VISTA Seminar

Seminar 77

October 16, 2024

10:00 am – 11:30 am EDT / 3:00 – 4:30 pm BST London / 4:00 pm – 5:30 pm CEST Paris / 10 pm – 11:30 pm CST Beijing

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**Quantum Mechanics Without Wavefunctions**

Bill Poirier

*Department of Chemistry and Department of Physics,*

*University of Vermont, 82 University Place, Burlington, VT 05405-0125,* [*Bill.Poirier@uvm.edu*](mailto:Bill.Poirier@uvm.edu)*,*

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This talk addresses an alternate formulation of quantum mechanics in which the wavefunction Ψ(*t,* **x**) is discarded entirely. Instead, quantum states are represented as ensembles of real-valued probabilistic trajectories, **x**(*t*, **C**), where **C** is a trajectory label. Each of these worlds has well-defined real-valued particle positions and momenta, and is thereby classical-like. Unlike a classical ensemble, however, nearby trajectories/worlds can interact with each other dynamically, giving rise to quantum effects. The latter manifest as partial derivatives with respect to **C** in the dynamical equations, which thus constitute partial differential equations (like the Schrödinger equation itself), rather than ordinary differential equations (like Newton).

The quantum trajectory ensemble **x**(*t*, **C**) also satisfies a trajectory-based action principle, which allows quantum theory (via the Euler-Lagrange equation and Noether’s theorem) to be placed on the same footing as classical theories. The action principle also gives rise to trajectory-based symmetry and conservation laws (via Noether’s theorem). Several of these correspond to standard laws, e.g. conservation of energy. However, one such trajectory-based law (pertaining to curl-free velocity fields) appears to have no standard analog.

A full understanding of the new trajectory-based conservation law may require relativistic considerations. Whereas an earlier, non-relativistic version of the trajectory-based theory turns out to be mathematically equivalent to the time-dependent Schrödinger equation [1–5], the relativistic generalization (for single, spin-zero, massive particles) [6,7,8] is *not* equivalent to the Klein-Gordon (KG) equation—and in fact, avoids certain well-known problems of the latter. The new relativistic quantum trajectory equations could in principle be used in quantum chemistry calculations, and otherwise could lead to new physical predictions that could be validated or refuted by experiment.

These and other developments, e.g. for many dimensions, multiple particles, numerical implementations, etc., may also be discussed. The companion VISTA talk will address the spin ½ case, and also ramifications for quantum time.

**References**

[1] Bouda, A.; *Int. J. Mod. Phys. A,* **2003**, *18*, 3347–3368.

[2] Holland, P.; *Ann. Phys.*, **2005**, *315*, 505–531.

[3] Poirier, B.; *Chem. Phys.*, **2010**, *370*, 4–14.

[4] Schiff, J.; Poirier, B.; Communication, *J. Chem. Phys.*, **2012**, *136*, 031102.

[5] Poirier, B.; *Phys. Rev. X*, **2014**, *4*, 040002.

[6] Poirier, B.; **2012**, *arXiv:1208.6260 [quant-ph]*.

[7] Tsai, H.-M.; *J. Phys.*, **2016**, *701*, 012013.

[8] Poirier, B,; Tsai, H.-M.; *J. Phys*., **2020**, *1612*, 012022.

**Interacting Quantum Trajectories and Dwell Times for Particles with Spin 1/2**

Richard Lombardini1 and Bill Poirier2

*1St. Mary’s University (San Antonio, TX), Department of Physics (Associate Professor).*

*Email:* [*rlombardini@stmarytx.edu*](mailto:rlombardini@stmarytx.edu)

*2University of Vermont, Department of Chemistry (Chair). Email:* [*bill.poirier@uvm.edu*](mailto:bill.poirier@uvm.edu)

A diagram of magnet and magnet

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Time propagation of non-relativistic quantum systems of spin 1/2, traditionally modeled by spinor wavefunctions obeying Pauli equation, will be examined within the context of quantum trajectory methods (QTMs). First, a new variation of QTMs, known as the interacting quantum trajectory (IQT) method, which has been developed for non-relativistic spin-free particles,1 will be presented for both a free-particle system called the ‘quantum spin flipper’ and the Stern-Gerlach experiment. This method replaces the wavefunction or ‘pilot wave’ in the de Broglie-Bohm (dBB) theory with an ensemble of trajectories where the quantum effects manifest as interactions between the trajectories. The 1D cases will be presented where three real-valued field quantities, one particle position and two angles designating orientation of spin, each depending on time and a trajectory labeling coordinate, are guided by three non-linear coupled PDEs. Novel numerical techniques will be introduced in the propagation in order demonstrate stable dynamics. Second, quantum dwell times and dwell time distributions in the context of dBB QTMs, will be presented for a benchmark 3D spin-1/2 particle system which was analyzed in an earlier study using QTM-based arrival time distributions.2 Recent work has established a connection between QTMs and dwell times,3,4 but only in the context of time-independent stationary scattering applications. This present analysis extends these concepts to more general multi-dimensional and time-dependent cases. In addition, dwell time formulation in terms of bipolar quantum trajectories5 will be presented which offers another possible theoretical candidate for comparison to experimental quantum time measurements.

**References:**

[1] B. Poirier, *Chemical Physics* **370**, 4-14 (2010).

[2] S. Das, M. Nth, D. Drr, *Physical Review A* **99**, 052124 (2019).

[3] L. Dupuy, G. Parlant, B. Poirier, Y. Scribano, *Physical Letters A* **456**, 128548 (2022).

[4] L. Dupuy, G. Parlant, B. Poirier, Y. Scribano, *Chemical Physics* **572**, 111952 (2023).

[5] B. Poirier, *Journal of Chemical Physics* **121**, 4501-4515 (2004).

**How to connect**

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 77

Time: Oct 16, 2024 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting

<https://buffalo.zoom.us/j/97673320076?pwd=a2KEo3bbrCaEona84OQ2pDRAmbKQ8O.1>

Meeting ID: 976 7332 0076

Passcode: 036453