$, and $\phi(x,t) \rightarrow \phi(C,t)$
    - $\rho(x,t) = \frac{1}{x^{(1)}(C,t)}$ where $x^{(1)} = \left.\frac{\partial x(C,t)}{\partial C}\right|_t$, or in general, $x^{(n)} = \left.\frac{\partial^n x(C,t)}{\partial C^n}\right|_t$
- Three (coupled) time-evolution equations not involving wavefunction
- For the free 1D case:

$$m\ddot{x} = F_Q + F_{Q_S}$$

$$F_Q = -\frac{\hbar^2}{4m}\left(\frac{x^{(4)}}{[x^{(1)}]^4} - 8\frac{x^{(3)}x^{(2)}}{[x^{(1)}]^5} + 10\frac{[x^{(2)}]^3}{[x^{(1)}]^6}\right)$$

$$F_{Q_S} = -\frac{\hbar^2}{4m}\left(\frac{[\phi^{(1)}]^2 \sin^2\theta + [\theta^{(1)}]^2}{[x^{(1)}]^3}\right)^{(1)}$$

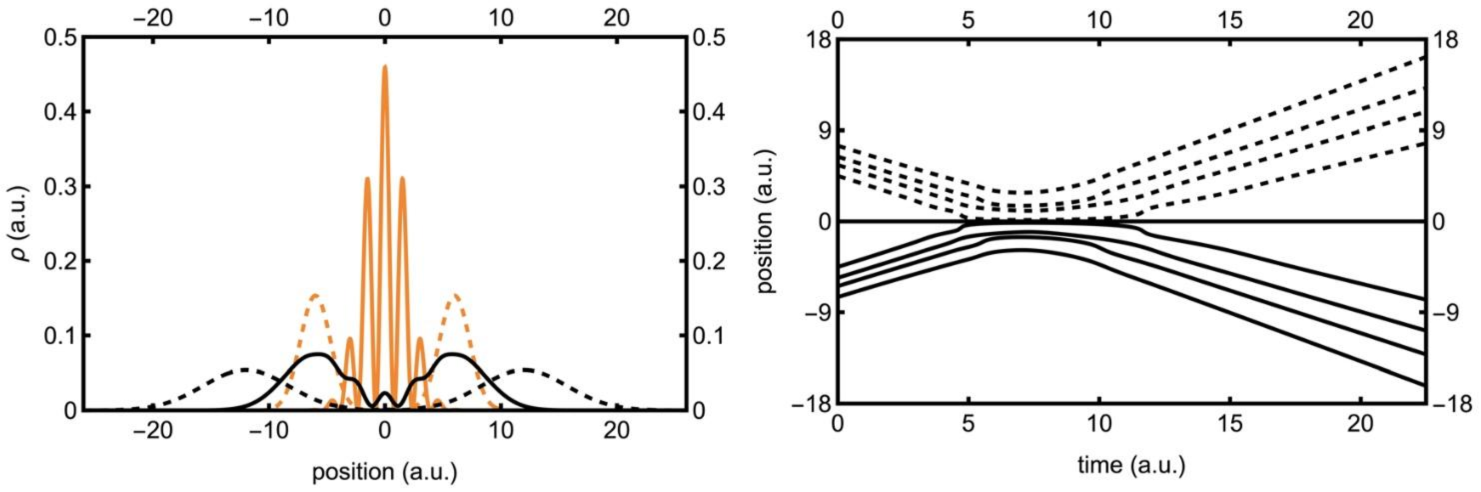
IQT Approach



- Stern-Gerlach experiment

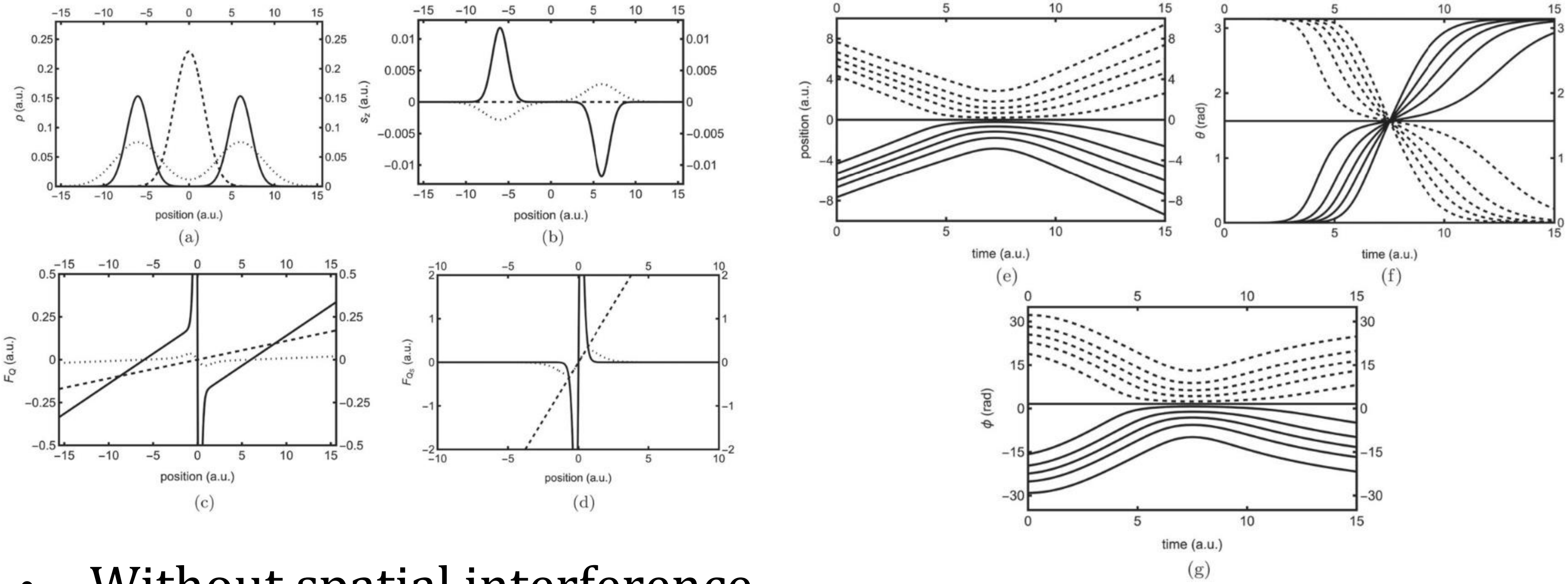
$$m\ddot{z} = F_Q + F_{Q_S} + \mu_B B_0' \cos\theta$$

Quantum Spin Flipper (Free Spinor)



- With spatial interference
  - Two spin-up coherent Gaussian waves approach each other and overlap.

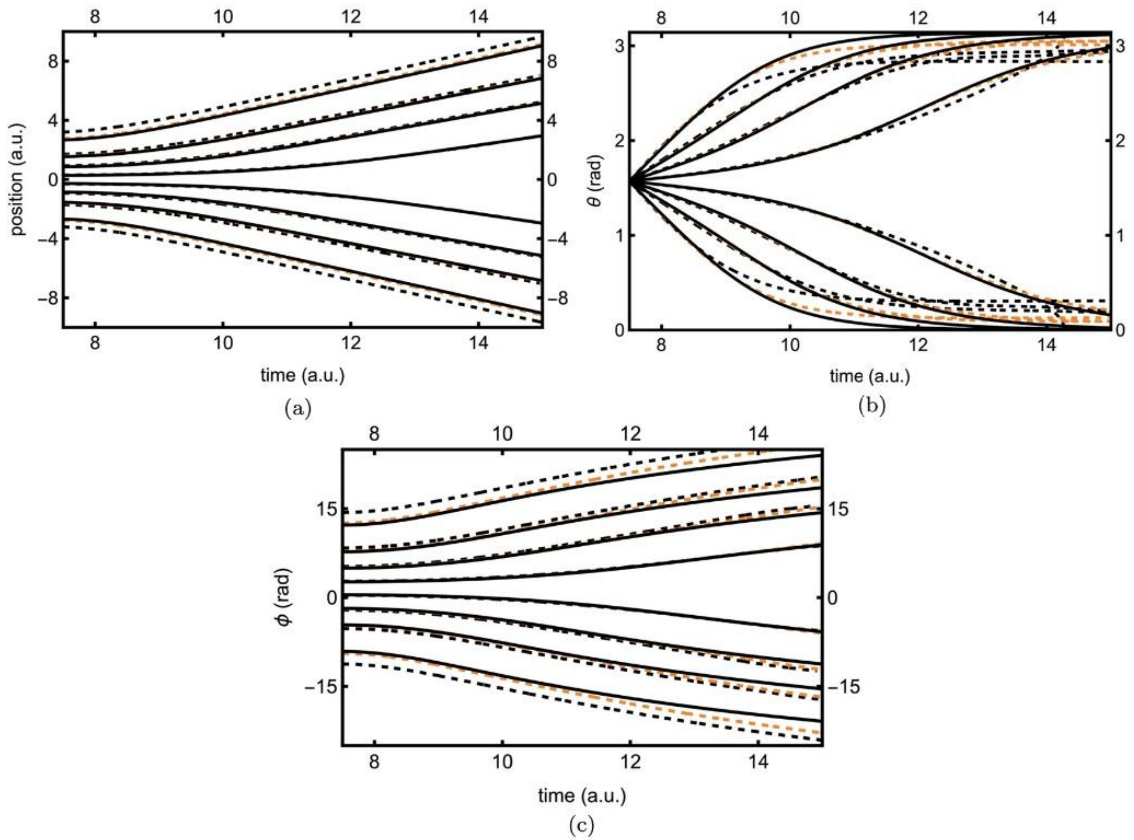
Quantum Spin Flipper (Free Spinor)



- Without spatial interference
  - Spin-up wave interacts with spin-down wave [spin flips—see (b)].

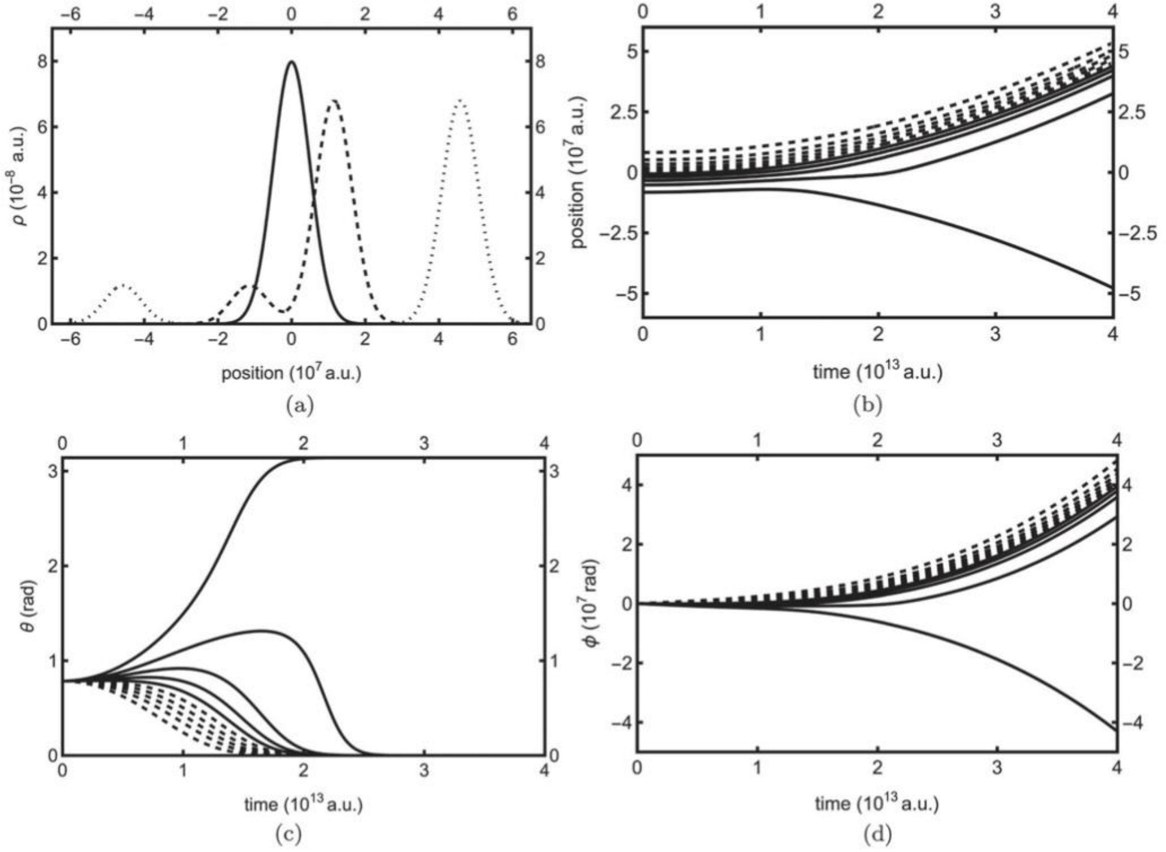
Quantum Spin Flipper (Free Spinor)

- IQT numerical calculations of free spinor with no interference
    - Used central finite difference approximation for derivatives in C.
    - Used Störmer-Verlet and Midpoint methods for time propagation.
    - NO WAVEFUNCTION NEEDED!!!



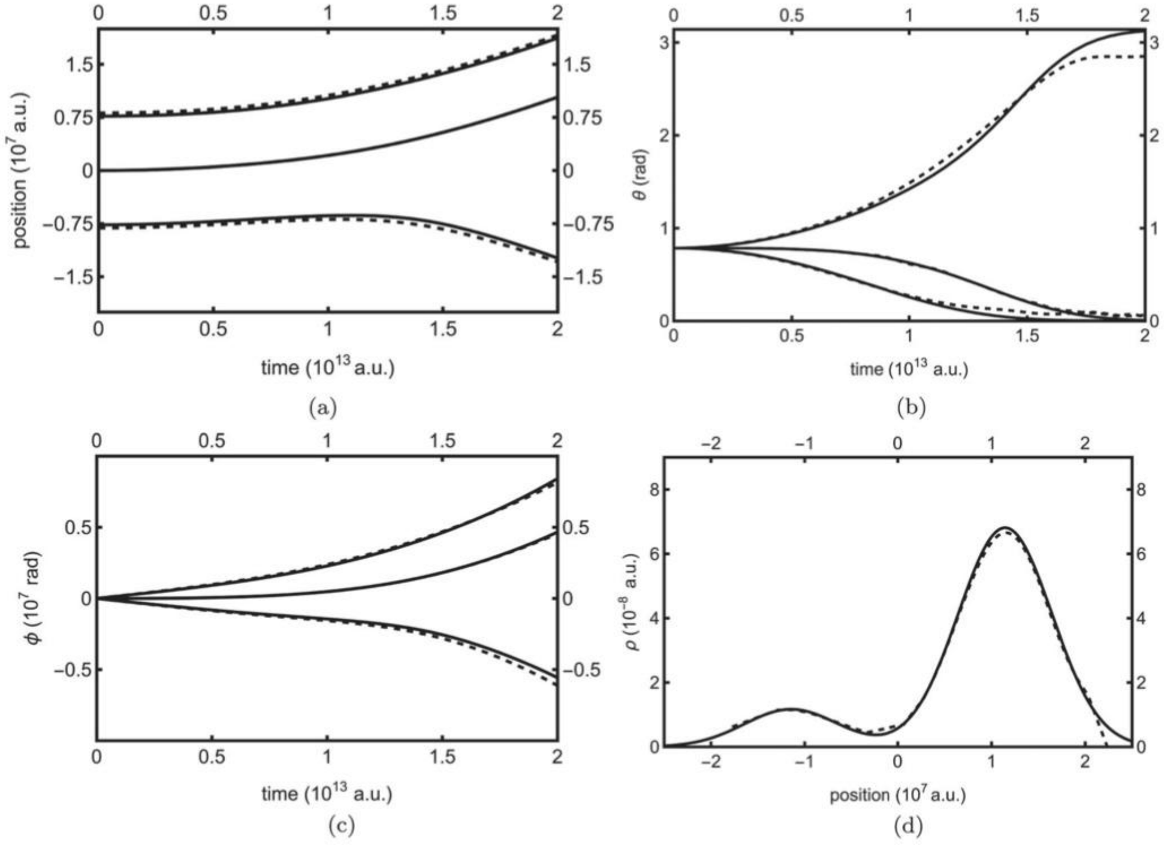
Stern-Gerlach Experiment

- Initial conditions: $\theta_0 = \frac{\pi}{4}$ rad and $\phi_0 = 0$
- $\cos^2 \frac{\pi}{8} \approx 85.36\%$ of silver atoms should measure spin-up.
- 9/10 or 90% trajectories end up in positive z region.



Stern-Gerlach Experiment

- IQT numerical calculations of Stern-Gerlach Experiment
  - Used central finite difference approximation for derivatives in C.
  - Used Störmer-Verlet and Midpoint methods for time propagation.
  - NO WAVEFUNCTION NEEDED!!!
    - Although, wavefunction can be recovered [see (d)].



Future Plans

- Improve upon numerical algorithms.
- Implement IQT on systems with multiple particles and spatial dimensions.
- Examine particles with higher spin.
- Develop IQT version of relativistic quantum mechanics for spin-1/2 particles.

Why Dwell Time?

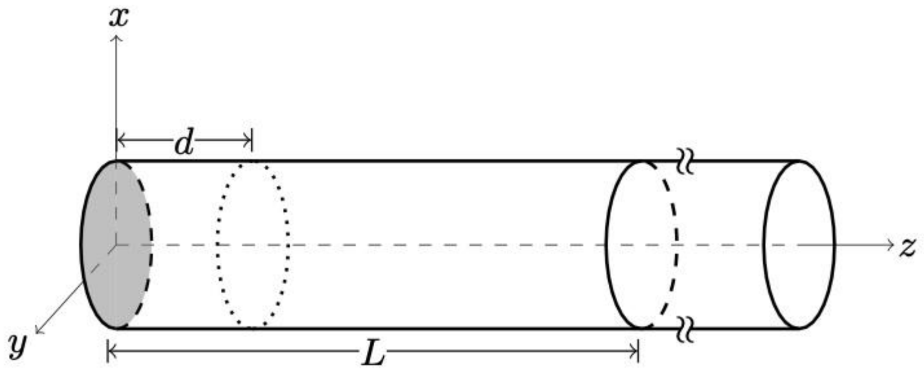
- For time-dependent QM, 1D dwell time τ in interval $[x_L, x_R]$:

$$\tau = \int_{-\infty}^{\infty} \left(\int_{x_L}^{x_R} |\psi(x,t)|^2 \, dx \right) dt$$

- Derived from an actual Hermitian dwell time operator.
  - J. Muñoz et al. Dwell-Time Distributions in Quantum Mechanics. [Time in Quantum Mechanics **2**, 97-125 (2009)].
- Previous work on dwell time calculations using QTMs for 1D time-independent stationary scattering applications.
  - L. Dupuy et al. Direct and accurate calculation of dwell times and time delays using quantum trajectories. [Phys. Lett. A **456**, 128548 (2022)].
  - L. Dupuy et al. Making sense of transmission resonances and Smith lifetimes in one-dimensional scattering: The extended phase space quantum trajectory picture. [Chem. Phys. **572,** 111952 (2023)].

Experimental Setup

- Inspired by dBB arrival time calculations for spin-1/2 particles
  - S. Das, M. Nöth, and D. Dürr. Exotic Bohmian arrival times of spin-1/2 particles: an analytical treatment. [Phys. Rev. A **99**, 052124 (2019)].



  - Spin state influences the quantum trajectory dynamics in dBB theory.

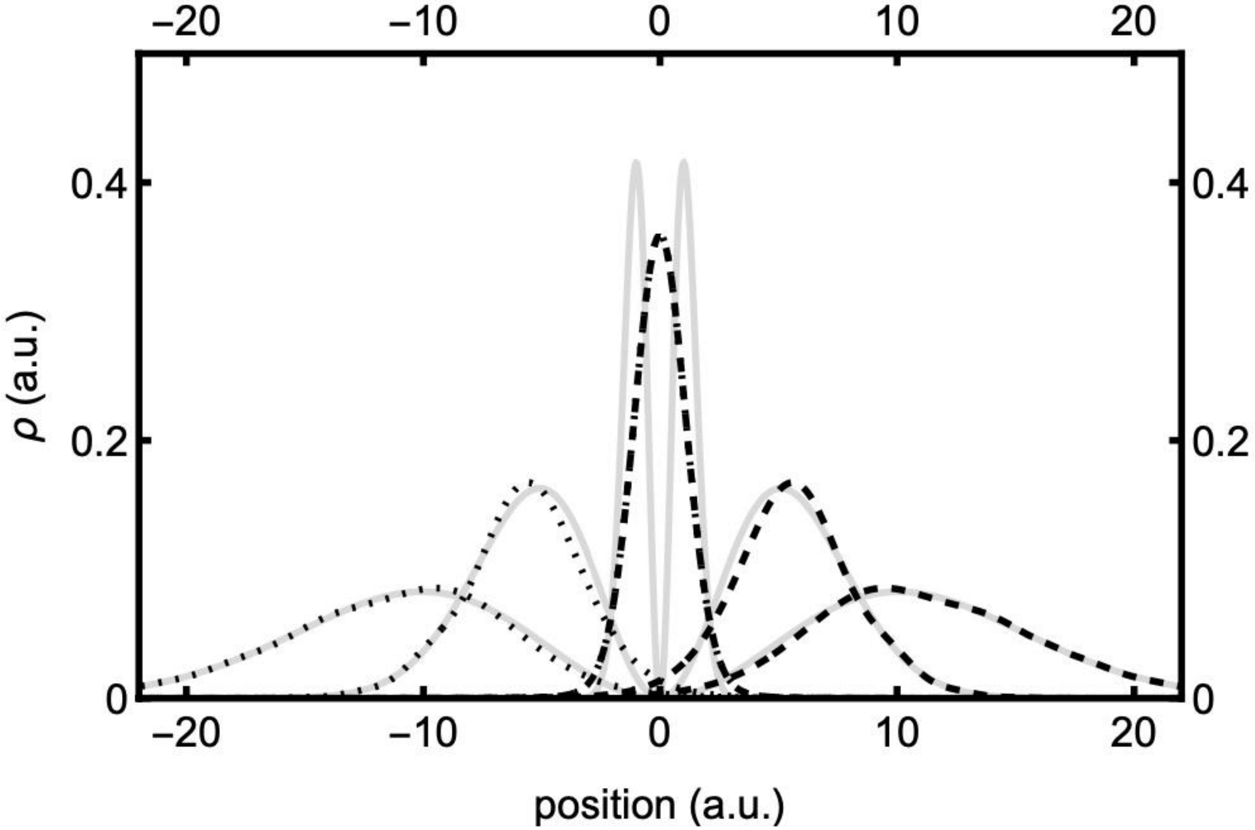
Experimental Setup

- We use same experimental setup except that:
  - Look at dwell-time distribution across trajectory ensemble $x(C, t)$ where C is a trajectory label.
  - Consider bipolar wavefunction decomposition:

$$\psi = \psi_+ + \psi_-$$

B. Poirier. Reconciling Semiclassical and Bohmian Mechanics I. Stationary States [J. Chem. Phys. **121**, 4501-4515 (2004)].

Probability Density Propagation

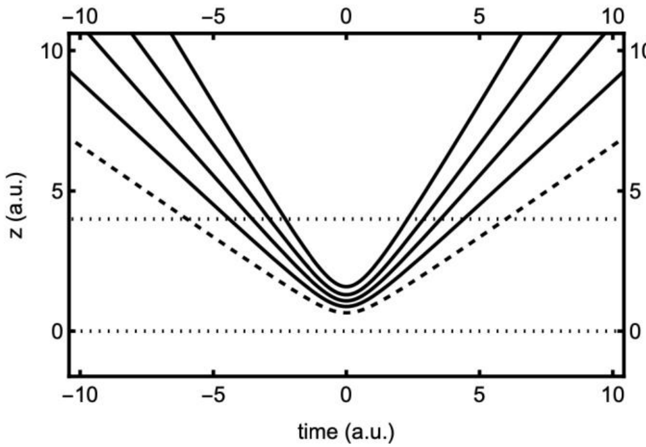


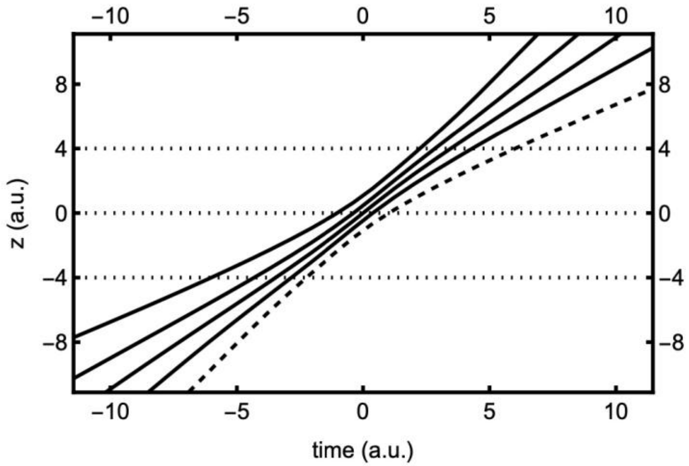
Spin States Examined

- Similar to Das et al. work, two spin states examined:
  - Spin up
    - Trajectory dynamics in z-direction can be decoupled from (x, y).
    - Unipolar dwell times τ calculated for $\psi_z(z, t)$.
    - Bipolar decomposition of $\psi_z(z, t)$.
      - $\langle\tau\rangle = \tau_+ + \tau_- = 2\tau_\pm$
      - Regard $z = 0$ as a $V \to \infty$ scattering center that reflects incoming ψ_- into outgoing ψ_+ in order to calculate $\tau^\pm$.
  - Spin up-down
    - Unipolar dwell times considered only

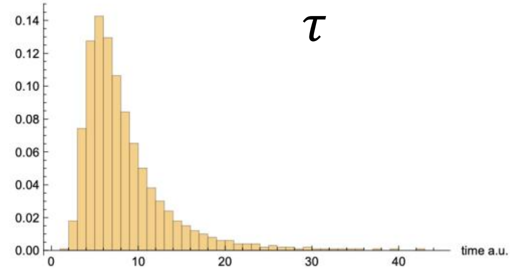
Spin Up Dwell Time Results

- 3 intervals considered: [10,20], [0,4], and [0,0.4]

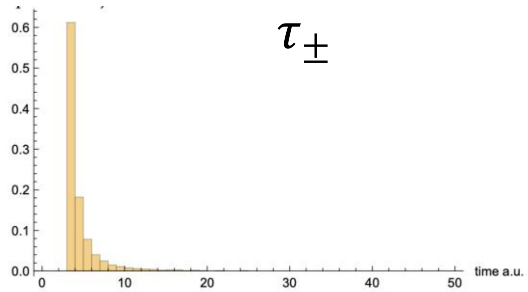




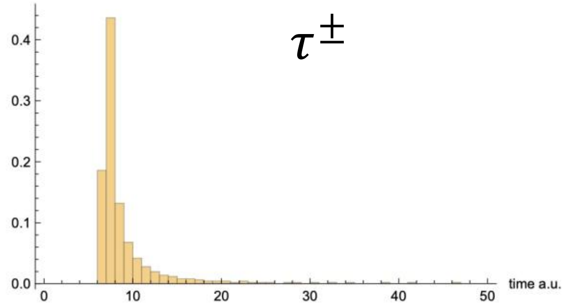
Interval	τ	$\langle \tau \rangle$	$\tau_{\pm}$	$\tau^{\pm}$	$\Delta\tau$	$\Delta\tau^{\pm}$
$[10, 20]$	22.47	22.59	11.30	22.59	14.74	7.15
$[0, 4]$	8.672	9.034	4.517	9.059	6.000	4.438
$[0, 0.4]$	0.089	0.905	0.452	0.906	0.076	0.486



τ



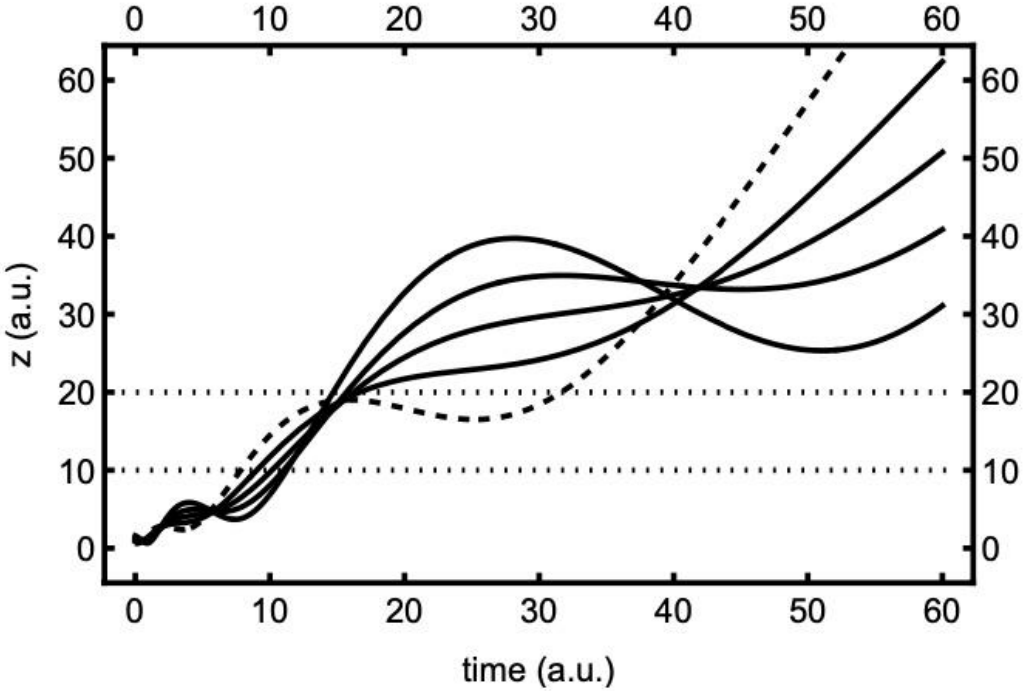
$\tau_{\pm}$



$\tau^{\pm}$

Spin Up-Down Dwell Time Results

- Asymptotic interval considered: [10,20]



spin-up case	N value τ value	100 21.99	200 22.20	500 22.38	1000 22.47
spin-up-down case	N^3 value τ value	5^3 19.82	20^3 21.58	46^3 21.40	