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Trajectory-based Representations of Quantum Transport Theory and their Connection with Semi-classical Physics

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It is argued that rigorous trajectory formulations of quantum transport phenomena are feasible and that trajectory based simulation methods corresponding to Ensemble Monte Carlo methods or Hydrodynamic modelling are possible provided the unavoidable accompanying pilot fields are included within the formalism.

1. Introduction

Most semiconductor device simulation relies on the computation of semi-classical trajectories in space-time: Monte Carlo simulation of particle histories or hydrodynamic / drift diffusion simulation of mean particle flows. Quantum mechanics enters only in an emasculated form through the dynamics: E-**p** relations; or via the perturbative evaluation of scattering rates between pairs of momentum states {**p**, **p**'}. These schemes cannot describe localisation, bound states, tunnelling, interference or diffraction phenomena, non-local effects, single electronic phenomena, quantum fluctuations and state entanglement phenomena. Although powerful mathematical tools exist for solving some classes of full quantum transport problems - Green function, path integral, density matrix methods - they have little continuity with Monte Carlo or Hydrodynamic methods and indeed are essentially field-theoretic, not particle based. They are impractical for full scale device modelling. It is often argued that the quantum mechanical "uncertainty" relations for position and momentum preclude specification of either a real space or phase space trajectory and because the underlying Schrödinger theory is a (complex) field theory there is no basis for an underlying particle (or hidden variable) description, except at the point of observation when one is reluctantly forced to admit that energy, momentum, charge are transferred locally. Nevertheless, it remains the case that people speak of particle tracks, orbits and indeed trajectories when describing quantum phenomena subjectively.

Experimental observations of apparent trajectories in cloud chambers, bubble chambers, spark chambers can be well accounted for in a pure wave picture as artefacts of the interplay of the conservation of linear momentum with the repeated inelastic scattering of a probe field on multiple scattering centres as described by Mott [1] . The geometrical optics limit of quantum theory is well understood in fields such as electron beam optics. Virtual trajectories appear in the formulation of Feynman Path integrals. Contours in phase space occur for certain classes of Wigner distribution and its relatives but cannot correspond to real particle trajectories because the formulation lacks compact support: the "trajectories" can occur in regions where the position probability density is zero.

The question thus arises: is it at all possible to maintain a particle trajectory picture as the transition is made from semi-classical transport to full quantum transport? The aim of this paper is to maintain that the answer is yes, but at a price. Our optimism is based on the observation that quantum mechanics is not a pure field theory: at the point of measurement energy and momentum is absorbed discontinuously and locally, by a detector, not continuously and dispersed as might be expected from a pure field model. Moreover the number of effective degrees of freedom for a single quanton, with respect to energy, momentum and other dynamical variables is 3 (space) plus whatever internal degrees of freedom are relevant (spin for example), whereas a pure field theory has an infinite number of degrees of freedom. In this paper we shall review progress towards revealing a quantum trajectory picture and discuss the prospects for particle simulation methods in determining full quantum transport properties. In passing we shall allude to trajectory interpretations of subtle quantum effects such as the time of arrival problem, wave packet collapse, Quantum Zeno effect and quantum measurement issues, all of which are crucial in achieving the goal of building deterministic quantum switches[2].

2. Trajectories from a classical field theory

Let us begin with the non-linear partial differential equation of motion for a particular classical field - the action $S(\mathbf{x},t)$ defined at field points $\{\mathbf{x},t\}$ in space-time:

$$\partial S(\mathbf{x},t))/\partial t + H(\nabla S(\mathbf{x},t), \mathbf{x},t) = 0 \qquad (1)$$

which is the Hamilton-Jacobi equation for a single particle and where H is a classical Hamiltonian. This is often converted quickly into a particle equation of motion by taking the gradient, identifying the form $\nabla S(\mathbf{r},t)$ as the momentum **p** of a particle at particle position $\{\mathbf{r},t\}$, in space-time and from the definitions of a drifted derivative and total differential obtaining an expression for the rate of change of momentum in terms of a local force. For specific classes of Hamiltonian such as $H = (\nabla S(\mathbf{x},t))^2/2m + V(\mathbf{x})$, the resulting "particle" equation of motion can be solved to give a complete picture of the evolution of the particle position and velocity along a well-defined particle trajectory in space-

0-7803-4369-7/98 $10.00

time. The field $S(\mathbf{x},t)$ appears to have been eliminated in favour of a local particle picture which only samples a one-dimensional orbit in the three dimensional support of S. If all possible initial boundary conditions are considered the corresponding infinite bundle of particle trajectories cover the full support of S.

A more instructive route is to adopt a *geometric* approach to equation (1), delaying any assumptions about the existence of particles. For brevity we assume a conservative Hamiltonian $H(\nabla S(\mathbf{x},t), \mathbf{x},t)$. The time-dependence of S may then factored into two components via the transformation $S = W(\mathbf{x}, \mathbf{P}) + S'(\mathbf{P},t)$ where the three components of $\mathbf{P}$ are the constants of integration $P_1 = E$, P_2, P_3 of (1). Equation (1) separates into:

$$\partial S'(\mathbf{P},t)/\partial t = -E \tag{2a}$$

$$H(\nabla W, \mathbf{x}) = E \tag{2b}$$

or by introducing the vector $\mathbf{p}$ by

$$\mathbf{p} = \nabla S = \partial S/\partial \mathbf{x} = \partial W/\partial \mathbf{x} \tag{3}$$

$$H(\mathbf{p}, \mathbf{x}) = E \tag{2c}$$

Integration of (2a) yields (β is a constant of integration)

$$S'(\mathbf{P},t) = -Et + \beta.$$

Now introduce three surfaces defined by the vector $\mathbf{X}$:

$$\mathbf{X} = \partial S/\partial \mathbf{P} \tag{4a}$$

$$X_1 = \partial W/\partial E - t \tag{4b}$$

$$X_2 = \partial W/\partial P_2 \tag{4c}$$

$$X_3 = \partial W/\partial P_3 \tag{4d}$$

where the components X_i are *constants*. Equations (4c) and (4d) describe two fixed *surfaces* $\mathbf{S}_1$ and $\mathbf{S}_2$ in space. The two surfaces $\mathbf{S}_1$ and $\mathbf{S}_2$ intersect in a fixed *curve* C given by the simultaneous solution of (4c) and (4d). Equation (4b) on the other hand describes a surface $\mathbf{T}$ which moves as a function of time t. The intersection of surface $\mathbf{T}$ with curve C locates a *moving point* D described by a vector position $\mathbf{r} = \mathbf{r}(t)$ (Fig.1a) If D is initiated at $\mathbf{x}_0$, t_0 on the curve we may determine constants X_1, X_2 and X_3 in terms of $\mathbf{x}_0$, t_0 and the constants P_i by setting $\mathbf{x} = \mathbf{x}_0$ in (4b) to (4d). Consequently $\mathbf{r}$ evolves in time from an initial location $\mathbf{r}(t_0) = \mathbf{x}_0$ at $t=t_0$ to reveal a *trajectory* along curve C (the orbit). By solving (4b - 4d) for $\mathbf{r} = \mathbf{r}(t, \mathbf{x}_0, \mathbf{P})$, we obtain the trajectory explicitly as a parametric form generated by the time variable. To obtain the velocity of point D along the trajectory we first use equation (2c) to derive

$$\partial H/\partial \mathbf{p} \,.\, d\mathbf{p} + \partial H/\partial \mathbf{x} \,.\, d\mathbf{x} = 0 \tag{5}$$

which must also hold along the orbit C. Introducing $\mathbf{p}(t)$ as the parametric form for $\mathbf{p}$ at moving location D we obtain

$$\partial H/\partial \mathbf{p} \,.\, d\mathbf{p}/dt + \partial H/\partial \mathbf{r} \,.\, d\mathbf{r}/dt = 0 \tag{6}$$

$$d\mathbf{r}/dt = \partial H/\partial \mathbf{p} \tag{7}$$

$$d\mathbf{p}/dt = -\partial H/\partial \mathbf{r} \tag{8}$$

subject to initial conditions $\mathbf{r}(t_0) = \mathbf{x}_0$, $\mathbf{p}(t_0) = \mathbf{p}_0$. where $\mathbf{p}_0$ is easily deduced from $\mathbf{P}$. Equation (7) yields the velocity. The system point $(\mathbf{r},\mathbf{p})$ follows a single valued path in phase space, but for surfaces which have non-Euclidean topology (for example self intersecting) the trajectory may re-cross a given point in space (figure eight orbits in planetary dynamics).

We have thus obtained from the equation of a pure field a *geometric* construction of Hamilton's equations for a "particle" of momentum $\mathbf{p}$ located at D which evolves along a trajectory in space or in phase space. This derivation requires that the gradient $\mathbf{X} = \partial S/\partial \mathbf{P}$ is a constant. By selecting all possible values for $\mathbf{X}$ and $\mathbf{P}$ we generate all possible solutions for S and equivalently all possible trajectories for D. The independence of the initial conditions $\mathbf{r}_0$ and $\mathbf{p}_0$ lead to multi-valuedness in $p = \nabla S$. Trajectories emanating from a family of initial locations in phase-space generate trajectories which cross in direct space (more properly configuration space). It is straightforward to show that the condition $\mathbf{X} = \partial S/\partial \mathbf{P}$ corresponds to the existence of a *contact transformation* used in Jacobi's construction of dynamics. The contact transformation implies that the co-ordinates $\mathbf{r}$, $\mathbf{p}$ are connected with the initial values at $\mathbf{r}_0$, $\mathbf{p}_0$ which are new constant co-ordinates generated by a contact transformation effected by $W(\mathbf{r},\mathbf{P})$.

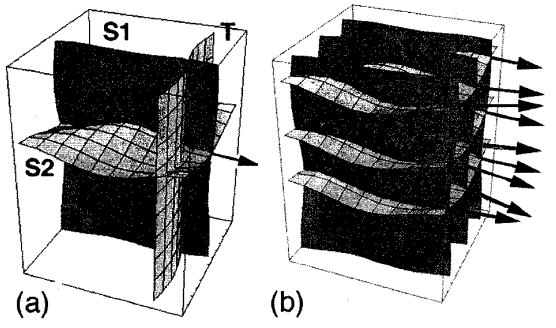

Fig. 1: (a) Classical action field: unique trajectory
(b) Quantum action field: multiple trajectories

3. Quantum trajectories

Consider now a simple conservative quantum Hamiltonian $H = T(\mathbf{p}) + V(\mathbf{x})$, where $\mathbf{x}$ and $\mathbf{p}$ are hermitian operators. For the moment let us specialise to $T(\mathbf{p}) = \mathbf{p}^2/2m$. Choosing $R(\mathbf{x},t)$ as the amplitude and $S(\mathbf{x},t)/h$ as the phase of the wave function we may separate out real and imaginary parts of the Schrödinger equation determined by H to obtain a continuity equation and a Hamilton-Jacobi like equation.

$$\partial \rho/\partial t + \nabla.\{\rho \nabla S)/m\} = 0 \tag{9}$$

$$-\partial S/\partial t = (\nabla S)^2/2m + V + V_Q \tag{10}$$

Here there are two equations for two pure fields R and S. V_Q is the quantum potential introduced by Bohm[3]. V_Q has a form that depends on the form of T(p); here

$$V_Q = -\hbar^2/(2m\,R)\nabla^2 R \qquad (11)$$

Crucially to obtain backward equivalence to the Schrödinger equation we must also put in a constraint on the boundedness of S corresponding to the wave function being single-valued, defining χ as a closed curve in space:

$$S = S \bmod h, \quad \text{or} \quad \int_\chi \mathbf{p}.\mathbf{dr} = nh \qquad (12)$$

Suppose that $R(\mathbf{x},t)$, and hence the quantum potential, is *known* as a function of space and time, from say an exact solution to Schrödingers equation. The quantity $S(\mathbf{x},t)$ then satisfies an effective Hamilton-Jacobi equation with an effective potential given by $V + V_Q$. We may follow the reasoning of section 2 to deduce the existence of a "particle" moving classically and *deterministically,* along a trajectory from some initial position and momentum $(\mathbf{r}_0, \mathbf{p}_0)$. The particle momentum is given by

$$p = \nabla S = \partial S/\partial \mathbf{r} \qquad (13)$$

Here, however, we cannot treat $\mathbf{p}_0$ as an independent boundary condition; instead the single-valuedness of the wave function implies the single-valuedness of ∇S, consequently the initial momentum at *any* starting point in space is given by

$$p_0 = \nabla S\,(\mathbf{r}_0, t_0) \qquad (14)$$

The *same* wave function thus gives rise to an infinite family of non-touching, non-crossing trajectories in configuration space (see Fig. 1b) corresponding to the set of initial moment described by the initial phase in (13). Thus a quantum state involves a delocalisation of the particle position in space. The theory is thus non-local.

If we define a probability density $P(\mathbf{x},t_0)$ for locating a particle in space at t_0, the continuity equation and the trajectory evolution equations allow us to derive $P(\mathbf{x},t)$ at any later time. *Experimentally*, we know that if an ensemble of identical states is probed to locate individual quanta they are located with probability density $P(\mathbf{x},t) = R^2(\mathbf{x},t)$. By making this choice for deciding on the initial random location in space *and* for consistency requiring that the *initial momenta* are given by equation (13) using the *initial phase* $S(\mathbf{x},t)$, we may use the entire trajectory bundle to propagate the field ∇S under guidance by the field R via a *particle -field* simulation. We have essentially re-derived Bohm's version of quantum mechanics [3] where condition (13) appears as an additional postulate.

The derivation again rests on the assumption $\mathbf{X} = \partial S/\partial \mathbf{P}$ is a constant. But what is the authority for this? We have introduced the localisation of quanta to relate the wave function amplitude to the probability density for occupying a trajectory. The assumption $\mathbf{X} = \partial S/\partial \mathbf{P}$ is equivalent to assuming the existence of a particle Hamiltonian with three degrees of freedom in which the position and momenta at one time are dependent on arbitrary initial conditions. We have additionally assumed that the evolution of R is known for all time and that S is known at some initial time. This initial condition appears to be in violation of the classical contact transformation and leads to curious properties for the trajectories. For example, the quantum trajectories in the entire bundle *cannot touch or cross.* a non-classical result. This implies a correlation between momentum and position.

4. Simulation

Either the field R or the field S must be known if the particle trajectories are to be computed. The trajectories are a geometric feature of the pilot fields. It is tempting to use Monte Carlo simulation to create the trajectories self-consistently and thus derive the fields R and S. The argument would be: (a) start with an initial set of N virtual particles distributed in space with a density given by $R^2(\mathbf{x}, t_0)$ and each with a momentum $p_0 = \nabla S(\mathbf{x}, t_0)$. (b) This ensemble would be evolved over a short time Δt using the equation of motion for $d\mathbf{p}_i/dt = \mathbf{F}(\mathbf{r}_i) + \mathbf{F}_Q(\mathbf{r}_i)$ where i denotes the i^{th} particle. Here the quantum force $\mathbf{F}_Q$ is derived from the gradient of the initial quantum potential. (c) The new particle density and hence R is calculated from the new positions or from the continuity equation. An updated quantum potential is obtained and the procedure repeated. By integrating the velocity field we might obtain S and thus the wave function would be recovered. Unfortunately, there are two particular problems: first, the continuity equation (which is trivially reflected in the continuity of the trajectories) maps the non-nodal regions of the pilot field R (where $R \neq 0$) into themselves along the trajectories:

$$\rho(\mathbf{r}(t)) = \rho(\mathbf{r}_0(t))\exp\left(-\int_{t_0}^{t} \nabla.\mathbf{v}(\mathbf{r}(t'))dt'\right) \qquad (15)$$

The quantum force is derived from $\rho = R^2$, and it prevents particle trajectories crossing nodal lines. Thus this particle based or fluid based simulation cannot change the original nodal structure. Second, the phase condition (12) is automatically satisfied in the initial state and is secure whilst the nodal pattern is fixed. However in a full wave-mechanical treatment, the nodal pattern not only evolves but there are discontinuous changes in the phase number n possibly leading to changes in the current quantisation (appearing as a quantised vorticity). Either the full wave function must be computed at each time step (the trajectories are then trivially derived from Bohm's theory) or *either* of the two fields R or S. It is easier to compute R.

A possible scheme is to use the quantum Hamilton Jacobi equation (10) together with (11) to compute R at each time step, subject to *field boundary conditions* rather than particle boundary conditions. We thus solve:

$$\hbar^2/(2m)\nabla^2 R = \Omega(\mathbf{x},t)\,R \qquad (16)$$

$$\Omega = (\partial S/\partial t + (\nabla S)^2/2m + V) \qquad (17)$$

where Ω is obtained from the trajectory dynamics by simple Monte Carlo. With this approach there is no need to impose an initial probability distribution (alternative views are in [4]); it may be derived from the stationary wave equation for R using initial values for $\partial S/\partial t$ and ∇S. This scheme is quite useful for handling 1-D particle in a box problems including the non-trivial adiabatic and non-adiabatic problems of a particle in a box with moving walls. It works very well when the spatial wave function is real. It describes evolving nodal patterns but in general it cannot pick up changes in quantised current coming from the phase condition.

It is also feasible to use a complex quantum Hamilton Jacobi equation for the complex phase $S' = S - i\hbar\nabla\rho/2\rho$:

$$-\partial S'/\partial t = (\nabla S')^2/2m + V + V'_Q \qquad (18)$$

$$V'_Q = i\hbar/(2m)\nabla^2 S' \qquad (19)$$

This equation preserves all the phase conditions and nodal properties and if solved with pure wave boundary conditions is equivalent to the Schrödinger equation. A virtual particle simulation may be possible provided the wave boundary conditions are suitable transformed.

A deeper interpretation of Bohm's picture [5] suggests that the quantum Hamilton Jacobi equation is in fact an ensemble average over an underlying stochastic picture in which the trajectories are *stochastic:* akin to Brownian motion paths. The resulting re-formulation is similar to Nelson's [6] stochastic version of quantum mechanics but it utilises the phase condition(12) to derive the stochastic forces. There are similar problems in a self-consistent simulation of the random trajectories.

Quantum hydrodynamics has similarities to the Bohm picture and encounters exactly the same problem of being unable to provide a self-consistent simulation of transport without *a priori* knowledge of the quantum state [7].

5. Arrival time on a trajectory

If occupancy of a quantum trajectory is established the particle has a precise time of arrival at any subsequent point on the orbit. Thus traversal times, a controversial problem in tunnelling theory are easily established. The mean traversal time τ between two points is obtained by computing the time $T(\mathbf{x}_1, \mathbf{x}_2; \mathbf{x}_0)$ for a particle initially on a trajectory at $\mathbf{x}_0$ with probability density $R^2(\mathbf{x}_0)$

$$\tau = \int d^3x T(\mathbf{x}_1, \mathbf{x}_2; \mathbf{x}_0) R^2(\mathbf{x}_0) . \qquad (20)$$

Leavens [8] gives a precise description of the various tunnelling times on this basis. It should be noted however that in the stochastic picture [5, 6] the trajectory evolution is quite different and a different value for the traversal time τ must be expected. No experimental tests exist at present.

6. Information theory

It is interesting to note that there is no requirement for "wave packet collapse" to be invoked in understanding the measurement problem if we adopt either the deterministic or stochastic Bohm picture. For example, if we calculate the R and S fields for inelastic scattering of an electron wave packet on an atom, the scattered wave contains wave packet components distributed in shells which recede apart at different velocities as time elapse. If the electron has an *a priori* probability P_i to be in the i^{th} outgoing packet and is subsequently discovered there, it cannot evolve to join any other packet according to the trajectory model. From an information theoretic point of view we may then re-normalise R over this particular packet when assigning a new probability distribution for the particle. The remaining *empty wave packets* may be then ignored.

7. Conclusions

The existence of classical trajectories as unique geometric features of the classical action field has been emphasised. The quantum action field has a different property; it sustains a family of non-touching, single-valued trajectories (but not orbits) which correspond to the same quantum state. It is not possible to build a particle-only model or self-consistent quantum hydrodynamic model of quantum theory. This is because the pilot field S cannot be eliminated as in classical theory and induces instead a de-localisation of each classical trajectory. The pilot field R induces an information theoretic probability distribution over the trajectory family. In some cases, for example, when the circulation (12) is not quantised a self-consistent particle simulation may be constructed by a leap-frog method in which the R field and then the velocity field is computed using successive field and particle boundary conditions. The information theoretic interpretation of pilot field - trajectory models is sufficiently powerful to handle some problems associated with continuous measurement processes. In particular, the Quantum Zeno effect is easily incorporated if we use the modified density-matrix formalism [9].

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