The Towler Institute

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Quantum Monte Carlo in the Apuan Alps V

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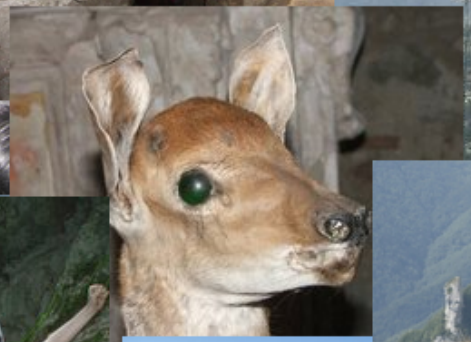


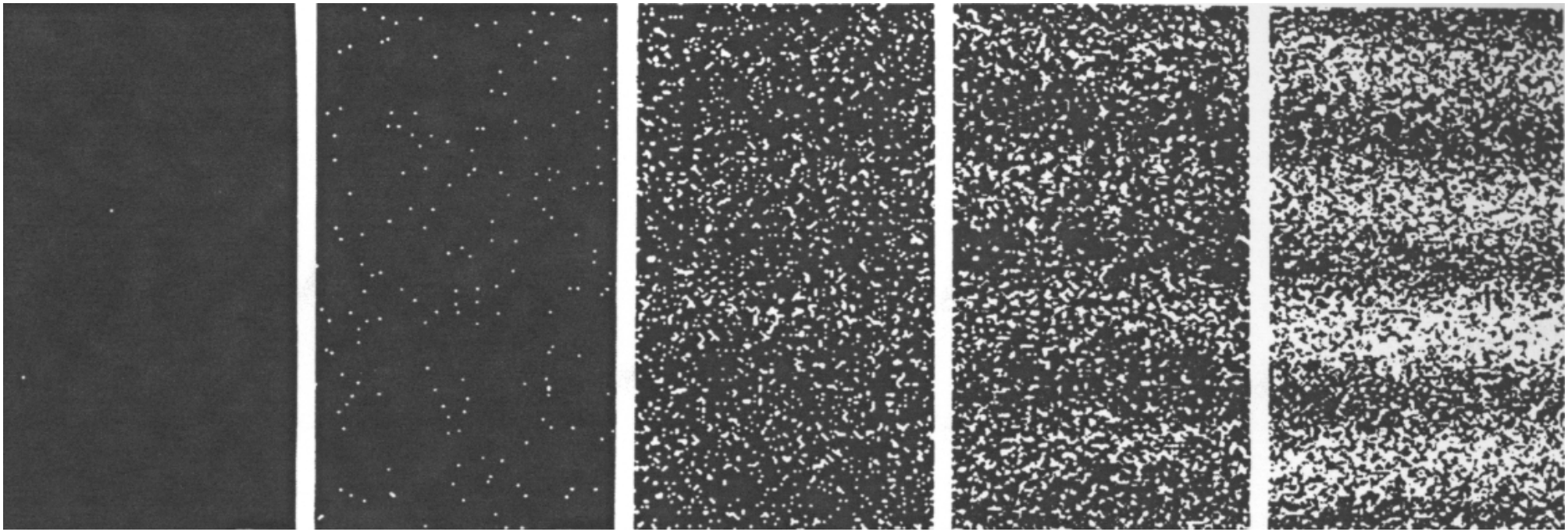





Pilot waves, Feynman path integrals, and quantum Monte Carlo

Quantum Monte Carlo in the Apuan Alps V

26th July 2009



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Pilot wave theory

(Bohmian mechanics, de Broglie-Bohm theory, Bohm interpretation, causal interpretation, ontological interpretation..)

What is pilot-wave theory?

- It is the original (not very well-known) interpretation of quantum mechanics (QM).
- It is a mathematical reformulation of QM equivalent in status to Feynman's path-integral theory.

Why are people interested in it?

- It shows that QM can simply be interpreted as just the statistical mechanics of particles with a non-classical dynamics. QM does not have to be 'weird'.
- It directly resolves all so-called paradoxes of orthodox QM, in particular the measurement problem/wave collapse. It does this without a massively expanded ontology of parallel worlds, shadow universes, multiple intersecting realities etc..
- The *quality of its explanation* is greatly superior to the orthodox theory (which anyway rejects the need for explanations on principle). We are suddenly able to understand Heisenbergs's uncertainty principle, Pauli exclusion, tunnelling, the classical limit, quantum jumps, angular momentum etc.
- If adopted widely, it would greatly reduce the amount of time spent trying to explain the unexplainable to novices.
- It can be used to do interesting calculations based on 'quantum trajectories' (there is a community of physical chemists who do this).

Basic idea of pilot-wave theory

We must first make a *metaphysical commitment*. Metaphysics is not a term of abuse - it means the study of reality; you have to specify 'what exists' - what is QM actually about? If you don't like doing this, feel free to use phrases like 'acts as if'.

(1) Particles

Change definition of single word - *probability* - such that $\Psi^2(\mathbf{x}, t)$ is the probability that the particle *is* at a precise location $\mathbf{x}$ at time t, rather than the probability of *finding it there in a suitable measurement*. This has the implication that particles exist continuously and have *trajectories*, independently of their being observed.

(2) Wave

What does the wave function Ψ mean? Often said it represents *information*, but clear from fact that we get interference effects in a two-slit experiment that 'something' wave-like passes along the different paths; to refuse to call it 'real' is merely to play with words. Thus we say a *wave field* exists and this is represented mathematically by the usual QM wave function evolving according to Schrödinger's equation.

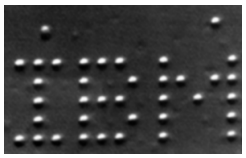
Wave-particle duality : both particles and wave exist!

These are the only changes required to orthodox QM to get the full pilot-wave theory. All equations and results follow directly from the established formalism.

1927 was a long time ago

Orthodox Copenhagen QM is both an algorithm for obtaining statistical predictions for the results of experiments and a prescription for *avoiding fundamental questions*. Bohr *et al.* designed it that way because in 1927 quantum entities were unobservable and thus [non sequitur] not real: "*. . . the idea of an objective real world whose smallest parts exist objectively in the same sense as stones or trees exist, independently of whether or not we observe them . . . is impossible.* " [Heisenberg, 1958]

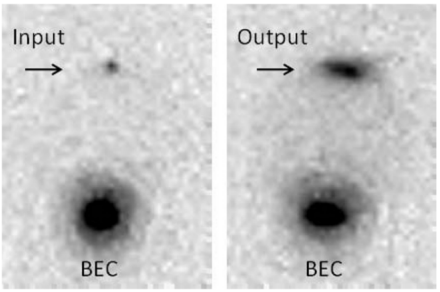
However, modern progress in experimental physics shows essentially without doubt that quantum entities are in fact real. They exist whether we 'observe' them, conduct experiments with them, or not.



Single atoms and even electrons can be isolated and trapped in containment vessels for long periods. Can repeat examination over and over again and get same data. Individual atoms can be 'pushed around', arranged into patterns (which can also be imaged) and otherwise manipulated. These experiments all yield *consistent* results and information about quantum entities using a variety of techniques and under different conditions.

"*Perhaps the most convincing proof of the reality of the quantum world would be to capture some of its creatures and hold them in place for all to see. This has become feasible.*" [Ho-Kim *et al.*, 2004]

Clear evidence for wave field existence from *matter wave optics*. Ultracold atomic gases have dominant wave behaviour. Can manipulate by 'optical devices'. Significant quantities of matter diffracted, focussed, reflected etc. Also 'matter wave amplification' experiments: production of output of atoms with particular properties from BEC reservoir of atoms in a trap) using process similar to stimulated emission of light in a laser. If matter wave can be subject to and utilized in such a process, it logically follows matter wave must exist in order to act and be acted upon.



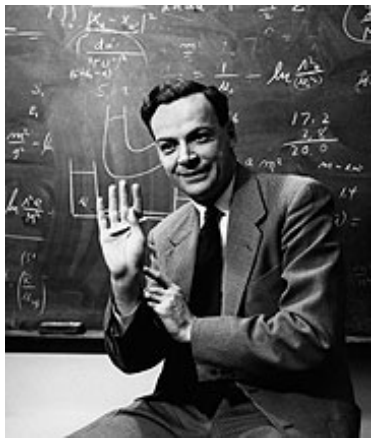
Many older physicists get really angry about this and clearly will never overcome the dominant though patterns of the prevailing paradigm of orthodox quantum theory (such as the denial of an independently existing quantum realm). Sadly, it will almost certainly be necessary to wait for them all to die.

Mathematical formulation of pilot-wave theory

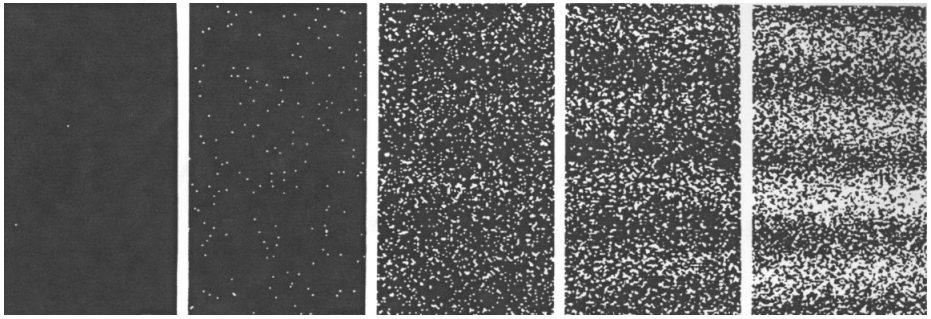
Wave field evolves according to Schrödinger equation $i\hbar\frac{\partial\Psi}{\partial t} = \sum_{i=1}^{N} -\frac{\hbar^2}{2m_i}\nabla_i^2\Psi + V\Psi$ but what are the particle trajectories? Recall standard result that quantum system behaves like 'probability fluid' $|\Psi|^2$ with an associated time-dependent quantum probability current, given by $\mathbf{j} = \frac{\hbar}{m}\mathrm{Im}(\Psi^*\nabla\Psi)$. Then velocity = current/density = $\frac{\hbar}{m}\mathrm{Im}\nabla\ln\Psi$. Using the complex polar form of $\Psi = |\Psi|\exp[iS/\hbar]$, we see the *phase* of the wave function $S(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N, t)$ is defined by $S = \hbar\mathrm{Im}\ln\Psi$. Thus we deduce trajectories $\mathbf{x}_i(t)$ are given by the *de Broglie guidance equation* for the velocity:

$$\mathbf{v}_i = \frac{d\mathbf{x}_i}{dt} = \frac{\nabla_i S}{m_i}$$

- A particle is thus 'pushed along' by the wave (by a 'quantum force') along trajectories perpendicular to surfaces of constant phase, as well as by the classical force' from the other particles.
- Guidance equation identical to trajectory equation in Hamilton-Jacobi theory (a standard form of classical mechanics like Hamiltonian or Lagrangian dynamics). There S is indefinite integral of classical Lagrangian with respect to t (note the 'action' is the *definite* integral with fixed endpoints).
- Can also guess guidance equation from de Broglie relation $\mathbf{p} = \hbar\mathbf{k}$ (connects particle and wave properties). Wave vector $\mathbf{k}$ defined only for plane wave. For general wave, obvious generalization of $\mathbf{k}$ is local wave vector $\nabla S(\mathbf{x})/\hbar$. Hence $\mathbf{v} = \nabla S/m$.
- Can also write in second order $F = ma$ form by taking time derivative of guidance equation, i.e.: $m_i\ddot{\mathbf{x}}_i = -\nabla_i(V + Q)$ where $Q = -\sum_i \frac{\hbar^2}{2m_i}\frac{\nabla_i^2|\Psi|}{|\Psi|}$ (the *quantum potential*).
- Operators on Hilbert space and all that play no fundamental role, but are exactly right mathematical objects to provide compact representation of the statistics in a de Broglie universe.



Two-slit experiment with electrons



- "*A phenomenon which is impossible, absolutely impossible, to explain in any classical way, and which has in it the heart of quantum mechanics. In reality it contains the only mystery.*"

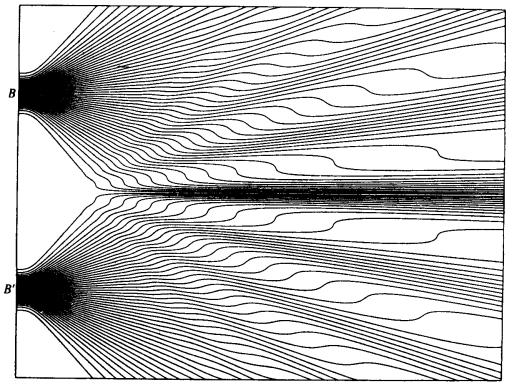
- "*Do not keep saying to yourself, if you can possibly avoid it, 'But how can it be like that?' because you will get 'down the drain,' into a blind alley from which nobody has yet escaped. Nobody knows how it can be like that.*"

- "*Many ideas have been concocted to try to explain the curve for* P_{12} [that is, the interference pattern] *in terms of individual electrons going around in complicated ways through the holes. None of them has succeeded.*"

- This experiment "*has been designed to contain all of the mystery of quantum mechanics, to put you up against the paradoxes and mysteries and peculiarities of nature one hundred per cent.*"

- "*How does it really work? What machinery is actually producing this thing? Nobody knows any machinery. Nobody can give you a deeper explanation of this phenomenon than I have given; that is, a description of it.*"

Pilot-wave theory: while each particle track passes through just one slit, the wave passes through both; the interference profile that consequently develops in the wave generates similar pattern in the trajectories guided by the wave.



Compare Feynman commentary with that of John Bell:

"*Is it not clear from the smallness of the scintillation on the screen that we have to do with a particle? And is it not clear, from the diffraction and interference patterns, that the motion of the particle is directed by a wave? De Broglie showed in detail how the motion of a particle, passing through just one of two holes in the screen, could be influenced by waves propagating through both holes. And so influenced that the particle does not go where the waves cancel out, but is attracted to where they cooperate. This idea seems to me so natural and simple, to resolve the wave-particle dilemma in such a clear and ordinary way, that it is a great mystery to me that it was so generally ignored.*"

Energy and diffusion

What is energy? Little or no attention paid in physics to general definition. In classical mechanics, energy defined as *capacity of physical system to perform work*, and work defined in terms of *forces*. This definition has severe limitations and is actually useless in many cases (consider cylinder with hot and cold gases in compartments separated by a heat conducting piston). In fact energy is real attribute of physical systems with following characteristics: it is conserved, can be stored, exists in different interconvertible forms, and can be transferred through space or from one material body to another. A *field* is nothing more than a spatial distribution of energy which varies with time.

Problem with usual definition of *potential energy*: often stated to be a property of *particles* - cannot be correct. Energy conservation can also be satisfied by debiting field with an energy loss equal to KE gained by particle. Must also distinguish between (position-dependent) PE available to particle in a field (e.g. qEy for particle between charged plates), and total energy stored in field (e.g. $\frac{1}{2}\epsilon dAE^2$).

- Why does time-dependent Schrödinger equation describe propagation of the wave field?
- Why is its mathematical form similar to the *diffusion* or *heat equation* of classical physics?

$$i\hbar\frac{\partial\Psi(\mathbf{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{x},t) \qquad \frac{\partial u(\mathbf{x},t)}{\partial t} = D\nabla^2 u(\mathbf{x},t)$$

Main difference is imaginary i - ultimately traceable to use of *complex* wave functions (just mathematical convenience as Schrödinger can be rewritten as two coupled DEs involving two *real* functions).

- Standard heat equation derivation with no sources proceeds by specifying energy 'flux' from one region to another due to temp variation. Resulting equation describes transfer of heat energy.
- Schrödinger equation describes propagation through space of physical field with no sources (in classical sense) and finite energy content. Wave field time development conserves energy - thus describes energy transfer between spatial regions. The two equations therefore have the same form..

A new language

'Wave field' exists objectively in ordinary 3d space. Mathematically represented by usual Schrödinger wave function in *configuration space* (to account for forces or 'entanglement' between particles). Wave field is repository of potential energy in a quantum sytem, and acts on quantum particle similar to an external field and receives or imparts energy and momentum to the particle.

'Quantum potential' $Q = -\sum_i \frac{\hbar^2}{2m_i}\frac{\nabla_i^2|\Psi|}{|\Psi|}$ is the potential energy function of the wave field. It represents a portion of the energy contained in the wave field and is the amount of energy available to the particle at its specific position in the field. Q independent of intensity of wave field. Facilitates nonlocal connections in many-particle system.

'Quantum force' or *quantum-mechanical force* $\mathbf{F} = -\nabla Q$ - additional to four accepted fundamental forces! Non-classical: strength need not decrease with distance (connected with 'nonlocality'). Existence of QM force not generally recognized; indeed - possibility *not even known* to most physicists! Circumstances in which force is present but not acknowledged:

- QM force acts but resulting phenomenon merely described as 'quantum effect' with no classical analogue (e.g. Aharanov-Bohm - QM force on particles non-zero even when other forces absent).
- Another force postulated which is QM force with different name (e.g. 'Pauli force/Pauli repulsion').
- QM force acts with accepted fundamental forces but is not recognized (e.g. covalent bonding).

Useful concept to gain more comprehensive understanding of natural processes in which quantum effects are manifest (superconductivity, metal-insulator transition etc..).

'Quantum equilibrium'. Particle distribution ρ logically distinct from $|\Psi|^2$. But can show if particles not initially distributed as $|\Psi|^2$ then become so under Schrödinger evolution and thereafter remain so distributed (in '*quantum equilibrium*'). Hence can *derive* Born rule. See numerical simulations later.

Better explanations

- Measurement problem, Schrödinger's cat, wave collapse: Wave doesn't collapse (i.e. momentarily stop obeying Schrödinger's equation and change shape at infinite speed when someone looks at it). Things are made of particles. If wave field branches, particles deterministically end up in some branch with appropriate probability (one cat, one universe not bazillions of them).
- Classical limit: Classical limit emerges from the theory rather than having to be postulated. Classical domain is where wave component of matter is passive and exerts no influence on corpuscular component, i.e. state of particle independent of state of field ($Q = 0$, essentially).
- Tunnelling: Effective 'barrier' encountered by particle not V but $V + Q$ - may be higher or lower than V and may vary outside 'true' barrier. For tunnelling need only $-\partial S/\partial t \geq V + Q$ then particle may enter/cross barrier region. Basically, particles shoved over barrier by 'quantum force'.
- Angular momentum: Due to rotational motion of electron trajectories 'orbiting' the nucleus! If ψ eigenfunction of $\hat{L}_z$, $\hat{\mathbf{L}}^2$ actual values and eigenvalues coincide. Traditionally x- and y-components 'undefined' but in fact well defined e.g. $L_x = -m\hbar \cot\theta \cos\phi, \quad L_y = m\hbar \cot\theta \sin\phi, \quad L_z = m\hbar$. Along trajectory L_x, L_y are *not conserved* (unlike $\hat{L}_z$, $\hat{\mathbf{L}}^2$).
- Quantum jumps: Standard belief: *systems can only possess certain values of physical quantities corresponding to spectra of Hermitian operators*. In pilot-wave theory quantities well-defined and continuously variable for all quantum states - values for subset of eigenstates have no *fundamental* physical significance. One of characteristic features of QM - existence of discrete energy levels - due to *restriction of basically continuous theory to motion associated with subclass of eigenfunctions*. Such states may possess particular physical importance in relation to stability of matter, but particle momentum and energy just as unambiguously defined when wave is superposition of eigenstates. No 'quantum jumps' in sense of process that is instantaneous or beyond analysis.

Rest of talk: some numerical applications of pilot-wave theory

1. The problem of quantum equilibrium - why are particles distributed as $|\Psi|^2$?

2. Quantum trajectory methods

3. Quantum trajectories and the Feynman path-integral method

4. Connections between pilot-wave theory and quantum Monte Carlo

5. 'Time-dependent quantum Monte Carlo'

Quantum equilibrium: dynamical origin of quantum probabilities

Proc. Roy. Soc. A **461**, 253 (2005).

In this paper, Valentini and Westman show using explicit numerical simulations that $\rho \to |\Psi|^2$ *arises naturally even from a grossly non-equilibrium particle distribution.*

- System is a single particle in a 2D box with configuration $q = (x, y)$ and a (pure state) wave function $\psi(x, y, t)$ satisfying Schrödinger equation ($\hbar = 1$)

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} - \frac{1}{2}\frac{\partial^2\psi}{\partial y^2} + V\psi.$$

- Have ensemble of independent particles each guided by same ψ, so define density $\rho(x, y, t)$ of actual configurations. Guidance law $\mathrm{d}\mathbf{q}/\mathrm{d}t = \mathrm{Im}\,\nabla \ln\psi = \nabla S$ defines velocity field $(\dot{x}, \dot{y})$ which determines evolution of ρ via continuity equation:

$$\frac{\partial\rho}{\partial t} + \frac{\partial(\rho\dot{x})}{\partial x} + \frac{\partial(\rho\dot{y})}{\partial y} = 0$$

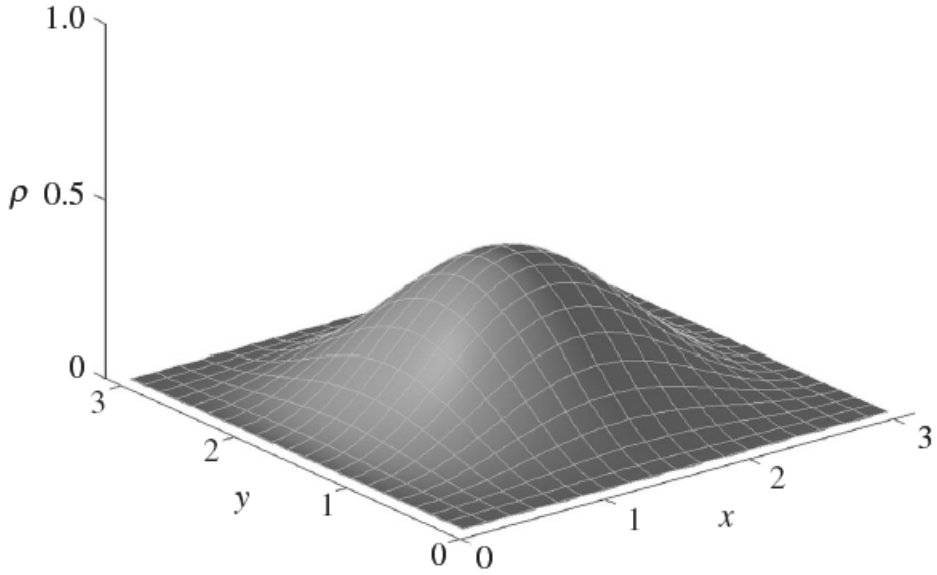
- Box has sides of length π with infinite barriers. The energy eigenfunctions are

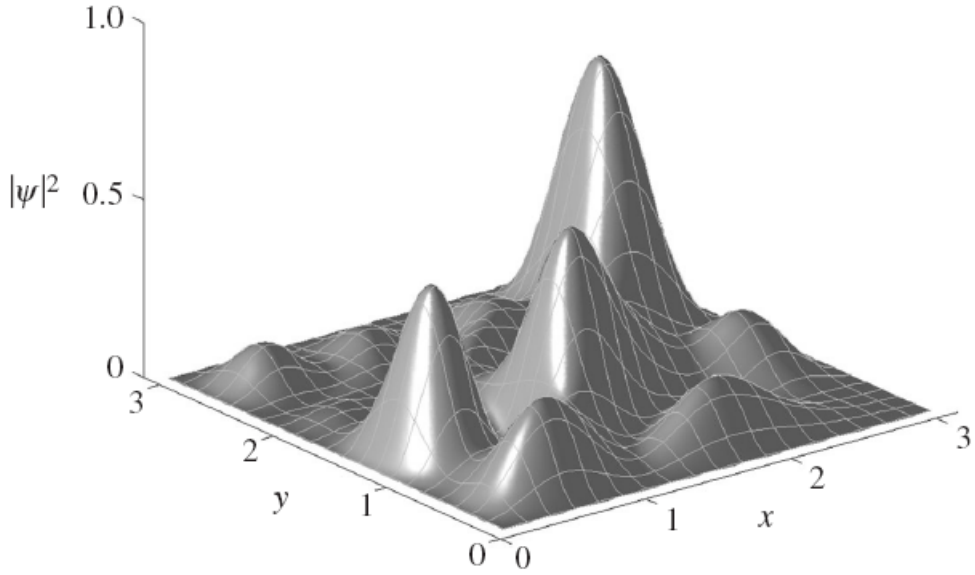
$$\phi_{mn}(x, y) = \frac{2}{\pi}\sin(mx)\sin(ny)$$

with energy eigenvalues $E_{mn} = \frac{1}{2}(m^2 + n^2)$, where $m, n = 1, 2, 3, \ldots$

Dynamical origin of quantum probabilities: numerical simulations

Starting conditions for the simulation: initial $\rho \neq |\Psi|^2$





Want grossly non-equilibrium starting distribution for particles. Choose distribution equal to square of ground-state wave function:

$$\rho(x, y, 0) = |\phi_{11}(x, y)|^2$$

.

Initial ψ is superposition of first 16 modes, $m, n = 1, 2, 3, 4, \ldots$ with equal amplitudes but randomly chosen phases θ_{mn}:

$$\psi(x, y, 0) = \sum_{m,n=1}^{4} \frac{1}{4} \phi_{mn}(x, y) \exp(i\theta_{mn})$$

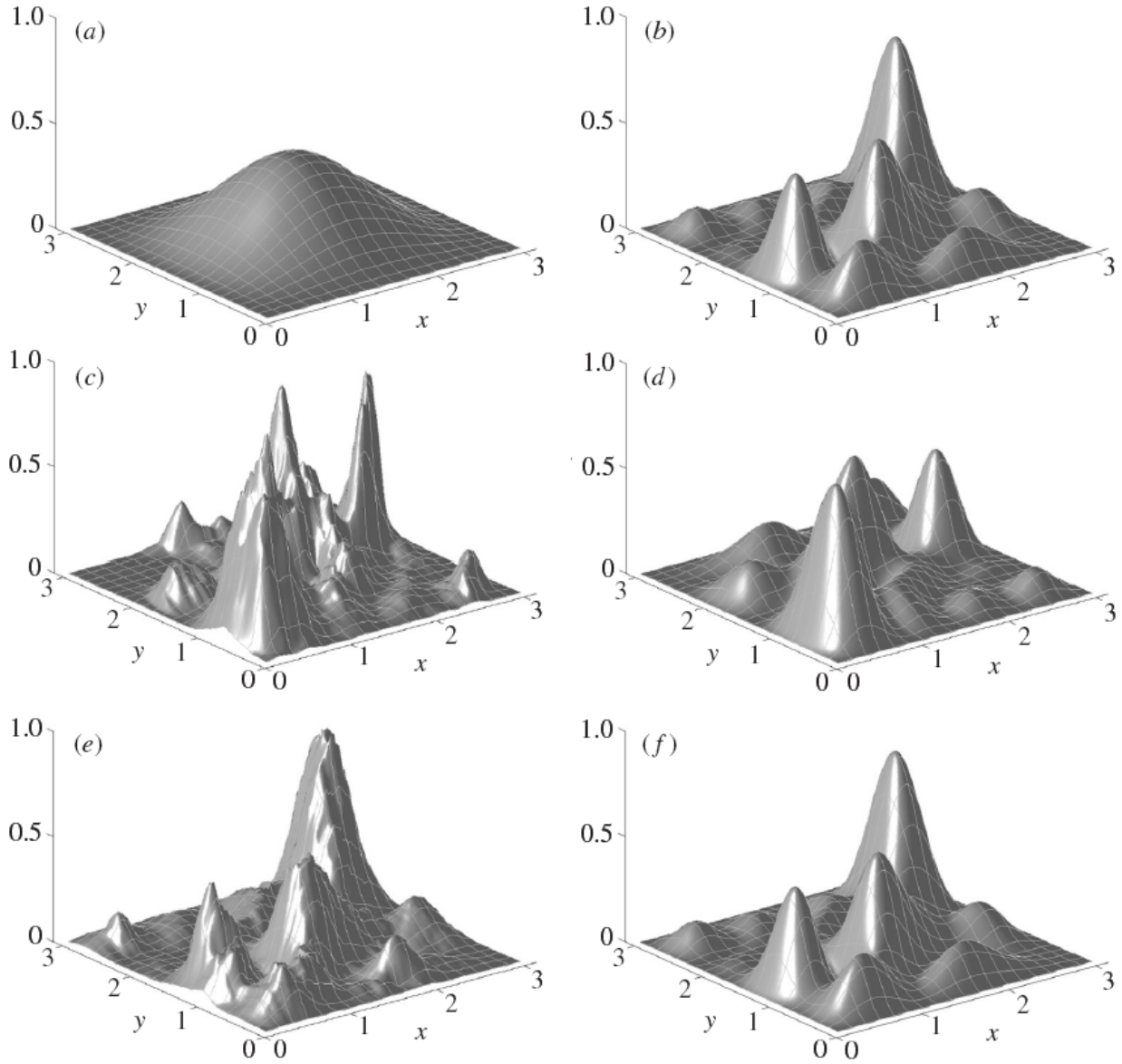
$$\psi(x, y, t) = \sum_{m,n=1}^{4} \frac{1}{4} \phi_{mn}(x, y) \exp i(\theta_{mn} - E_{mn}t)$$

Note ψ periodic in time with period 4π (since $4\pi E_{mn}$ is always an integer multiple of 2π).

Dynamical origin of quantum probabilities: numerical simulations

Results of evolution

ρ



$|\Psi|^2$

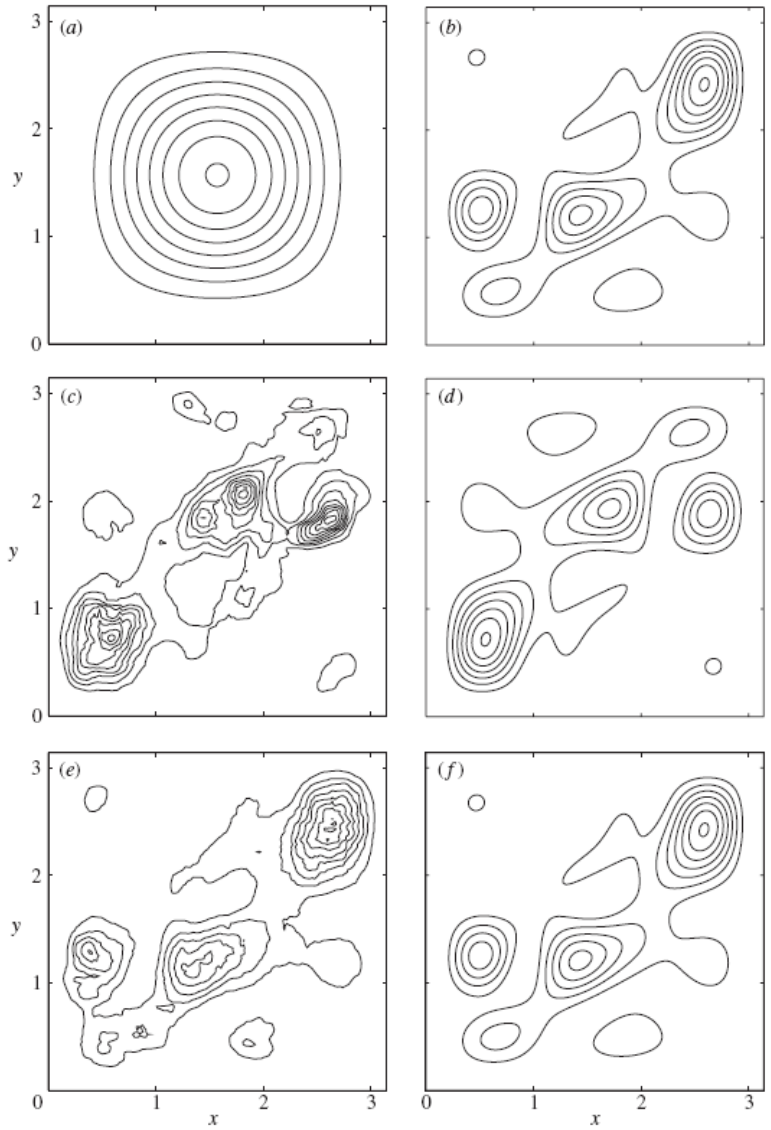
Results for $t = 0$ (a,b), for $t = 2\pi$ (c,d) and for $t = 4\pi$ (e,f).

While $|\Psi|^2$ recurs to its initial value, the smoothed particle distribution ρ shows a remarkable evolution towards quantum equilibrium!

Dynamical origin of quantum probabilities: numerical simulations

Results of evolution: contour plots

ρ



$|\Psi|^2$

Results for $t = 0$ (a,b), for $t = 2\pi$ (c,d) and for $t = 4\pi$ (e,f).
Same data as previous slide displayed as contour plots.

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Dynamical origin of quantum probabilities: numerical simulations

Character of the trajectories

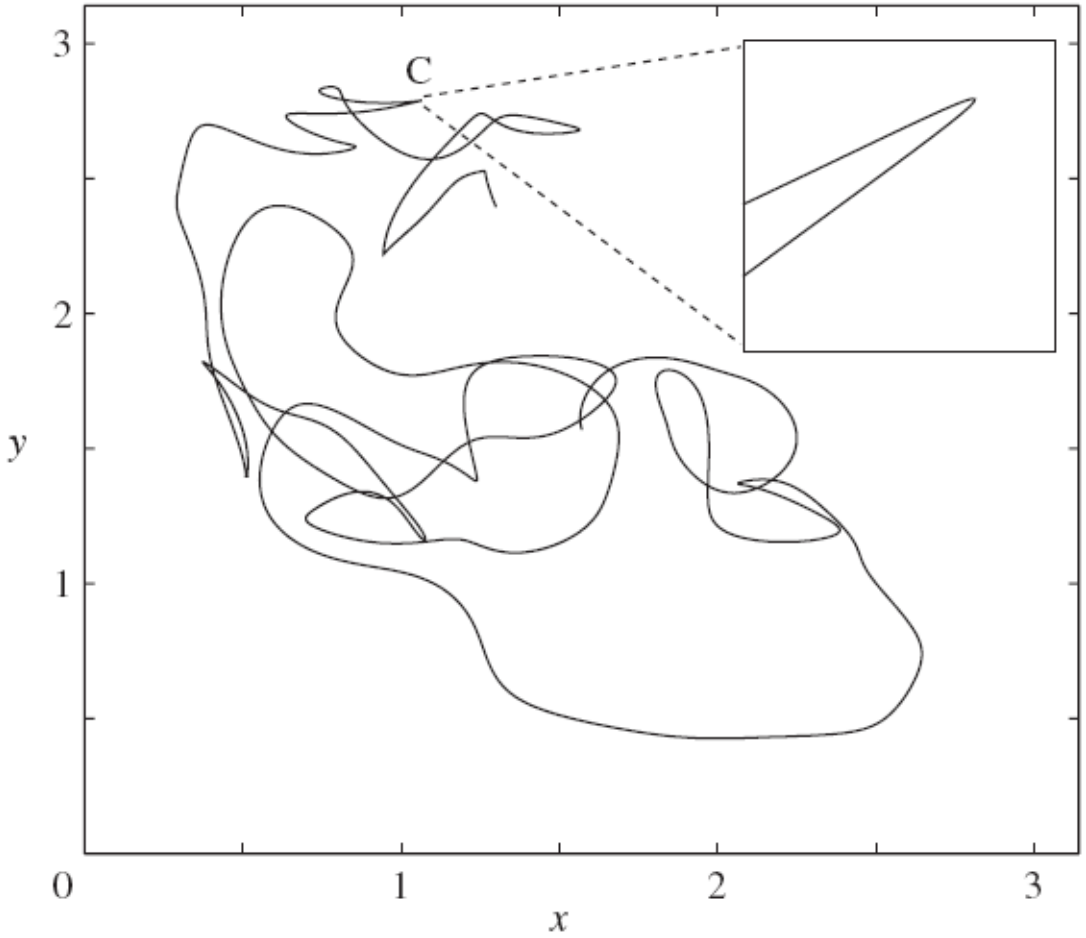
Particle velocity components at t:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{i}{2|\psi|^2}\left(\psi\frac{\partial\psi^*}{\partial x} - \psi^*\frac{\partial\psi}{\partial x}\right)$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = \frac{i}{2|\psi|^2}\left(\psi\frac{\partial\psi^*}{\partial y} - \psi^*\frac{\partial\psi}{\partial y}\right)$$

Calculate trajectory $x(t), y(t)$ by numerical integration of above. Typical trajectory shown here - in general they are rather irregular.

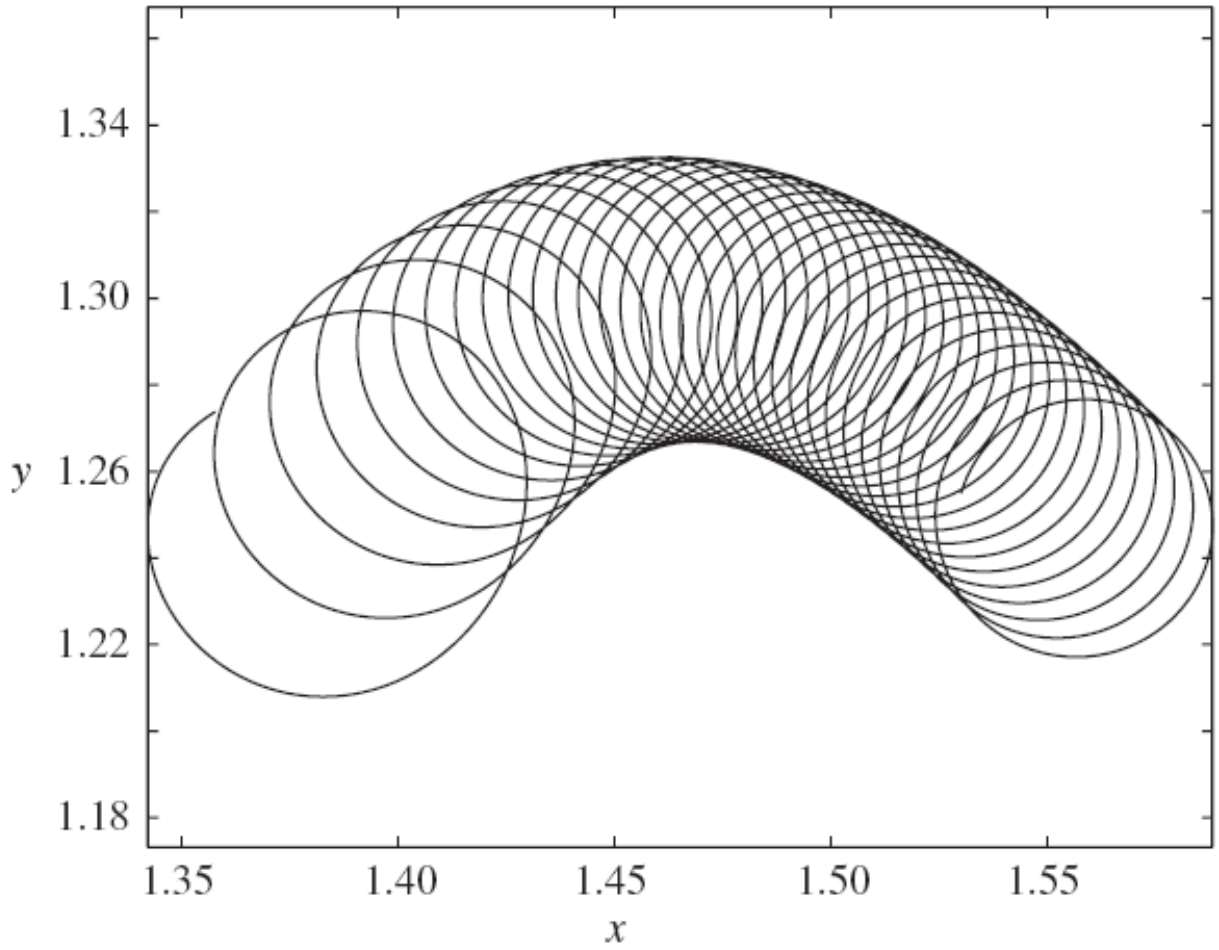
Point C looks like a cusp but tangent not actually discontinuous (particle turning round *slowly*).



Note velocities ill-defined at nodes (where $|\psi| = 0$) and tend to diverge as nodes are approached. This is because - close to a node - small displacements in x and y can generate large changes in phase $S = \mathrm{Im}\ln\psi$ corresponding to large gradient ∇S. Because ψ is smooth, single-valued function, small displacement $(\delta x, \delta y)$ produces small change $\delta\psi$ in complex plane. However, close to a node $\delta\psi$ lies near origin of complex plane and so can correspond to large phase change δS.

Dynamical origin of quantum probabilities: numerical simulations

Close-up of a trajectory near a node



Motion rapid in regions where $|\psi|$ is small. Above close-up of trajectory near nodal or quasi-nodal point where $|\Psi|$ very small (but not known to be strictly zero). Spatial region shown *ca.* 0.3% of whole box. Particle follows rapid circular motion around point moving from right to left - and moving point is a node or quasi-node at which $1/|\psi|$ is highly peaked.

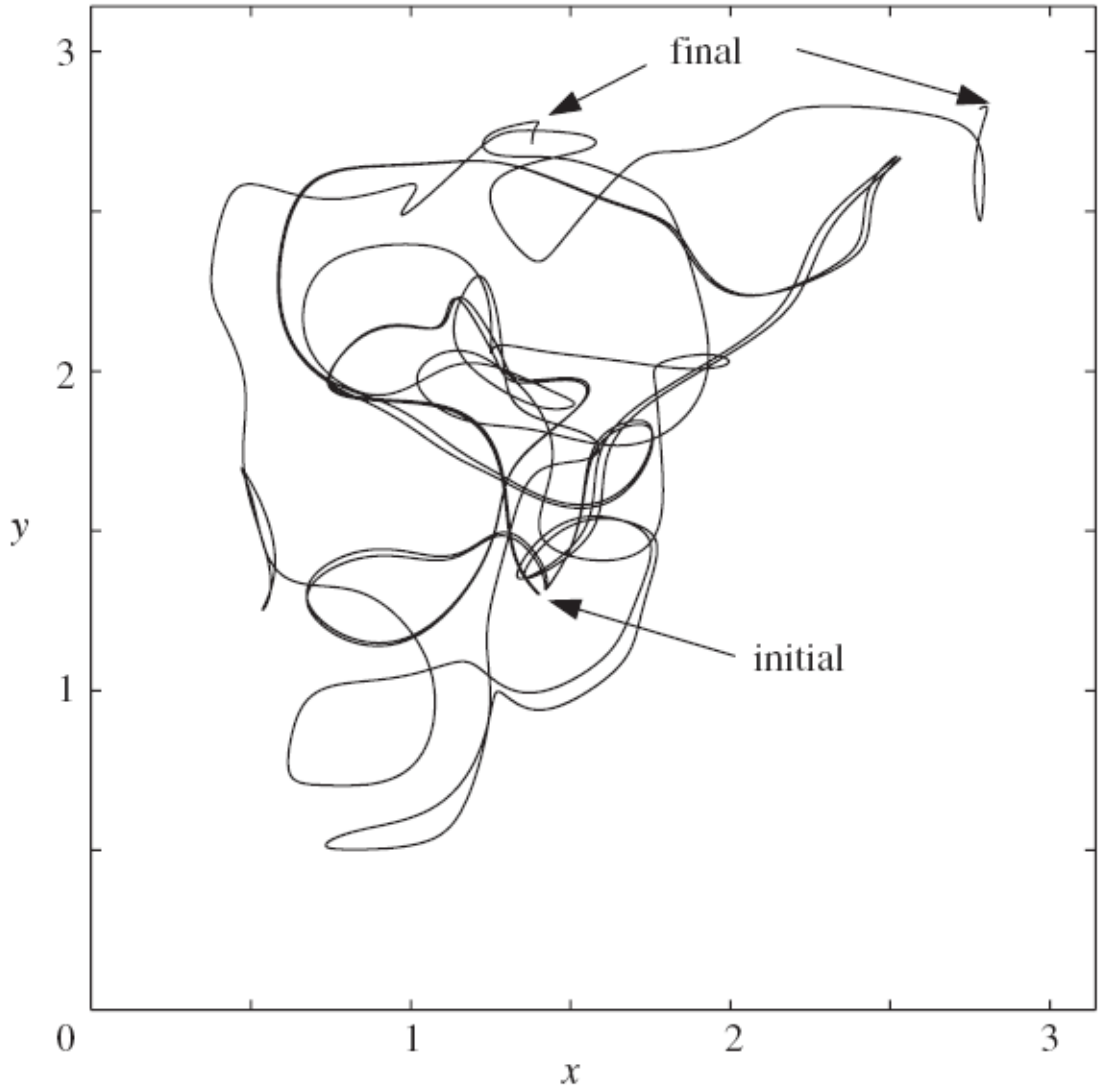
Dynamical origin of quantum probabilities: numerical simulations

Chaotic nature of the trajectories

Two distinct but very close initial positions evolve after $t = 4\pi$ *into widely separated final positions.*

Relevant quantity is *Lyapunov exponent* which characterizes rate of separation of infinitesimally close trajectories. Separation rate depends on orientation of initial separation vector, thus whole spectrum of n Lyapunov exponents - where n is dimensionality of the phase space. Usually use largest one - the *Maximal Lyapunov exponent* (MLE) as it determines predictability of a dynamical system. Positive MLE usually taken as indication that system is *chaotic*.

Difficulty to even *define* 'quantum chaos' in standard QM with no trajectories!



In pilot-wave dynamics, one sees the importance of *nodes* in generating chaotic motion. Numerical simulations suggest a proportionality between Lyapunov exponent and number of nodes.

[See e.g. Frisk *Phys. Lett. A* **227**, 139 (1997)]

Summary of these simulations

Normally say get fast relaxation to equilibrium on coarse-grained level for large numbers of particles. Clear from these simulations that large N in fact not needed for relaxation to occur. Even for one particle, relaxation occurs rapidly if its Ψ is a superposition of even a modest number of energy eigenfunctions.

Relaxation occurs because ρ and $|\Psi|^2$ evolve like two fluids 'stirred' by same velocity field. Most efficient mixing found to occur in neighbourhood of nodes or quasi-nodes, where Ψ is small. These points move around inside box, rather like 'electric mixers' or stirring devices moving through a fluid, generating an efficient relaxation everywhere.

Typicality and other views

Opposing camps exist in pilot-wave world differing in approach to $\rho = |\Psi|^2$. Having world's worst PR problem perhaps should be nicer to each other but the opposing camps typically dismiss the others' views with barbed footnotes† in their papers.

- **Bell**: 'It is *assumed* that the particles are so delivered initially by the source'.
- **Holland**: Lists the $|\Psi|^2$ distribution as one of four basic postulates of pilot-wave theory.
- **Dürr, Goldstein, Zanghì** *et al.*: $|\Psi|^2$ regarded as natural measure of probability or 'typicality' for initial configurations of whole universe (taking Ψ as the universal wave function), yielding Born rule for all subsystems at all times. [See Dürr and Teufel book for good discussion].

Valentini finds these 'incorrect and deeply misleading'; postulates about initial conditions should have no *fundamental* status in theory of dynamics. Fair enough.

† *Some people [hawk, spit!] believe that [FILL IN VIEW HERE] is a suitable position but they're obviously madder than a bucket of frogs.*

QM computations with trajectories

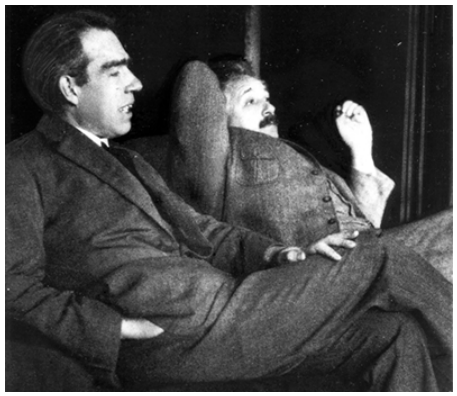
Computing the wavefunction from trajectories: particle and wave pictures in quantum mechanics and their relation

P. Holland (2004)

"The notion that the concept of a continuous material orbit is incompatible with a full wave theory of microphysical systems was central to the genesis of wave mechanics. Early attempts to justify this assertion using Heisenberg's relations were subsequently shown to be flawed, and indeed no credible proof forbidding the treatment of quantum processes in terms of precisely defined spacetime trajectories has ever been offered. The idea nevertheless entered the folklore of the subject and even now is invoked to highlight alleged paradoxical implications of quantum mechanics (e.g. Schrödinger's cat). So great was the philosophical bias that not only was the material orbit ruled out as an aid to comprehension, but the possibilities of using the trajectory as a computational tool, or even as the basis of an alternative representation of the quantum theory - the twin subjects of this paper - were foregone."

Note the wonderfully self-confident tone..

Feynman too has trouble with Bohr..



The Pocono conference (1948)

"Bohr was also at the meeting. After I had tried many times to explain what I was doing and didn't succeed. I talked about trajectories, then I would swing back - I was being forced back all the time. I said that in quantum mechanics one could describe the amplitude of each particle in such and such a way. Bohr got up and said 'Already in 1925, 1926, we knew that the classical idea of a trajectory or a path is not legitimate in quantum mechanics: one could not talk about the trajectory of an electron in the atom, because it was something not observable.' In other words, he was telling me about the uncertainty principle. It became clear to me that there was no communication between what I was trying to say and what they were thinking. Bohr thought that I didn't know the uncertainty principle, and was actually not doing QM right either. He didn't understand at all what I was saying. I got a terrible feeling of resignation. "

Feynman was of course talking about his *path-integral formulation* of quantum mechanics, whose connections with pilot-wave theory we shall discuss in a minute.

Classical mechanics

Given a set of initial conditions - the theory allows us to calculate deterministic trajectories of particles obeying Newton's laws. There are various equivalent mathematical formulations of this i.e. different equations leading to same trajectories:

$\mathbf{F}_i(q_1, q_2, \ldots, q_N) = m_i \ddot{\mathbf{q}}_i$ Newtonian mechanics

$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}(\mathbf{q}, \mathbf{p})$ $\dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}}(\mathbf{q}, \mathbf{p})$ Hamiltonian dynamics $\rightarrow$ standard QM

Solve a canonical system of 1st-order ODEs ($2n$ equations for $2n$ functions of a parameter t in which all variables' first derivatives are given by partial derivatives of the same function).

$\delta \int_{t_0}^{t_1} L\left(\mathbf{q}(t), \dot{\mathbf{q}}(t)\right) dt = 0$ Lagrangian dynamics $\rightarrow$ path-integral QM

Solve the basic calculus of variations problem of finding n functions $q_1, \ldots, q_n$ of a parameter t that make stationary a line integral (i.e. solve n 2nd-order ODEs).

$\frac{\partial S}{\partial t}(\mathbf{q}, t) + H(\mathbf{q}, \frac{\partial S}{\partial \mathbf{q}}) = 0$ Hamilton-Jacobi dynamics $\rightarrow$ pilot-wave theory

Solve a single 1st-order PDE in which the unknown function does not occur explicitly.

Feynman's path integral method (required later)

Feynman proposed the following postulates:

1. Probability for event given by square modulus of a complex amplitude Ψ.
2. Amplitude for event given by summing contributions of all histories which include that event.
3. Amplitude contributed by a particular history proportional to $e^{iS_{cl}/\hbar}$ where S_{cl} is classical *action* of that history i.e. time integral of classical Lagrangian $T - V$ along corresponding phase space path of system.

Dirac and Feynman

Overall amplitude for process from summing amplitudes of the infinite number of all possible histories between initial and final states. Path integral gives all histories (even barmy ones) amplitude of same magnitude but different phase. Contributions wildly different from classical suppressed by interference of similar cancelling histories.

Feynman showed this is equivalent to standard QM. An amplitude computed according to Feynman's principles also obeys the Schrödinger equation for the Hamiltonian corresponding to given action.

In limit of action large compared to $\hbar$, path integral dominated by solutions in neighbourhood of stationary points of the action, as there amplitudes of similar histories tend to constructively interfere. For paths far from such stationary points, complex phase varies rapidly for similar paths and amplitudes tend to cancel. Important parts of integral - the significant possibilities - in limit of large action consist simply of solutions of Euler-Lagrange equation, and classical mechanics is correctly recovered.

Does pilot-wave theory have a practical use?

- Historical discussion concerning 'hidden-variables' (such as the particles in pilot-wave theory) has tended to concentrate on their existence and properties as theoretical entities underlying the quantum formalism. Benefits perceived largely in terms of *insight they provide into quantum reality* i.e. they are primarily concerned with **quantum foundations**.
- Less consideration has been given to possible *practical* value of hidden variables theories in solving technical problems in QM. For example, can they help in solving the Schrödinger equation in a way analagous to, say, the computation of thermodynamic relations from microstates in statistical mechanics?
- In short, how do we *calculate things from quantum trajectories?*

Other questions

- What sort of problems can be addressed with quantum trajectory methods?
- Are they expensive with computer time, and how do they scale with system size?
- How are they related to other methods apparently involving trajectories such as Feynman's path-integral approach?
- How are they related to state-of-the-art techniques such as *quantum Monte Carlo* involving electrons hopping around and sampling the many-body wave function?

The basic idea

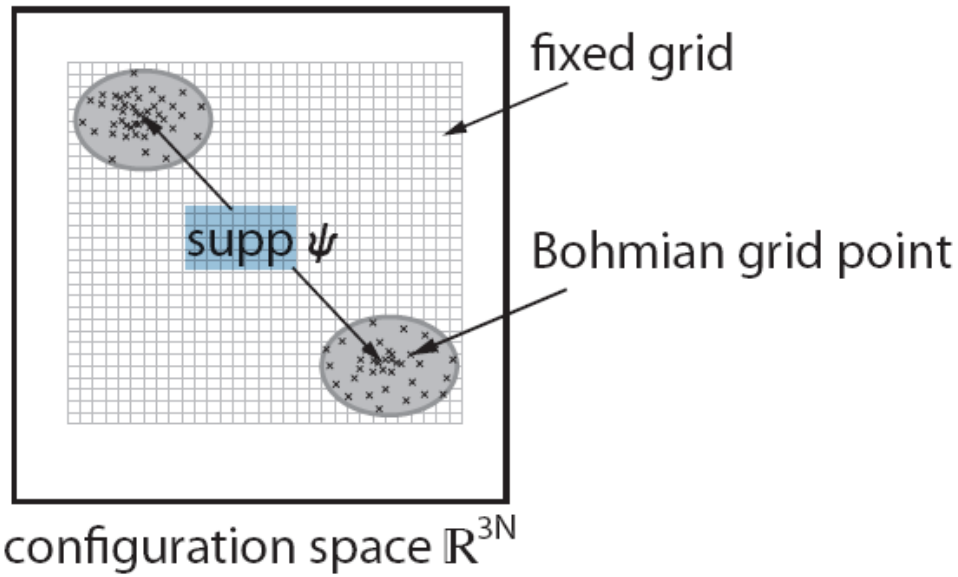
What we want to do is to integrate the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial\Psi(\mathbf{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{x},t) + V(\mathbf{x},t)\Psi(\mathbf{x},t) = \hat{H}\Psi(\mathbf{x},t)$$

where $\mathbf{x} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N\}$. Usually use atomic units: $\hbar = 1, m = 1$.

To be specific, given a starting wave function $\Psi_0(\mathbf{x},t)$ known only on a mesh of M grid points at time t, we want to find a numerical approximation to the real solution at later times using some physically meaningful and not too disastrously inaccurate approximation.

Direct numerical solution of many-body time-dependent Schrödinger equation in fact feasible only for simple few-body quantum systems (quasi-exponential scaling). We shall see how pilot-wave theory can help by transporting grid points along quantum trajectories.. Solution unfolds in a Lagrangian ('moving-with-the-fluid') reference frame, eliminating need to solve the problem on a large grid or mesh - a sort of grid 'importance sampling'.



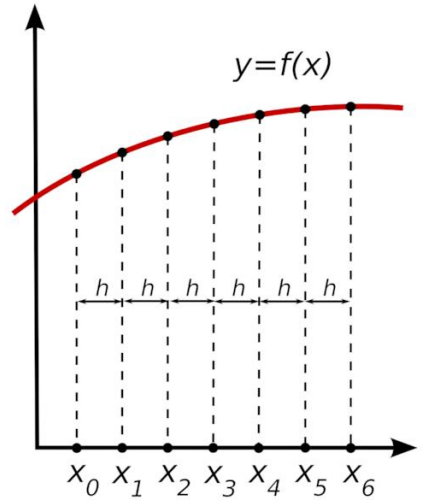
Some preliminaries - finite differencing

Finite-difference methods approximate solutions to differential equations by replacing derivatives with approximately equivalent difference quotients, i.e.

$$f'(a) = \lim_{h\to 0} \frac{f(a+h)-f(a)}{h} \quad \longrightarrow \quad f'(a) \approx \frac{f(a+h)-f(a)}{h} \approx \frac{f(a)-f(a-h)}{h} \approx \frac{f(a+\frac{1}{2}h)-f(a-\frac{1}{2}h)}{h}$$

Expressions to right of arrow - respectively *forward difference*, *backward difference*, and *central difference* - are all reasonable approximations to the derivative for some small value of h. With these can approximate solutions to differential equations with no calculus.

For approximate solution first discretize problem's domain - usually by dividing into uniform grid. Finite-difference methods give sets of discrete numerical approximations to derivative, often in 'time-stepping' manner.



Example 1: $u'(x) = 3u(x)+2$. Solve this ODE by substituting finite difference quotient $\frac{u(x+h)-u(x)}{h}$ for $u'(x)$. We find $u(x+h) = u(x) + h(3u(x)+2)$ - a finite-difference equation giving us approximate solutions to the ODE.

Example 2: 1D heat equation $\partial U/\partial t = \partial^2 U/\partial x^2$. Approximate *both* derivs by finite differences: uniform mesh in x (step h) and in t (step k). Points $u(x_j, t_n) = u_j^n$ give numerical approximation to $U(x_j, t_n)$. *Explicit* method: forward difference at t_n and 2nd-order central difference at position x_j gives $u_j^{n+1} = (1-2r)u_j^n + ru_{j-1}^n + ru_{j+1}^n$ with $r = k/h^2$. Using backwards or central difference for t deriv gives *implicit* or *Crank-Nicholson* methods (which differ in stability, accuracy, and cost).

In three dimensions complications evidently arise (too many grid points, bad scaling and cost).

Quantum trajectory calculations

Schrödinger equation for both stationary and nonstationary states may be solved exactly by propagating quantum trajectories, at least *in principle*. Probability amplitude and phase of Ψ transported along trajectories and observables computable directly in terms of this information. Investigations that employ quantum trajectories may be broadly divided into two classes:

The analytic approach:

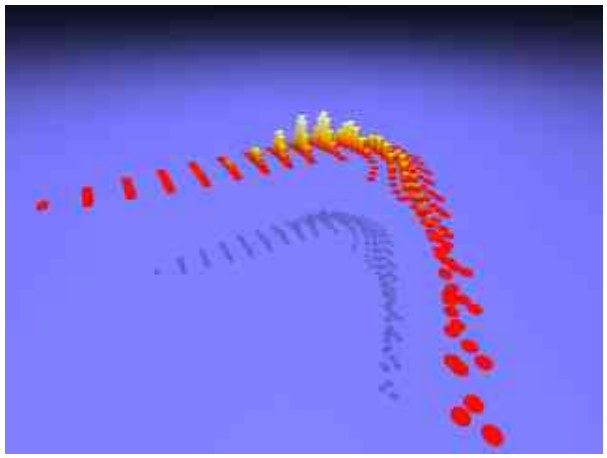
First solve TDSE using conventional techniques (fixed grids/basis set expansions). Individual 'particles' then evolved along quantum trajectories $\mathbf{x}(t)$ with velocities generated by Ψ-field via guidance equation $\dot{\mathbf{x}} = \frac{\hbar}{m} \mathrm{Im} \nabla \ln \Psi = \nabla S/m$. Patterns developed by trajectories emanating from ensemble of 'launch points' exactly define evolving system history. Used as means of understanding and exploring quantum behaviour i.e. point is not to solve TDSE but to provide *insight*.

The synthetic approach:

Rather than guiding quantum trajectories with a precomputed wave function, *the trajectories and wave function are computed concurrently, on the fly*. Wave packets are evolved by propagating ensembles of quantum trajectories, which become the *computational tool* for solving the 'quantum hydrodynamic' equations of motion.

Today we concentrate on the latter approach.

The synthetic approach to quantum trajectory calculations



Flow of quantum-mechanical probability density through configuration space is that of a compressible fluid. The evolution of this fluid is to be described in terms of a relatively small number of correlated fluid elements evolving along quantum trajectories.

- Initial wave packet (assumed known) discretized in terms of N fluid elements - small chunks of the probability fluid. The equations of motion for the set of elements are integrated in lockstep from one time step to the next. Along each trajectory the probability density and phase function (and thus the complex-valued wave function) are computed by integrating two coupled equations of motion.
- Fluid elements correlated with one another through global action of wave field (or, if you like, through the quantum potential). Each evolving fluid element influenced by motion of the other elements, even when external potential vanishes (source of quantum effects in the dynamics).

Natural language for theory through analogy with fluid mechanics or hydrodynamics. Probability density proportional to fluid density, and phase of Ψ is a velocity potential. Novel feature of quantum fluid is appearance of 'quantum stresses' (usually represented through quantum potenial Q).

The quantum hydrodynamic equations of motion

$$\frac{\partial \rho}{\partial t} = -\rho \nabla \cdot \mathbf{v} \quad \text{(continuity equation)}$$

$$\frac{\partial S}{\partial t} = L(t) = \frac{1}{2} m v^2 - (V + Q) \quad \text{(quantum H – J equation)}$$

$$m \frac{\partial \mathbf{v}}{\partial t} = -\nabla (V + Q) \quad \text{(Bohm)} \qquad \text{or} \qquad \mathbf{v} = \frac{\nabla S}{m} \quad \text{(de Broglie)}$$

First-order de Broglie form preferred since no ∇Q (a 3rd-order derivative of the wave amplitude R). Solve equations of motion using various 'finite-differencing' schemes:

Eulerian: Fluid elements (grid points) are stationary. Less useful.

Lagrangian: Grid points move along trajectories with velocities matching flow velocity of probability fluid (allows *compact* description of Ψ).

ALE (arbitrary Lagrangian-Eulerian): Arbitrary grid point velocity. Numerical advantages.

Wave mechanics might be said to correspond to Eulerian picture and trajectory theory to Lagrangian picture. Watch fluid go by, or 'go with the flow'.

Historical note: Computer implementation of synthetic approach to hydrodynamic formulation of QM first done as late as 1999 e.g. *quantum trajectory method* (QTM) of Lopreore and Wyatt, and *quantum fluid dynamics* (QFD) of Rabitz *et al.*

The problem with spatial derivatives

Given wave function of form $\Psi(\mathbf{x},t) = R(\mathbf{x},t)\mathrm{e}^{\frac{iS(\mathbf{x},t)}{\hbar}}$ then at each t state of system is specified by the **descriptor**:

$$D(t) = \{\mathbf{x}_i(t), R_i(t), S_i(t)\}_{i=1}^{N}.$$

This lists location of each fluid element along with amplitude and phase function at position of each element. Full wave function can be constructed from this information.

- Spatial derivatives appearing in functions ∇S, Q and $\nabla \cdot \mathbf{v}$ make equations of motion difficult to integrate since information ('hydrodynamic fields' R and S) only available at positions of fluid elements, and locations of these elements dictated by equations of motion i.e. they form an *unstructured (non-Cartesian) grid*.
- Spatial derivatives in equations of motion bring *nonlocal effects* into the dynamics; it is through the spatial derivatives that each fluid element is influenced by the surrounding hydrodynamic fields.
- Evaluation of accurate derivatives on unstructured grids is one of most challenging and important problems in numerical analysis, but many good approximate techniques have been developed for specific applications.

Wave function synthesis along quantum trajectory

$$\Psi = R(x,t)\mathrm{e}^{\frac{iS(\mathbf{x},t)}{\hbar}}$$

Propagation of the amplitude

Along trajectory $\mathbf{x}(t)$ from $(\mathbf{x}_0, t_0)$ to $(\mathbf{x}_1, t_1)$ rate of change of density $\frac{\partial \rho}{\partial t} = -\rho \nabla \cdot \mathbf{v}$.
Amplitude $R = \rho^{\frac{1}{2}}$ so $\frac{\partial R}{\partial t} = -\frac{R}{2}\nabla \cdot \mathbf{v}$. Integrate to get new R in terms of value at t_0.

$$\frac{\mathrm{d}R}{R} = -\frac{1}{2}\nabla \cdot \mathbf{v}\ \mathrm{d}t \xrightarrow{\text{integrate}} \ln R + c = -\frac{1}{2}\int_{t_0}^{t_1} \nabla \cdot \mathbf{v}\ \mathrm{d}t \xrightarrow{\text{exponentiate}} A\exp(\ln R) = \exp\left[-\frac{1}{2}\int_{t_0}^{t_1} \nabla \cdot \mathbf{v}\ \mathrm{d}t\right]$$

$$R(\mathbf{x}_1, t_1) = \exp\left[-\frac{1}{2}\int_{t_0}^{t_1} (\nabla \cdot \mathbf{v})_{\mathbf{x}(t)}\ \mathrm{d}t\right] R(\mathbf{x}_0, t_0)$$

To propagate R we integrate the *divergence of the velocity field* along the trajectory.

Propagation of the exponential of the phase

Quantum H-J eqn is $\frac{\partial S}{\partial t} = L(t) = \frac{1}{2}mv^2 - (V + Q)$. From $S(t_1) = S(t_0) + \int_{t_0}^{t_1} \frac{\partial S}{\partial t}\ \mathrm{d}t \xrightarrow{\times \frac{i}{\hbar} \text{ and exponentiate}}$

$$\mathrm{e}^{\frac{iS(\mathbf{x}_1,t_1)}{\hbar}} = \exp\left[\frac{i}{\hbar}\int_{t_0}^{t_1} L(t)\ \mathrm{d}t\right] \mathrm{e}^{\frac{iS(\mathbf{x}_0,t_0)}{\hbar}}$$

To propagate $e^{\frac{iS(\mathbf{x},t)}{\hbar}}$ we integrate the *quantum Lagrangian* along the trajectory.

Wave function synthesis along quantum trajectory

We multiply the expressions for the R propagator and the $\mathrm{e}^{\frac{iS(\mathbf{x},t)}{\hbar}}$ propagator to obtain an expression for updating the full wave function along the trajectory:

$$\Psi(\mathbf{x}_1, t_1) = \exp\left[-\frac{1}{2}\int_{t_0}^{t_1} (\nabla \cdot \mathbf{v})_{\mathbf{x}(t)}\, \mathrm{d}t\right] \exp\left[\frac{i}{\hbar}\int_{t_0}^{t_1} L(t)\, \mathrm{d}t\right] \Psi(\mathbf{x}_0, t_0).$$

Hydrodynamical wave function propagator (HWFP): $K^Q(\mathbf{x}_1, t_1; \mathbf{x}_0, t_0)$

An alternative derivation

Evolving along quantum trajectory from t to $t + \mathrm{d}t$, new wave function given by

$$\Psi(t + \mathrm{d}t) = \Psi(t) + \frac{\partial \Psi}{\partial t}\mathrm{d}t + (\mathbf{v} \cdot \nabla \Psi)\mathrm{d}t.$$

Now use TDSE to evalute $\frac{\partial \Psi}{\partial t}$, use $\mathbf{v} = \frac{\nabla S}{m}$, and use polar form of Ψ throughout, then we find after some algebra:

$$\Psi(t + \mathrm{d}t) = \left\{1 - \frac{1}{2}(\nabla \cdot \mathbf{v})\, \mathrm{d}t + \frac{i}{\hbar}\left[\frac{1}{2}mv^2 - (V + Q)\right] \mathrm{d}t\right\} \Psi(t).$$

Term in braces $\{\ldots\}$ is *wave function propagator* for time increment $\mathrm{d}t$. After a number of these small time steps, composite propagator identical to HWFP above.

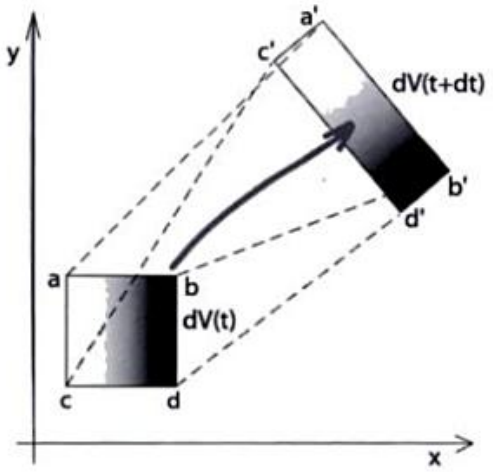
Wave function propagation and the Jacobian

$$R(\mathbf{x}_1, t_1) = \exp\left[-\frac{1}{2}\int_{t_0}^{t_1} (\nabla \cdot \mathbf{v})_{\mathbf{x}(t)}\, \mathrm{d}t\right] R(\mathbf{x}_0, t_0)$$

What does $\nabla \cdot \mathbf{v}$ mean here?

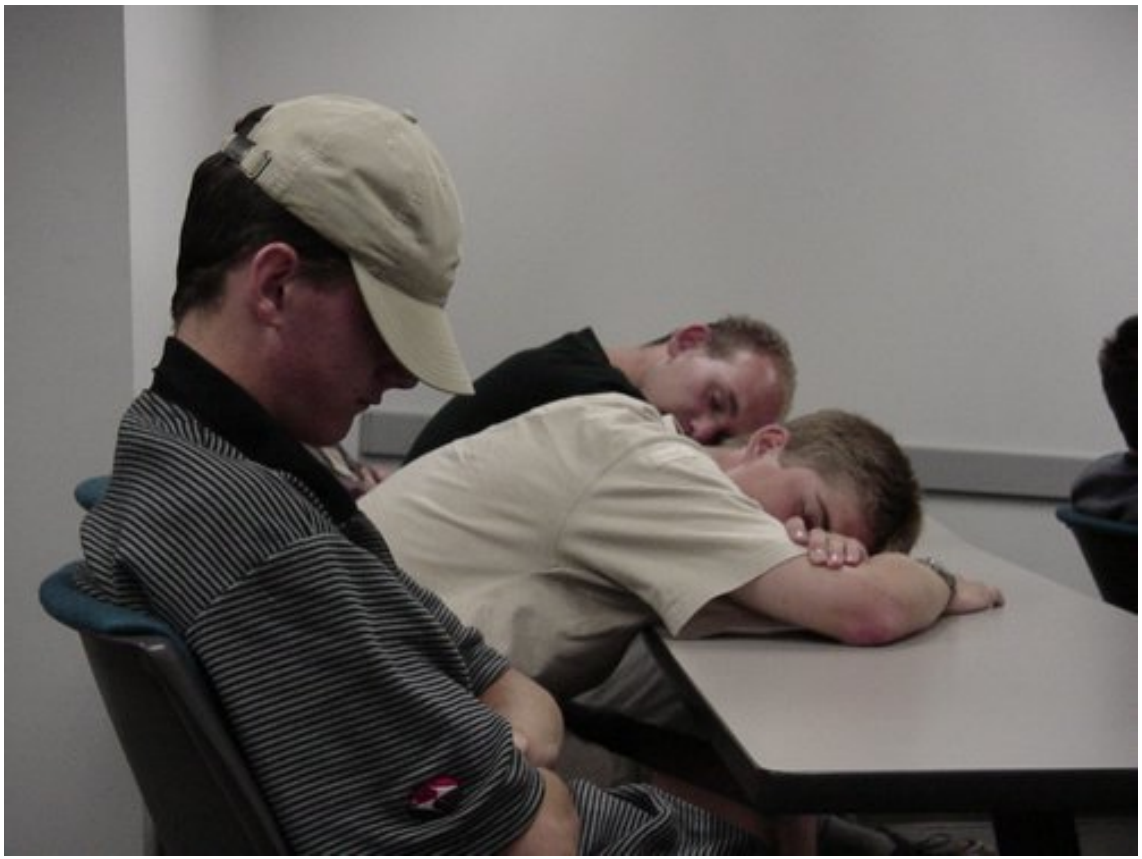
At time t have volume element $\mathrm{d}V(t)$. Element corners defined by trajectory positions $\{a, b, c, d\}$. Increment time by $\mathrm{d}t$ and equations of motion shift corners to $\{a', b', c', d'\}$ and volume element changes to $\mathrm{d}V(t+\mathrm{d}t)$. Ratio of new to old volumes is the *Jacobian*: $\mathrm{d}V(t+\mathrm{d}t) = J(t+\mathrm{d}t, t)\mathrm{d}V(t)$. Can be shown Jacobian is:

$$J(t_1, t_0) = \exp\left[\int_{t_0}^{t_1} \nabla \cdot \mathbf{v}\, \mathrm{d}t\right].$$



- Implies if velocity field has positive divergence (velocity vectors 'point away from each other') then Jacobian increasing and local volume element *expanding* along flow. So velocity divergence locally measures rate of change of geometric quantity.
- If flow is *incompressible* ($\nabla \cdot \mathbf{v} = 0$) Jacobian is invariant. Not usually the case in QM, but note *classical* flow in phase space *is* incompressible (Liouville's theorem).
- Fact that $\rho(\mathbf{x}, t)J(t, t_0) = \rho(\mathbf{x}_0, t_0)$ shows *conservation of the product* ρJ along quantum trajectory. As $\mathrm{d}V$ changes along flow, density adjusts such that ρJ retains value specified by initial condition.
- Note the R-propagator $\exp\left[-\frac{1}{2}\int_{t_0}^{t_1} \nabla \cdot \mathbf{v}\, \mathrm{d}t\right]$ is thus just $J(t)^{-\frac{1}{2}}$.

Never mind the numerical derivatives



OK, look - I was only joking about the least squares fitting - I won't bore you with it. However, it is *the* crucial step in evaluating the spatial derivatives required to use the propagators we have just derived for solving the TDSE. To get a feel for the issues, see Deckert, Dürr and Pickl's paper in *J. Phys. Chem. A* **111**, 10325 (2007) where they show least squares fitting allows pilot-wave trajectories to cross, and that one should use polynomial fitting instead. Robert Wyatt's book '*Quantum dynamics with trajectories*' has a comprehensive overview of the various techniques.

But here's something interesting..

Quantum trajectories and Feynman path integrals

- In the expression $\Psi(\mathbf{x}_1, t_1) = K^Q(\mathbf{x}_1, t_1; \mathbf{x}_0, t_0)\Psi(\mathbf{x}_0, t_0)$ that propagates the wave function along the quantum trajectory, the propagator K^Q may - expressing the R-propagator in terms of the Jacobian - be written as

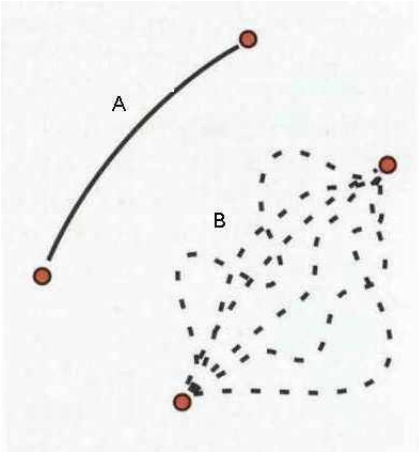
$$K^Q(\mathbf{x}_1, t_1; \mathbf{x}_0, t_0) = \frac{1}{J(t)^{\frac{1}{2}}} \exp\left[\frac{i}{\hbar}\int_{t_0}^{t_1} L(t)\,\mathrm{d}t\right].$$

- In *Feynman's path integral formulation of quantum mechanics* the equivalent propagator may be written as

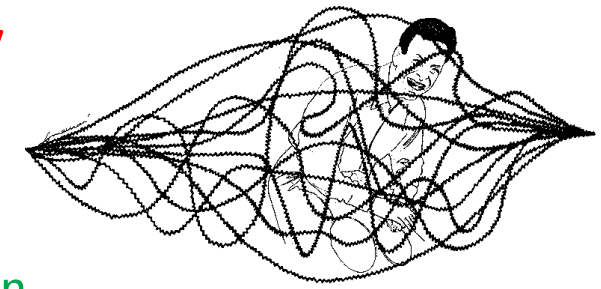
$$K^F(\mathbf{x}_1, t_1; \mathbf{x}_0, t_0) = N \sum_{\text{all paths}} \exp\left[\frac{i}{\hbar}\int_{t_0}^{t_1} L_{cl}(t)\,\mathrm{d}t\right].$$

Here propagator linking two spacetime points calculated by linearly superposing amplitudes $e^{iS/\hbar}$ (obtained by integrating **classical** Lagrangian $L_{cl}(t) = \frac{1}{2}mv^2 - V$) associated with infinite number of **all possible paths** connecting the points.

In pilot-wave approach, achieve same effect by integrating the **quantum** *Lagrangian* $L(t) = \frac{1}{2}mv^2 - (V + Q)$ *along precisely* **one** *path. Bet you didn't know that..*



Paths in Feynman's theory



How to construct the wave function

Feynman: Sum over infinite number of independent but interfering paths, the phase for each path determined by a classical Lagrangian. Nonlocality from explicitly summing over every point in universe.

de Broglie-Bohm: Use *one* unique pilot-wave trajectory influenced by underlying hydrodynamic fields (i.e. the global wavefunction). Nonlocality since trajectory 'aware' of Ψ in surrounding region through influence of amplitude curvature ($Q = \frac{\hbar^2}{2m}\frac{\nabla^2 R}{R}$) and curvature of the phase $\nabla \cdot \mathbf{v} = \frac{\nabla^2 S}{m}$.

What are Feynman's paths?

We really mean *all* paths - including the one heading off (very quickly) into space, orbiting three times around Alpha Centauri, popping down the road for some chips, before arriving, exhausted, at $\mathbf{x_1}, \mathbf{t_1}$. Is it perhaps one of these paths that a particle actually follows?

If path integral formalism provided probability distribution ρ on space of all paths could assume Nature chooses one at random from ρ. Same ontology as pilot-wave theory but different law of motion. Unfortunately there is no probability measure on path space that is a real number, so this suggestion cannot be taken literally. Status of paths more like "possible paths along which a part of the *wave* may travel" to the extent that waves travel along paths.

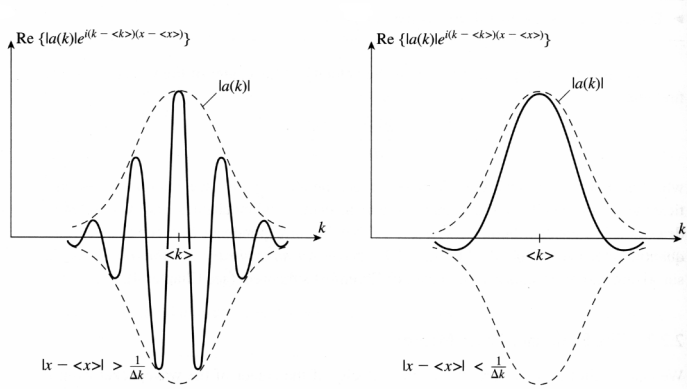
Feynman's paths are **mathematical tools** *for computing the evolution of Ψ, while one among de Broglie paths is actual motion of particle, which exists in addition to Ψ. Keep in mind path integrals not exclusive to QM; can write any linear field equation (e.g. Maxwell) in terms of path integrals.*

Feynman stage 2

The Feynman propagator K^F is a many-to-many mapping i.e. all points are linked by all possible paths. So full $\Psi(\mathbf{x}_1, t_1)$ found from *Huygen's principle* by summing contributions coming from *all possible start points* - multiply amplitude at $\mathbf{x}_0, t_0$ by transition amplitude K^F for 'hopping' to $\mathbf{x}_1, t_1$. Then sum (integrate) over all $\mathbf{x}_0$.

$$\Psi(\mathbf{x}_1, t_1) = \int K^F(\mathbf{x}_1, t_1; \mathbf{x}_0, t_0)\Psi(\mathbf{x}_0, t_0)\, \mathrm{d}x_0$$

- Note Feynman propagator (a Green's function) is a kind of wave function; if initial wave function $\Psi(\mathbf{x}_0, t_0)$ spiked at point $\mathbf{x}_0 = \mathbf{a}$, i.e. $\Psi(\mathbf{x}_0, t_0) = \delta(\mathbf{x}_0 - \mathbf{a})$ is a Dirac delta function then resulting wave function at point $\mathbf{x}_1$ is the propagator $\Psi(\mathbf{x}_1, t_1) = K^F(\mathbf{x}_1, t_1; \mathbf{a}, t_0)$. Classical trajectory linking endpoints gives *stationary phase* contribution to integrand in definition of K^Q.
- In quantum trajectory method achieve same end as path integral - computation of Ψ given initial value - in quite different and conceptually simpler manner with two spacetime points connected by at most a single path. Two steps in Feynman's approach (propagator then Huygens) condensed into one. Ψ generated from initial form by *single-valued continuum of trajectories*. Pilot-wave theory thus not just interpretation but an alternative mathematical representation of QM.



Stationary phase argument

Quantum trajectory methods: summary

- Association of pilot-wave approach with fluid mechanics yields significant computational benefit (appreciated only recently): (i) pilot-wave trajectories can be computed independently of Ψ (only initial Ψ required), and (ii) they exhibit sufficient structure to provide a method to generate the time-dependence of Ψ.
- Note this is not standard pilot-wave theory as it uses only the trajectories and not its theory of matter (where one path is labelled preferentially and occupied by a material corpuscle). We recover pilot-wave theory if we add 'dust particles' to the fluid flow. Shows us trajectories are not "superfluous ideological superstructure".
- In hydrodynamic analogy, wave mechanics corresponds to the Eulerian picture, and the particle theory (as outlined here) to the Lagrangian picture. Ψ encodes the temporal history of a space point, while v encodes its 'spatial' history. Given the wave function, the time-dependence of either state function can be computed and implies the other - a kind of *wave-particle duality*!
- For full mathematical equivalence of the models, the hydrodynamic variables must satisfy conditions inherited from Ψ, which in turn provide physical insight into the original conditions. For example, single-valuedness requirement on Ψ corresponds to appearance of *quantized vortices* in the fluid.
- I have skipped essentially all modern developments of this theory. For relatively up-to-date references in rapidly changing field see Wyatt's talk listed below.

Relevant things to read

R.E. Wyatt, *Overview: dynamics with quantum trajectories*. Talk slides at `http://cnls.lanl.gov/qt/Agenda.html`

P. Holland, *Computing the wavefunction from trajectories*, Ann. Phys. **315**, 505 (2005) and `quant-ph/0405145`.

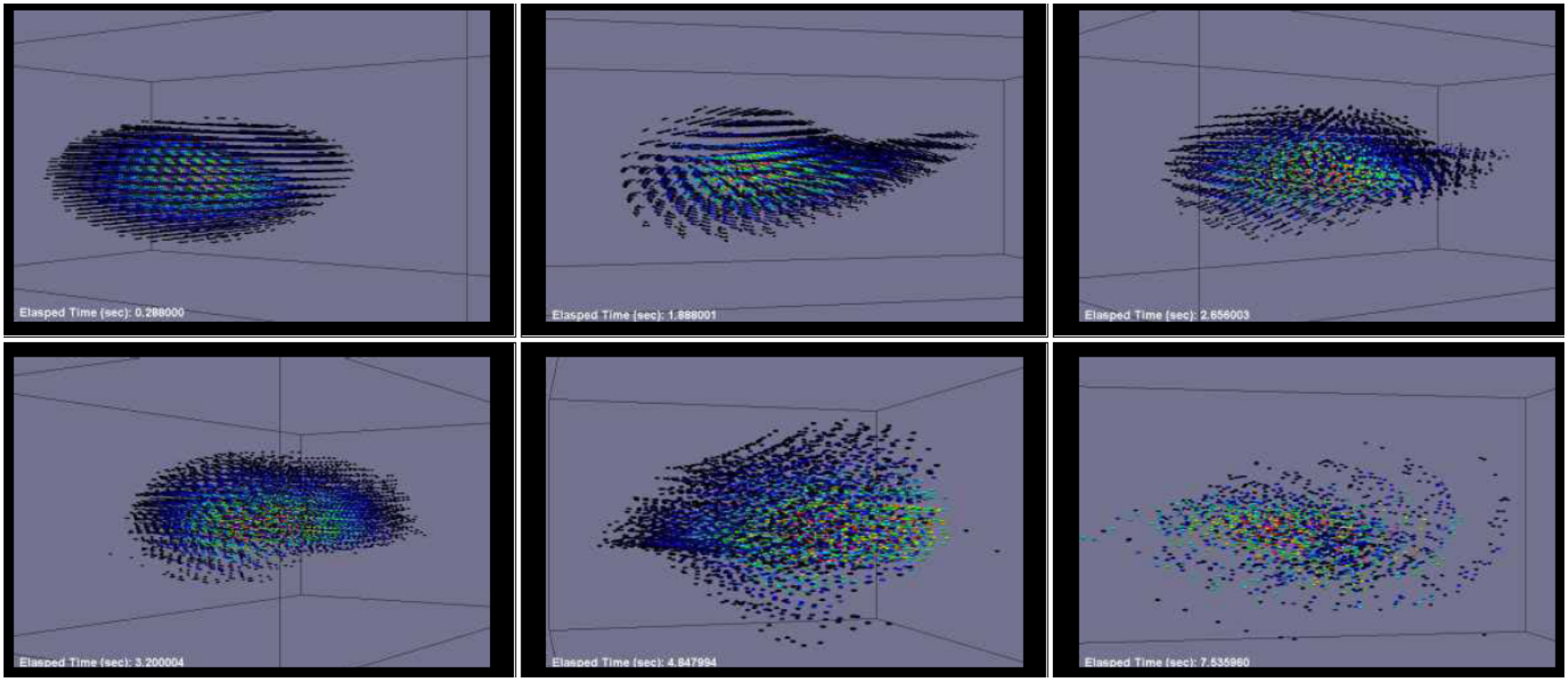
R.E. Wyatt, *Quantum dynamics with trajectories*, Springer (2005)

P. Holland, *Schrödinger dynamics as a two-phase conserved flow*, J. Phys. A: Math.Theor. **42**, 075307 (2009).

An example

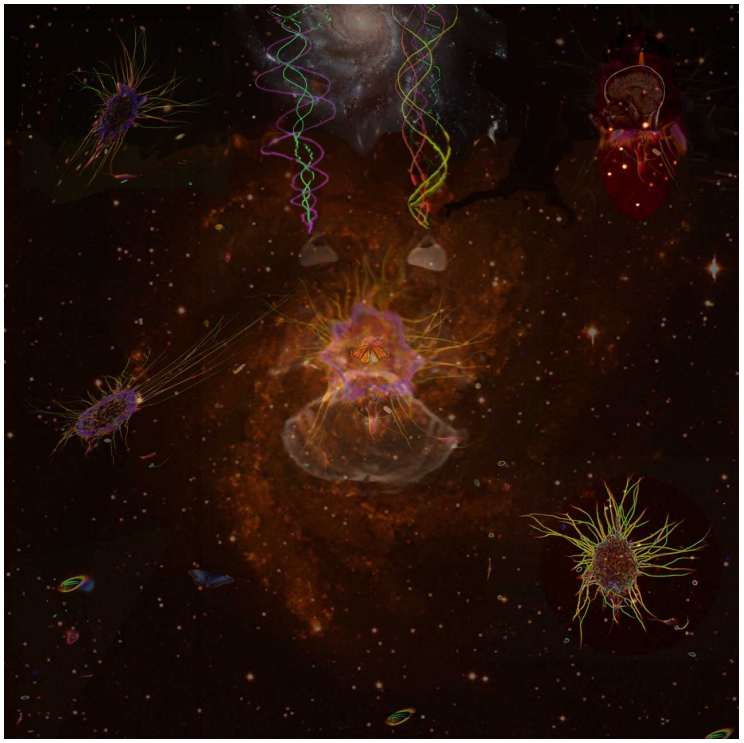
Disclaimer: Much more difficult than I thought to find pretty 3D pictures to show you for applications (we did prettier 2D analytic trajectories last week). This is best I could come up with in a short search..

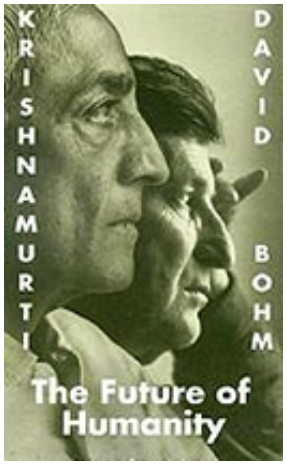
Pictures by Guzman *et al.*'*Visualizing energetics of dissociation of a metastable molecule*'. Used model molecule composed of two fragments, A and B. Starting from the molecular state AB, what is probability that AB will dissociate into separated components A + B? Solution unfolds in Lagrangian ('moving-with-the-fluid') frame, eliminating need to solve problem on large grid. Fluid in pictures is probability density discretized into small elements. Visualize outcome: number of particles escaping from system at lower right, for example, represents overall probability of dissociation at a given energy. Tendency of molecular system to remain intact represented by high-probability-density particles (colored red) that remain in center of picture; low-probability-density particles colored blue.

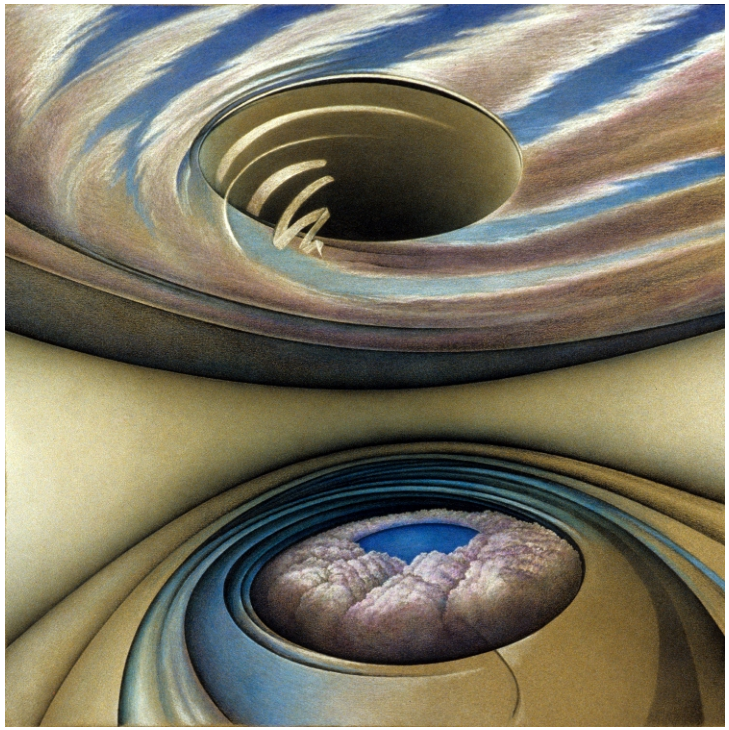


Ensemble of probability densities at various times as the AB system dissociates into A+B.

Propagators and the implicate order







Bohm in his Indian guru mode sometimes used to take propagators a bit further, in terms of his concepts of the $\mathbf{implicate\ order}$ *and his concepts of enfolding and unfolding*:

All laws of movement in QM correspond to *enfoldment* and *unfoldment*. In particular, relation between wave function at one time and its form later determined by propagator or Green's function K through $\Psi(\mathbf{x},t) = \int K(\mathbf{x},t;\mathbf{x}',t')\Psi(\mathbf{x}',t')\ \mathrm{d}x'$. Simple picture of movement is that waves from whole space enfold into each region and waves from each region unfold back into whole space. Propagator ultimately derived from Cartesian order by solving differential equations. But if we question this order holds fundamentally can adopt view that propagator is more basic than the differential equation.

See Bohm and Hiley's "*The Undivided Universe*", *p. 354.*

Quantum trajectories and quantum Monte Carlo

What connection, if any, is there between quantum trajectory methods and the various state-of-the-art techniques - like **quantum Monte Carlo** *(QMC) - that accurately solve the time-independent Schrödinger equation sampling the full many-electron* Ψ*?*

Quantum Monte Carlo methods

The most highly-evolved QMC variant with broad scope is *diffusion Monte Carlo* (DMC). It is probably the most accurate method known for solving the many-electron Schrödinger equation that also scales reasonably with the number of particles. It remains tractable (and highly accurate) for large system sizes; simulations of periodic systems with over 2000 electrons per cell have been reported.

It propagates an arbitrary starting wave function using a (Green's function) propagator just like the ones we have been discussing. The main difference is that the propagation occurs in *imaginary time* τ as opposed to real time t. This has the effect of 'improving' the wave function i.e. making it look more like the ground state as imaginary time passes (see later).

$$\Psi(\mathbf{x}, \tau + \delta\tau) = \int K(\mathbf{x}, \mathbf{x}', \delta\tau)\Psi(\mathbf{x}', \tau)\, d\mathbf{x}'$$

Evolving wave function represented by distribution in space and time of randomly-diffusing electron positions over an ensemble of copies of the system. From pilot-wave perspective, this is something like calculating expectation values by 'sampling trajectories' (from ensemble of different launch points).

Further reading

Quantum Monte Carlo simulations of solids, W.M.C. Foulkes, L. Mitas, R.J. Needs and G. Rajagopal, Rev. Mod. Phys **73**, 33 (2001).
The quantum Monte Carlo method, M.D. Towler, Phys. Stat. Solidi **243**, 2573 (2006).

Why do we propagate Ψ in imaginary time in DMC?

Consider Schrödinger equation (in a.u.) with constant offset E_T to zero of potential:

$$-\frac{\partial \Psi(\mathbf{x},t)}{i\partial t} = \left(\hat{H} - E_T\right)\Psi(\mathbf{x},t).$$

For eigenstate, general solution is clearly

$$\phi(\mathbf{x},t) = \phi(\mathbf{x},0)\mathrm{e}^{-i(\hat{H}-E_T)t}.$$

Then expand an *arbitrary* ('guessed') $\Psi(\mathbf{x},t)$ in complete set of eigenfunctions of $\hat{H}$.

$$\Psi(\mathbf{x},t) = \sum_{n=0}^{\infty} c_n\phi_n(\mathbf{x})\mathrm{e}^{-i(E_n-E_T)t}$$

Substitute it with *imaginary time* $\tau = it$. Oscillatory behaviour becomes exponential.

$$\Psi(\mathbf{x},\tau) = \sum_{n=0}^{\infty} c_n\phi_n(\mathbf{x})\mathrm{e}^{-(E_n-E_T)\tau}$$

Get imaginary time independence by choosing constant E_T to be ground state eigenvalue E_0. As $\tau \to \infty$, Ψ comes to look more and more like the ground state ϕ_0.

$$\Psi(\mathbf{x},\tau) = c_0\phi_0 + \sum_{n=1}^{\infty} c_n\phi_n(\mathbf{x})\mathrm{e}^{-(E_n-E_0)\tau}$$

How do we propagate Ψ in imaginary time in DMC?

- We use a Green's function propagator $K(\mathbf{x}, \mathbf{x}', \delta\tau)$:

$$\Psi(\mathbf{x}, \tau + \delta\tau) = \int K(\mathbf{x}, \mathbf{x}', \delta\tau)\Psi(\mathbf{x}', \tau)\, d\mathbf{x}'$$

- How do we find an expression for the propagator K? Consider imaginary-time Schrödinger equation in two parts:

$$\begin{aligned} \frac{\partial\Psi}{\partial\tau} &= \frac{1}{2}\nabla^2_{\mathbf{x}}\Psi \quad \text{(diffusion equation)} \\ \frac{\partial\Psi}{\partial\tau} &= -V\Psi \quad \text{(rate equation)} \end{aligned}$$

- Propagator for diffusion equation well-known: it is a $3N$-dimensional Gaussian with variance $\delta\tau$ in each dimension. Propagator for rate equation known - gives so-called 'branching factor' which can be interpreted as a position-dependent *weight* or *stochastic survival probability* for a member of an ensemble.

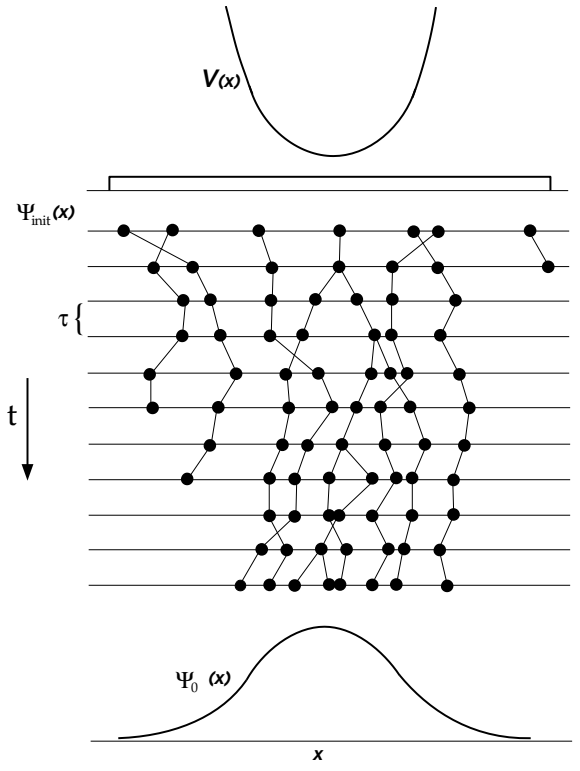
$$K(\mathbf{x}, \mathbf{x}', \delta\tau) = \frac{1}{(2\pi\delta\tau)^{\frac{3N}{2}}} \exp\left(-\frac{|\mathbf{x} - \mathbf{x}'|^2}{2\delta\tau}\right) \times \exp\left[-\delta\tau\left(\frac{V(\mathbf{x}) + V(\mathbf{x}') - 2E_T}{2}\right)\right]$$

Multiplying the two together to get the propagator for the imaginary-time Schrödinger equation is an *approximation* valid in the limit of small $\delta\tau$.

A Diffusion Monte Carlo simulation

- Interpret Ψ as a *probability density*, then diffusion equation $\frac{\partial \Psi}{\partial \tau} = \frac{1}{2}\nabla^2_{\mathbf{x}}\Psi$ represents movement of N diffusing particles. Turning this around, can represent $\Psi(\mathbf{x}, \tau)$ by *ensemble* of such sets of particles. Member of ensemble called a 'configuration'.
- Interpret propagator $K(\mathbf{x}, \mathbf{x}', \delta\tau)$ as probability of configuration moving from $\mathbf{x}'$ to $\mathbf{x}$ in a time $\delta\tau$. Branching factor determines population of configurations: in regions of high V configurations will be killed off; in low V regions configurations will multiply. It is this that 'changes the shape of the wave function' as it evolves.
- Propagate distribution in imaginary time, and after sufficiently long time excited states will have decayed away to leave the ground-state Ψ. Can then continue propagation and accumulate averages of observables.

Guess that the ground-state wave function for a single electron in a harmonic potential well is a constant over some range (stupid!). Start with seven copies of the system over which ensemble the electrons are distributed according to this constant probability distribution. Propagate the particle distribution in imaginary time according to the prescription above, and watch the electrons become distributed according to the proper Gaussian shape of the exact ground-state wave function. The change in shape is produced by the branching factor occasionally eliminating configurations in high V regions and duplicating ones in low V regions..

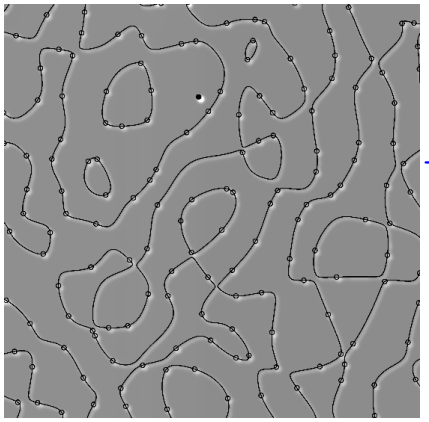


Importance sampling and the fixed-node approximation in DMC

The basic DMC algorithm sounds nice but *doesn't work* in practice. This is because:

- Ψ can only be a probability distribution if of one sign everywhere (e.g. H atom, boson system). For multi-particle fermion systems it necessarily has positive and negative bits. Obvious ways of getting round this (e.g. separate probabilities for different signs) fail on account of signal-to-noise problems ('*fermion sign problem*').
- Branching factor $\exp\left[-\frac{\delta\tau}{2}\left(V(\mathbf{x})+V(\mathbf{x}')-2E_{\mathrm{T}}\right)\right]$ contains potential V varying from $-\infty$ to $+\infty$. Sampling of points e.g. near nucleus leads to massive fluctuations in branching factor and significant numerical instabilities.

Fix problem by introducing *importance sampling* via a guessed trial function Φ_T (from a HF or DFT calculation, say). Require propagation to produce distribution $f(\mathbf{x},\tau)=\Psi(\mathbf{x},\tau)\Phi_T(\mathbf{x})$ - forced to be of one sign by demanding fixed Φ_T and variable Ψ functions have same *nodal surface* i.e. same zeroes ('*fixed-node approximation*').



New 'imaginary time Schrödinger equation' (Fokker-Planck)

$$-\frac{\partial f(\mathbf{x},\tau)}{\partial\tau}=-\frac{1}{2}\nabla_{\mathbf{x}}^2 f(\mathbf{x},\tau)+\nabla_{\mathbf{x}}\cdot\left[\mathbf{F}(\mathbf{x})f(\mathbf{x},\tau)\right]-\left(E_{\mathrm{L}}(\mathbf{x})-E_{\mathrm{T}}\right)f(\mathbf{x},\tau)$$

$\mathbf{F}(\mathbf{x})\equiv\frac{\nabla_{\mathbf{x}}\Phi_T}{\Phi_T}$ 'drift vector' $E_L=\frac{\hat{H}\Psi}{\Psi}$ 'local energy'

$$f(\mathbf{x},\tau+\delta\tau)=\int K(\mathbf{x}',\mathbf{x},\delta\tau)f(\mathbf{x},\tau)\,d\mathbf{x}'$$

Problem solved - more or less

Final propagator consists of diffusion, drift and branching processes:

$$K(\mathbf{x}',\mathbf{x},\delta\tau) = \frac{1}{(2\pi\delta\tau)^{\frac{3N}{2}}} \exp\left[-\frac{(\mathbf{x}'-\mathbf{x}-\delta\tau\mathbf{F}(\mathbf{x}))^2}{2\delta\tau}\right] \exp\left[-\frac{\delta\tau}{2}\left(E_{\mathrm{L}}(\mathbf{x})+E_{\mathrm{L}}(\mathbf{x}')-2E_{\mathrm{T}}\right)\right]$$

To be compared with the original propagator without importance sampling:

$$K(\mathbf{x},\mathbf{x}',\delta\tau) = \frac{1}{(2\pi\delta\tau)^{\frac{3N}{2}}} \exp\left(-\frac{(\mathbf{x}-\mathbf{x}')^2}{2\delta\tau}\right) \exp\left[-\frac{\delta\tau}{2}\left(V(\mathbf{x})+V(\mathbf{x}')-2E_T\right)\right]$$

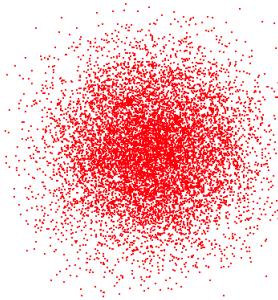
- Mixed distribution $f = \Psi\Phi_T$ of one sign everywhere so no more sign problem (at cost of reducing flexibility by fixing the nodes).
- Branching term now contains local energy $E_L = \hat{H}\Psi/\Psi$ which fluctuates much less than the potential V (for an eigenstate, E_L is constant everywhere in configuration space). No more numerical instability in the branching.
- Importance sampling from drift term $\mathbf{F}(\mathbf{x}) = \nabla\Phi_T/\Phi_T$ enhancing density of configs where Φ_T is large i.e. there is a *drift* or *osmotic velocity* directed towards large Φ_T on top of the random diffusion - like electric field on Brownian motion.

Fixed-node approximation most serious error in DMC, but still recover 95-100% of the total energy error made in a Hartree-Fock calculation (the 'correlation energy') for typical systems. Error typically increases with increasing atomic number.

Stochastic pilot-wave theories

To put DMC in de Broglie-Bohm context, must first understand concept of stochastic pilot-wave theories. Additional random motion introduced in 1954 by Bohm and Vigier in context of why particles distributed as $|\Psi|^2$ (though no need - see earlier).

Imagine a deeper 'sub-quantum' level which imparts additional intrinsic randomness to particle motion (like in Brownian motion with pollen grains being hit by clouds of atoms). Velocity of individual particle is $\mathbf{v} = \frac{\nabla S}{m} + \xi(t)$ with $\xi(t)$ a chaotic contribution to the velocity fluctuating randomly with zero average. Usual $\frac{\nabla S}{m}$ trajectory produced by guiding equation thus *average* velocity rather than *actual* one.



- Assume - whatever its origin - stochastic process treatable as simple *diffusion*. With prob density P, diffusion constant D, there is diffusion current $\mathbf{j} = -D\nabla P$ and a conservation equation $\partial P/\partial t = -D\nabla^2 P$. Leads clearly to *uniform distribution* (change in P stops at zero density curvature, like ink drop spreading in water).

- If want *non-uniform* final distribution there must be another field giving rise to an *osmotic velocity*. **Example**: Einstein showed if add gravitational field in z-direction this velocity is $u = D\frac{mg}{kT}z$, the conservation equation becomes $\frac{\partial P}{\partial t} = -D\nabla\left[\frac{mg}{kT}zP + \nabla P\right]$. In equilibrium when $\frac{\partial P}{\partial t} = 0$ we have $\frac{\nabla P}{P} = \frac{mg}{kT}z + c$ or $P = A\exp(-\frac{mgz}{kT})$ which is just the Boltzmann factor.
- In stochastic pilot-wave theory require random diffusion process whose equilibrium state corresponds to prob density $P = |\Psi|^2 = \rho$ and mean current $\mathbf{j} = \rho\mathbf{v} = \rho(\frac{\nabla S}{m})$. Consistent possibility if $\Psi = \sqrt{\rho}\exp(\frac{iS}{\hbar})$ as this implies conservation equation $\frac{\partial \rho}{\partial t} + \nabla\cdot\mathbf{j} = 0$. Can be shown suitable osmotic velocity is $\mathbf{u} = \frac{D\nabla\rho}{\rho}$ - then follows there is an equilibrium state with $P = \rho$ in which the osmotic velocity is balanced by the diffusion current so the mean velocity is $\frac{\nabla S}{m}$.

DMC vs. stochastic pilot-wave theories

In the various theories at each timestep get change in particle position $\mathrm{d}\mathbf{r}$ from some combination of guided velocity, random diffusion and a drift (osmotic) velocity. The χ in the diffusion part is a random variable with zero mean and unit variance. Atomic units are dispensed with ($\hbar$ and m are back).

Standard pilot wave	$d\mathbf{r} = \frac{\nabla S}{m}\mathrm{d}t$
Stochastic pilot wave	$d\mathbf{r} = \frac{\nabla S}{m}\mathrm{d}t + \chi\sqrt{\frac{\hbar}{m}}\mathrm{d}t + \frac{\hbar}{2m}\frac{\nabla\lvert\Psi\rvert^2}{\lvert\Psi\rvert^2}\mathrm{d}t$
DMC	$d\mathbf{r} = \chi\sqrt{\frac{\hbar}{m}}\mathrm{d}t + \frac{\hbar}{m}\frac{\nabla\lvert\Phi_T\rvert}{\lvert\Phi_T\rvert}\mathrm{d}t$
DMC2†	$d\mathbf{r} = \frac{\nabla S}{m}\mathrm{d}t + \chi\sqrt{\frac{\hbar}{m}}\mathrm{d}t + \frac{\hbar}{m}\frac{\nabla\lvert\Phi_T\rvert}{\lvert\Phi_T\rvert}\mathrm{d}t$

† If use complex Φ_T and retain imaginary part of complex drift vector $\nabla\Phi_T/\Phi_T$ (since for $\Psi = R\mathrm{e}^{iS/\hbar}$ have $\frac{\hbar}{m}\frac{\nabla\Psi}{\Psi} = \frac{\hbar}{m}\nabla\ln\Psi = \frac{\hbar}{m}\frac{\nabla R}{R} + i\frac{\nabla S}{m}$). In this view, $\nabla S/m$ is that part of osmotic velocity accounting for target distribution changing shape in real time.

So methods have practically identical Langevin-type equations describing particle motion as result of drift and diffusion, and similar propagators K (one in real, one in imaginary time).

Notes

- In DMC complex Ψ hardly used: real arithmetic faster and real Ψ easier to map into probabilities.
- Where complex Ψ have been used one employs *fixed-phase approximation* instead of fixed-node i.e. you say phase S is fixed and equal to phase of trial function Φ_T. DMC algorithm used to solve for modulus of Ψ. Discussions in literature generally unclear (at least to me).
- Note no-one ever does DMC for *time-dependent* wave functions - always stationary states.

Some random ideas

Repeat DMC imaginary time analysis with complex time $\tau = t + it'$*:*

Choose constant offset E_T in TDSE to be ground-state energy E_0 then, as $\tau \to \infty$, Ψ comes to look more like ground state ϕ_0 (as before). Difference is that exponentially-decaying bit now has t-dependent moving nodal surface. (Recall that a linear combination of stationary TDSE solutions with different energies, each with its own t-dependent phase factor, gives overall t-dependence in $|\Psi|^2$.)

$$\Psi(\mathbf{x}, \tau) = c_0\phi_0 + \sum_{n=1}^{\infty} c_n\phi_n(\mathbf{x})\mathrm{e}^{i(E_n-E_0)t}\mathrm{e}^{-(E_n-E_0)t'}$$

- With t-dependent complex Ψ there are no nodal surfaces, just nodal lines where surfaces of real and imaginary functions intersect. No barriers to particle motion.
- Valentini's calculations showed us how particles guided by the wave field with rapidly-moving nodes quickly became distributed according to $|\Psi|^2$. Also saw that nodal lines moving through particle distribution acted as 'particle mixers'; trajectories become 'more chaotic' with more nodes.
- Might think that while imaginary time propagation improves Ψ, real time propagation allows nodal surface to relax and Ψ to be optimized more efficiently, unconstrained by fixed nodes. As excited-state contributions die away and distribution approaches stationary state, $\frac{\nabla S}{m}$ (and hence guided particle velocity) tends to zero (only diffusion and real part of drift velocity remain for computing statistical data and expectation values).

Is there a way this sort of thing can be useful in developing better QMC algorithms?

Time-dependent quantum Monte Carlo

Only reference in literature to anything like this is Bulgarian chap I.P.Christov's time-dependent quantum Monte Carlo (TDQMC) method from 2007. Involves moving electrons guided by de Broglie-Bohm pilot waves!

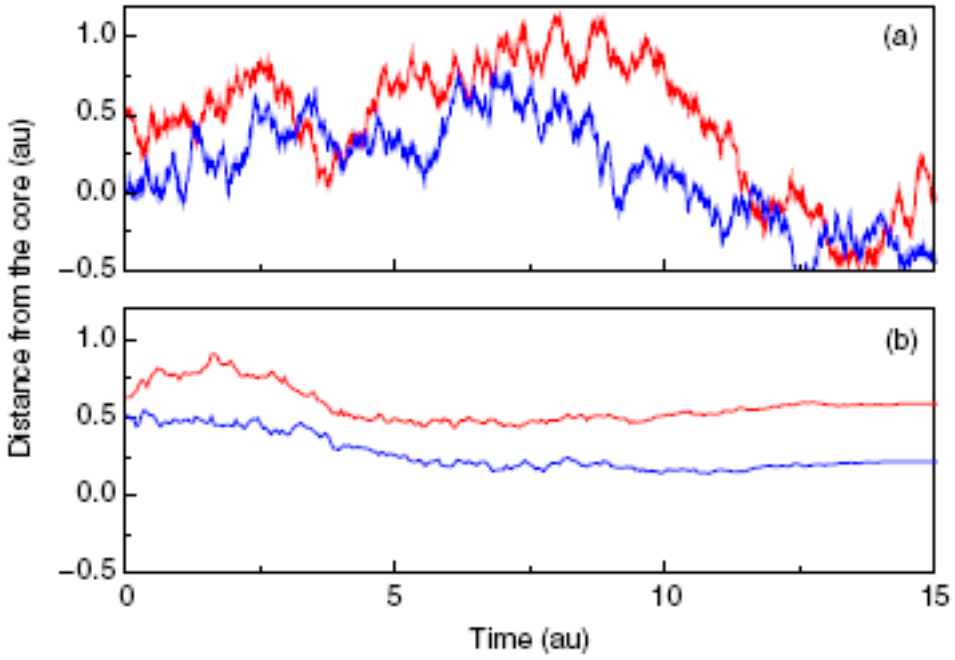
Important-sounding claims:

- Particle distribution in configuration space corresponds to $|\Psi|^2$; method thus not sensitive to sign of many-body wave function (apparently thereby claims to solve fermion sign problem..).
- Guide waves and *nodal surface* evolve with particles. No initial guess for Ψ required.
- Can do *time-dependent* problems e.g. involving external electromagnetic fields.
- Easier numerically than QTM and similar methods outlined earlier.

What it does

- Sort of synthesis of QMC and quantum hydrodynamics. Each *electron* represented by ensemble of configs moving on quantum trajectory implied by guidance equation (normal or stochastic).
- Guide functions are 'one-electron orbitals' evolving according to time-dependent Schrödinger equation. Time evolution by simple numerical integration (not Green's function propagators).
- *Complex time* used in evolution; imaginary part causes guide waves to relax to ground state, real part gives time-dependent phase which guides configs to stationary positions. Amplitude of random diffusion part decreasing function of time.
- Nodal structure (and hence symmetry properties of many-electron Ψ) from Slater determinants of individual time-dependent orbitals. Trajectories never cross nodes and nodes are *time-dependent*.

TDQMC - relaxation to ground state



Time evolution of coordinates of two arbitrary configs for 1D He (a) for DMC and (b) for TDQMC.

Different methods for guiding configs: TDQMC trajectories tend towards steady-state positions (distributed as $|\Psi_{GS}|^2$ over ensemble), DMC trajectories undergo random jumps at all times. Once TDQMC ground state achieved, can switch to real time and turn on external fields to study t-dependent dynamics, since $P(\mathbf{x},t) = |\Psi(\mathbf{x},t)|^2$ and will stay that way (e.g. Christov calculates t-dependent dipole moment for 1D He atom).

Problems

- Calculations (over 4 papers) only for embarassingly trivial systems (1D helium atoms etc..).
- Uses *Numerical Recipes*-style Crank-Nicholson finite-differencing in Eulerian picture to propagate pilot-waves. More sophisticated technology required for more complex systems.
- Uses 'effective Coulomb interactions' instead of proper ones as he doesn't like singularities. Ugly Hartree-style approximation $R(\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N) = R_1(\mathbf{x}_1)R_2(\mathbf{x}_2)\ldots R_N(\mathbf{x}_N)$ which means no non-local quantum correlations (though he has an 'effective potential correction' to patch this up).
- Very low tech compared to what is routinely done today by people like us. Solutions of fermion sign problem need to demonstrate explicitly suitable scaling with system size etc. Long way from 1D He to e.g. 1000+ atom solid magnetic NiO calculations currently being done with DMC.

Nevertheless ideas like these may yet prove very interesting. Not many people studying them either!

Gissa job