

The Towler Institute

2010 Conference Programme

Quantum Monte Carlo in the Apuan Alps VI

Vallico Sotto, Tuscany, Italy : 24th -31st July 2010

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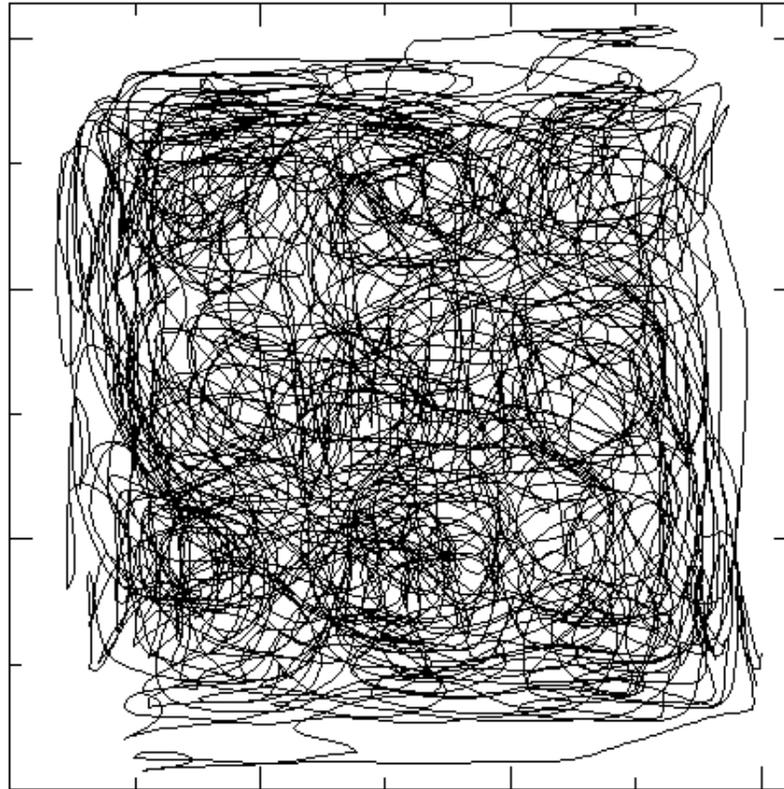
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The magic of moving nodes..

..or, an account of Mike's attempt to write an entirely new computer code for the first time in years.

QMC in the Apuan Alps VI, 29th July 2010



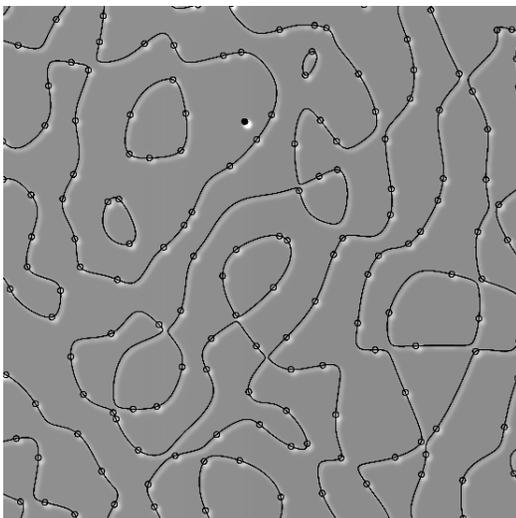
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Nodes - the QMC perspective



In FN-DMC calculations, we normally deal only with:

- **Stationary states with real wave functions:** Time-independent $3N - 1$ dimensional hypersurface where Ψ is zero. Fixed-node approximation most significant error in DMC.
- **Stationary states with complex wave functions:** Less common but used in e.g. twist-averaging, non-collinear spins, magnetic fields. Fixed-phase approximation in DMC.

It is normally stated that e.g. "*very little is known about wave function nodes, and a systematic study has never been attempted*" (Bressanini, Ceperley, Reynolds). So in this talk I shall make things easier for myself by dealing with er.. ***non-stationary states with (necessarily) complex wave functions evolving in real time.***

What do the nodes of such wave functions look like?

In general, we expect them to have a different topology to those for real functions. Imagine something like: for complex functions in 3D get nodes along lines where zero surfaces of real and imaginary functions cross. Similarly, in 2D lines become nodal points. Fewer barriers to movement of configurations?

Student overhead: the time-dependent Schrödinger equation

Solve $i\hbar\frac{\partial}{\partial t}\Psi(x, t) = H\Psi(x, t)$ by separation of variables to give the following **particular solutions** (which have the counterintuitive property of predicting time-independent observables):

$$\Psi(x, t) = \phi_E(x)e^{-\frac{i}{\hbar}Et} \quad |\Psi(x, t)|^2 = |\phi_E(x)|^2$$

Where has the time gone? It is restored to us by a **general solution** to the TDSE - an arbitrary superposition of the particular solutions:

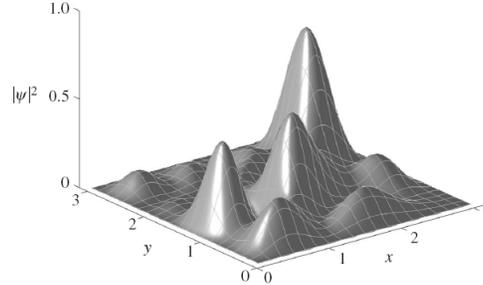
$$\begin{aligned} \Psi(x, t) &= \sum_{n=1}^{\infty} a_n \phi_n(x) e^{-\frac{i}{\hbar}E_n t} && \text{(discrete spectrum)} \\ &= \int_0^{\infty} a(E) \phi_E(x) e^{-\frac{i}{\hbar}Et} dE && \text{(continuous spectrum)} \end{aligned}$$

Quite generally, a *wave packet* - a superposition of states having different energies - is required in order to have a time-dependence in the probability density and in other observable quantities, such as the average position or momentum of a particle. Simplest example: a linear combination of just two particular solutions $\Psi(x, t) = a\phi_E(x)e^{-\frac{i}{\hbar}Et} + b\phi_{E'}(x)e^{-\frac{i}{\hbar}E't}$. The probability density is given by:

$$|\Psi(x, t)|^2 = |a|^2|\phi_E(x)|^2 + |b|^2|\phi_{E'}(x)|^2 + 2\text{Re} \left\{ a^* b \phi_E^*(x) \phi_{E'}(x) e^{-i\frac{(E'-E)t}{\hbar}} \right\}$$

All the time-dependence is contained in the interference term.

Example test case: particle in a 2D box



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

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

- 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 $m, n = 1, 2, 3, \dots$

- Initial *non-stationary* Ψ is superposition of first N modes ($m, n = 1, 2, 3, 4, \dots$) with equal amplitudes but randomly chosen phases θ_{mn} . Note Ψ periodic in time with period 4π (since $4\pi E_{mn}$ is always an integer multiple of 2π).

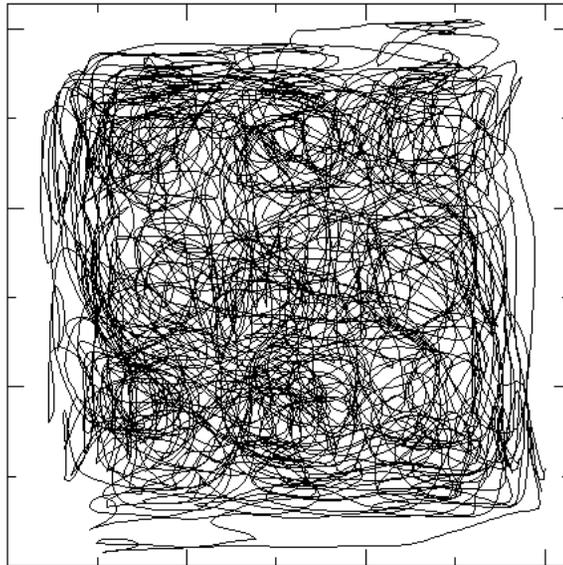
$$\Psi(x, y, 0) = \sum_{m,n=1}^{\sqrt{N}} \frac{1}{\sqrt{N}} \phi_{mn}(x, y) e^{i\theta_{mn}} \quad \Psi(x, y, t) = \sum_{m,n=1}^{\sqrt{N}} \frac{1}{\sqrt{N}} \phi_{mn}(x, y) e^{i(\theta_{mn} - E_{mn}t)}$$

Electron trajectories

In order to study this, I will make a hypothesis of *what exists*.

(1) We say that the wave function is a mathematical representation of a real objectively-existing 'wave field'.

(2) We say that 'particles' objectively exist, and that they follow trajectories - which are just the streamlines of the usual quantum probability current.



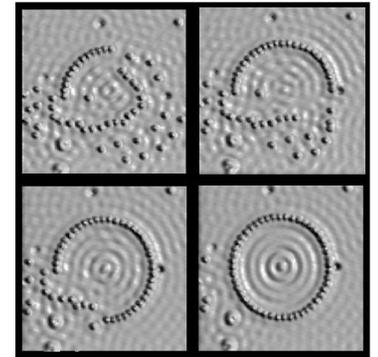
This is the *de Broglie-Bohm* interpretation of quantum mechanics

QM is the statistical mechanics of particles following non-classical trajectories. (!)

This is forbidden, of course, but 1927 was a long time ago..

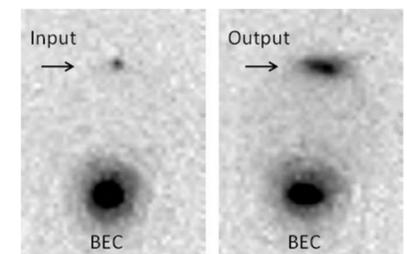
Orthodox Copenhagen QM is both an algorithm for obtaining statistical predictions for the results of experiments and a prescription for *avoiding fundamental questions*. Bohr *et al.* designed it that way because in 1927 quantum entities were unobservable and thus [non sequitur] not real: “. . . *the 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 technological progress shows essentially without doubt that quantum entities exist whether we ‘observe’ or do experiments with them, or not. Single atoms and even electrons can be isolated and trapped in containment vessels for long periods. Can repeat examination many times and get same data. Individual atoms can be ‘pushed around’ and arranged into patterns (which can also be imaged). These experiments all yield *consistent* results and information about quantum entities using a variety of techniques and under different conditions.



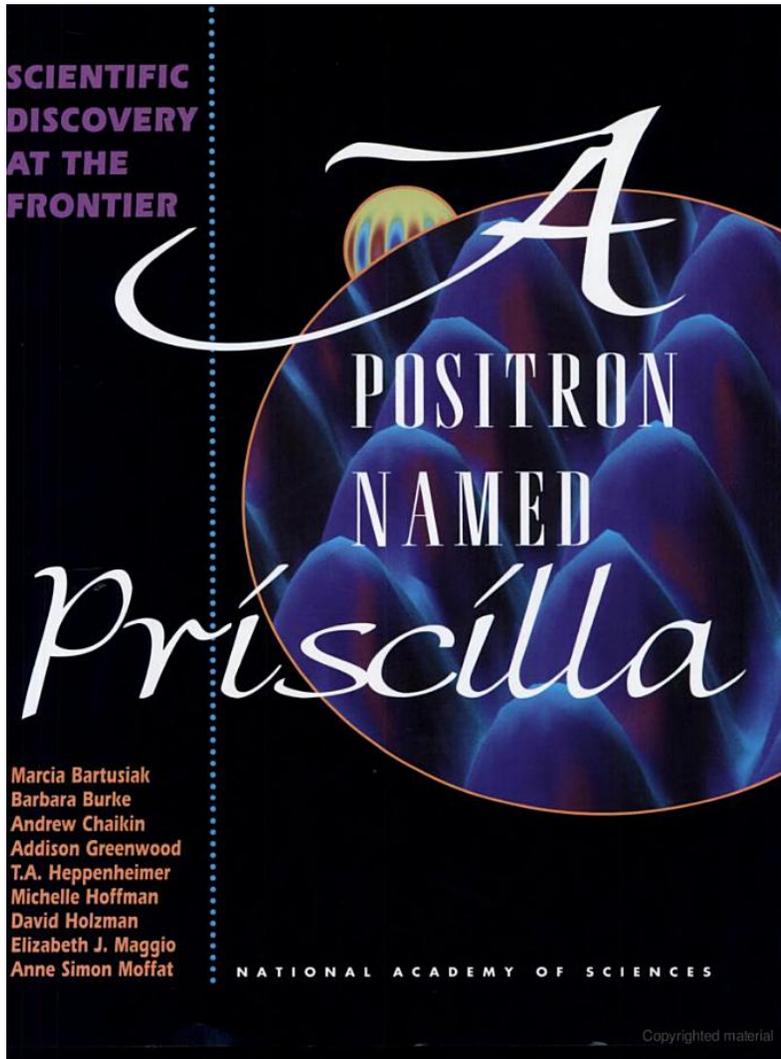
“Perhaps the most convincing proof of the reality of the quantum world would be to capture some of its creatures and hold them in place for all to see. This has become feasible.” [Ho-Kim *et al.*, 2004]

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 thought patterns of the prevailing paradigm of orthodox quantum theory (such as the denial of an independently existing quantum realm). So be it.

The impossible observed



Hans Dehmelt has carried out exquisitely precise studies of *individual electrons and positrons* - including measuring their magnetic moments to twelve decimal places - by capturing them in electromagnetic traps. Because positrons do not exist naturally on Earth, he showed that the particular positron under study had no opportunity to swap with a different one. He has held that particle in place for as long as three months. He writes “*The well-defined identity of this elementary particle is something fundamentally new, which deserves to be recognized by being given a name, just as pets are given names of persons.*” So he called her **Priscilla**, and won the Nobel prize for it in 1989.

Bohr, Pauli and other Copenhagenists had conclusively proved in 1928 that the magnetic moment of a free electron could never be observed (an argument still being defended up to 1985). ‘*From these arguments we must conclude that it is meaningless to assign to the free electron a magnetic moment*’. Today this quantity may be the best measured number in all of science.

Moral: Be modest about the implications of your theories and never underestimate the cleverness of experimentalists.

Astrid the atom



Dehmelt also trapped a single barium atom that he named Astrid, and kept it floating like a pixie in a tiny ion-trap vacuum chamber for ten months. Under suitable conditions, she turned out to be visible to the naked eye..

It used to be claimed that no-one could ever see an atom with their naked eyes. The mistake here is assuming that *smallness* is the important issue; actually *brightness* and *isolation from other atoms* are what matters. A laser-stimulated barium atom produces 10^8 photons per second; your eyes can collect several thousand. The normal retina is sensitive to even a few photons, so you can see the atom, just as you would a distant star or any other bright, isolated object.

How do 'quantum trajectories' differ from classical trajectories?

i.e. when we say 'this is not explicable classically; it is a *quantum effect*' (Pauli repulsion, degeneracy pressure, covalent bonding, etc..) can we be more specific about what we mean?

Strategy: Work with statistical distribution ρ since particle positions unknown. Assuming *classical* Newtonian trajectories, derive differential equation giving time evolution of ρ . Can we deduce from this anything about form of force in *quantum* case?

- Probability distribution ρ must obey usual continuity equation $\partial\rho/\partial t = -\nabla \cdot (\rho\mathbf{v})$ so that it remains normalized as it changes shape over time (here \mathbf{v} is velocity vector).
- Assume particles obey classical dynamics. To calculate trajectories, don't use Newtonian $\mathbf{F} = m\mathbf{a}$ formulation; instead use the *entirely equivalent* Hamilton-Jacobi equation $-\frac{\partial S}{\partial t} = \frac{(\nabla S)^2}{2m} + V$ - where S is related to the 'action'.

For convenience, combine *continuity* and *classical Hamilton-Jacobi* equations (two *real* equations, note) into a single *complex* equation. To do this, introduce general complex function $\Psi = re^{i\theta} = \sqrt{\rho}e^{\frac{iS}{\hbar}}$ with \hbar an arbitrary constant giving a dimensionless exponent. Complex equation that results is:



$$i\hbar\frac{\partial\Psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V - Q \right) \Psi \quad \text{with} \quad Q = -\frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}.$$



This is the *time-dependent Schrödinger equation* - straight out of QM - with one difference: something like a potential (' Q ') is subtracted off the Hamiltonian. Note Ψ has same interpretation as in QM: a particle probability density. Tells us that if particles are to follow Newtonian trajectories, must subtract off an extra 'quantum force' $-\nabla Q$ (apparently due to a 'wave field' pushing the particles) from the usual classical force.

Derive the same thing directly in QM

- Wave field evolution from Schrödinger equation $i\hbar \frac{\partial \Psi}{\partial t} = \sum_{i=1}^N -\frac{\hbar^2}{2m_i} \nabla_i^2 \Psi + V\Psi$. Evolving quantum system behaves like 'probability fluid' of density $|\Psi|^2 = \Psi\Psi^*$ with an associated time-dependent quantum *probability current* $\mathbf{j} = \frac{\hbar}{m} \text{Im}(\Psi^* \nabla \Psi)$.
- Suspect particle trajectories follow streamlines of current: velocity $\mathbf{v} = \frac{\hbar}{m} \text{Im} \nabla \ln \Psi$ (current/density). Using complex polar form $\Psi = |\Psi| \exp[iS/\hbar]$, the wave function *phase* $S(\mathbf{x}_1, \dots, \mathbf{x}_N, t)$ is given by $S = \hbar \text{Im} \ln \Psi$ (similar to velocity expression). Thus deduce trajectories $\mathbf{x}_i(t)$ given by *de Broglie guidance equation* for velocity:

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

- Can write in 2nd-order ' $F = ma$ ' form by taking t derivative: $m_i \ddot{\mathbf{x}}_i = -\nabla_i(V + Q)$, where $Q = -\sum_i \frac{\hbar^2}{2m_i} \frac{\nabla_i^2 |\Psi|}{|\Psi|}$ (*quantum potential*). Extra 'quantum' force $-\nabla_i Q$ (big if large curvature in wave field). *Non-classical* dynamics since particles 'pushed along' by wave along trajectories perpendicular to surfaces of constant phase, as well as by classical force from 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). Suggests immediately how to obtain the classical limit, i.e. when $Q = \nabla Q = 0$ the wave component of matter is passive and the particles follow classical trajectories (impossible in orthodox QM!).

Example: fermionic repulsion in a trajectory theory

A total antisymmetrical wave function for a many-electron system can occur in a number of ways. For 2 electrons there are 3 states of interest where the electrons 'avoid each other'. Collectively called the 'triplet state' with total z -components of spin \hbar , $-\hbar$, 0 . Their wave functions (which are products of space and spin) all have antisymmetrical spatial components so $\Psi = 0$ if $\mathbf{x}_1 = \mathbf{x}_2$ and are given by:

$$\Psi = \{\psi_A(\mathbf{x}_1)\psi_B(\mathbf{x}_2) - \psi_A(\mathbf{x}_2)\psi_B(\mathbf{x}_1)\} \alpha(1)\alpha(2)$$

$$\Psi = \{\psi_A(\mathbf{x}_1)\psi_B(\mathbf{x}_2) - \psi_A(\mathbf{x}_2)\psi_B(\mathbf{x}_1)\} \beta(1)\beta(2)$$

$$\Psi = \{\psi_A(\mathbf{x}_1)\psi_B(\mathbf{x}_2) - \psi_A(\mathbf{x}_2)\psi_B(\mathbf{x}_1)\} \{\alpha(1)\beta(2) + \alpha(2)\beta(1)\}$$

Now let the spatial part be written in complex polar form: $\psi_A(\mathbf{x}_1)\psi_B(\mathbf{x}_2) - \psi_A(\mathbf{x}_2)\psi_B(\mathbf{x}_1) = R e^{i\frac{S}{\hbar}}$. When this is zero the amplitude R must be zero (since $e^{i\frac{S}{\hbar}}$ cannot be zero by definition). Thus, as a nodal region of the wave field is approached, the value of R will tend to zero. The (repulsive) quantum force on each particle is $\mathbf{F}_i = (d\mathbf{p}_i/dt) = -\nabla_i Q$ where $Q = -\hbar^2/2mR(\nabla_1^2 R + \nabla_2^2 R) +$ spin-dependent terms. Finding the negative gradient of Q (ignoring the spin-dependent terms since the spatial terms will dominate as R tends to zero) gives:

$$\mathbf{F}_i = \frac{\hbar^2}{2mR^2} \sum_{j=1}^2 \left[R \nabla_i (\nabla_j^2 R) - (\nabla_i^2 R) (\nabla_j R) \right]$$

It can be seen that as $R \rightarrow 0$ then $\mathbf{F}_i \rightarrow \infty$. The 'Pauli repulsion' force \mathbf{F}_i exerted by the wave field on the two fermions prevents them coming into close proximity of each other when their 'spins are the same' (i.e. in cases where the spatial part of Ψ is antisymmetric). More generally, the dynamics as shown by this trajectory theory **prevent fermions occupying the same quantum state**.

Electron trajectories? What do we think about this?

But do electrons really have trajectories? This is really a question of the *interpretation* of QM, but very few electronic structure people think about that. What do we *actually do in practice*?

Density functional theory people:

- Create movies using *ab initio* molecular dynamics, where the nuclear positions are evolved using Newton's equations. We therefore believe that nuclei are point particles with classical trajectories.
- The electrons have a sort of fuzzy charge density which is a 'solution to the Schrödinger equation' (in the Kohn-Sham sense) for a sequence of nuclear positions. So - because electrons are very light - either we don't believe they have trajectories at all, or we believe they move much faster than the nuclei and their (presumably non-classical) trajectories are 'smeared out'.
- Sometimes, for very light atoms such as H, we think that *quantum effects* such as zero-point motion or tunnelling are important. We then might do e.g. *ab initio* path integral molecular dynamics (e.g. Matt Probert's implementation in CASTEP).¹
- The 'exchange potential' - which gives rise to so-called 'quantum effects that cannot be described classically' - is presumably some kind of approximation to Q ?

"If we were to name the most powerful assumption of all, which leads one on and on in an attempt to understand life, it is that all things are made of atoms, and that everything that living things do can be understood in terms of the jiggings and wiggings of atoms." [Feynman]

¹It can be shown that Feynman path-integral QM - where you sum over the infinite number of possible trajectories each weighted by an expression involving the classical Lagrangian $T - V$ - is equivalent to just using a single term involving the trajectory that the electron actually follows along with the new 'quantum Lagrangian' $T - V - Q$. In principle one could just calculate $-\nabla Q$ to correct the quantum H atom trajectories.

Electron trajectories? What do we think about this?

Quantum Monte Carlo people:

- Both nuclei and electrons are treated as point particles (though the nuclei are usually clamped).
- We can compute forces (albeit with some difficulty) and if we bothered to implement coupled DMC-MD in CASINO [as Lucas did with Qwalk ages ago] then we would move the nuclei along classical trajectories just as with DFT. Widely differing timescales make it difficult to treat nuclei and electrons on the same quantum footing.
- In QMC the point electrons do not move along trajectories (we instead move them along a stochastic random walk to sample the distribution). However, importance-sampled diffusion Monte Carlo is something like the time-independent limit of a stochastic quantum trajectory method (this would be more apparent if we ever used time-dependent probability distributions).

Conclusions:

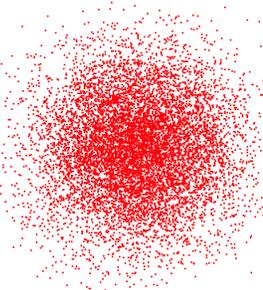
- Neither DFT people or QMC people are Copenhagenists, since such people explicitly state - as part of the ontology - that quantum particles *do not have positions* unless they are measured. It is explicitly understood that hidden variables descriptions (and particle positions and their consequent trajectories are hidden variables) are impossible.
- The 'quantum force' depends inversely on the mass. So when we decide whether particles follow classical trajectories, we appear to have developed a mental facility for estimating the size of \hbar . Clearly for heavier particles, \hbar will be small and the trajectories approximately classical. For lighter particles, this is not so and we must use quantum methods to calculate their dynamics.
- There is no justification for saying that electronic structure theorists do not believe in the reality of particle trajectories (either for electrons or nuclei). We may therefore proceed with a clear conscience to use arguments based on particle trajectories.

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 $\mathbf{u} = D \frac{mg}{kT} \mathbf{z}$, the conservation equation becomes $\frac{\partial P}{\partial t} = -D\nabla \cdot \left[\frac{mg}{kT} \mathbf{z} P + \nabla P \right]$. In equilibrium when $\frac{\partial P}{\partial t} = 0$ we have $\frac{\nabla P}{P} = \frac{mg}{kT} \mathbf{z} + c$ or $P = A \exp\left(-\frac{mgz}{kT}\right)$ 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 $\mathbf{j} = \rho \mathbf{v} = \rho \left(\frac{\nabla S}{m}\right)$. Consistent possibility if $\Psi = \sqrt{\rho} \exp\left(\frac{iS}{\hbar}\right)$ 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 $d\mathbf{r}$ 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.

Standard pilot wave	$d\mathbf{r} = \frac{\nabla S}{m} dt$
Stochastic pilot wave	$d\mathbf{r} = \frac{\nabla S}{m} dt + \chi \sqrt{\frac{\hbar}{m}} dt + \frac{\hbar}{2m} \frac{\nabla \Psi ^2}{ \Psi ^2} dt$
DMC	$d\mathbf{r} = \chi \sqrt{\frac{\hbar}{m}} dt + \frac{\hbar}{m} \frac{\nabla \Phi_T }{ \Phi_T } dt$
DMC2 [†]	$d\mathbf{r} = \frac{\nabla S}{m} dt + \chi \sqrt{\frac{\hbar}{m}} dt + \frac{\hbar}{m} \frac{\nabla \Phi_T }{ \Phi_T } dt$

[†] If use complex Φ_T and retain imaginary part of complex drift vector $\nabla \Phi_T / \Phi_T$ (since for $\Psi = \text{Re}^{iS/\hbar}$ 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 $\tau \rightarrow \infty$, 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 $|\Psi|^2$.)

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

- With t -dependent complex Ψ nodal surfaces dissolve into nodal lines where surfaces of real and imaginary functions intersect. Fewer barriers to motion of configurations?
- Simulations will show us how particles guided by the wave field with rapidly-moving nodes quickly became distributed according to $|\Psi|^2$. Also see 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?

My new calculations: dynamical relaxation to quantum equilibrium. Why $\rho = |\Psi|^2$?



Pauli objection: Taking a particular particle distribution $\rho = |\Psi|^2$ as an initial condition is unjustified in a fundamentally deterministic theory, therefore 'theories' of this kind are rubbish [in *Louis de Broglie: physicien et penseur* Festschrift, 1953].

However, Pauli is right: this should be *derived* from the dynamics, for QM truly to emerge as the statistical mechanics of an underlying deterministic theory.

Easy to show if $\rho(\mathbf{x}, t) = |\Psi(\mathbf{x}, t)|^2$ at any t it will always remain so under Schrödinger time evolution ('equivariance'). Can also show $|\Psi(\mathbf{x}, t)|^2$ is *only* distribution with this property i.e. 'quantum equilibrium' is unique [Goldstein, Struyve 2007]. It is analogous to thermal equilibrium $P = \frac{\exp(-H/kT)}{Z}$.

With deterministic hidden-variable theories the Born distribution should not be regarded as an axiom. It should be seen as dynamically generated, in same sense that one usually regards thermal equilibrium as arising from process of relaxation based on some underlying dynamics.

A quite general argument (due to Antony Valentini, 1992) for the relaxation $\rho \rightarrow |\Psi|^2$ may be framed in terms of an analogy with the *classical coarse-graining H-theorem*. One may also look at *numerical simulations*.

Approach to equilibrium in classical statistical mechanics

For a **classical** isolated system, both the probability density ρ and the volume element $d\Omega$ (on phase space) are preserved along trajectories (Liouville's theorem).

- Despite fact that $d\rho/dt = 0$ we find ρ evolves in a highly complex 'filamentary' manner over energy surface so *on a coarse-grained level* ρ becomes uniform as expected (whatever its initial shape). 'Coarse graining' involves dividing phase space into little cells of volume δV and working with *average* of ρ in each cell ($\bar{\rho}$).
- Can quantify difference between ρ and $\rho_{uniform}$ with *classical H-function*, i.e. $H_{class} = \int \rho \ln \rho d\Omega$. This is minus relative entropy of ρ with respect to $\rho_{uniform}$ (standard measure of difference between two distributions). H bounded below by zero, and equals zero if and only if ρ uniform on energy surface (equilibrium).
- Classical $H_{class} = \int \rho \ln \rho d\Omega$ is *constant in time*. If replace fine-grained ρ by coarse-grained $\bar{\rho}$ and assume $\bar{\rho}_0 = \rho_0$ at $t = 0$, then $\bar{H}_{class}(t) \leq \bar{H}_{class}(0)$ for all t - which is the **classical coarse-graining H-theorem**: i.e. \bar{H}_{class} either decreases or remains constant, $d\bar{H}_{class}/dt \leq 0$. Decrease of \bar{H}_{class} corresponds to formation of structure in ρ and consequent approach of $\bar{\rho}$ to uniformity.
- Relies on assumption $\bar{\rho}(0) = \rho(0)$ in phase space, i.e. no fine-grained microstructure in initial conditions (which could lead to 'unlikely' entropy-decreasing behaviour). Assumption necessary owing to time-reversibility of the theory.

Analogy with subquantum case if we let $d\Omega \rightarrow |\Psi|^2 dx$ and ρ be the density of quantum particles.

Subquantum H -theorem

Valentini's argument for the relaxation $\rho \rightarrow |\Psi|^2$ is framed in terms of an analogy with the classical coarse-graining H -theorem.

- For 'sufficiently complex' system assume have initial distribution $\rho(\mathbf{x}, 0)$ of configurations $\mathbf{x}(0)$ each guided by the same Ψ , with $\rho(\mathbf{x}, 0) \neq |\Psi(\mathbf{x}, 0)|^2$.
- By definition $\rho(\mathbf{x}, t)$ satisfies continuity equation $\partial\rho/\partial t + \nabla \cdot (\dot{\mathbf{x}}\rho) = 0$, and Schrödinger equation implies this is also satisfied by $|\Psi|^2$. Since $\dot{\mathbf{x}} = \nabla S/m$, clear that Ψ actually determines time evolution of ρ . So ratio $f = \rho/|\Psi|^2$ is preserved along trajectories: $df/dt = \partial f/\partial t + \dot{\mathbf{x}} \cdot \nabla f = 0$.
- Initial deviations $\rho \neq |\Psi|^2$ thus forever carried along trajectories and never disappear, appearing to imply equilibrium unreachable (as with the ρ in classical stat mech). We now define the *subquantum H -function*: $H = \int |\Psi|^2 f \ln f \, d\mathbf{x} = \int \rho \ln(\rho/|\Psi|^2) \, d\mathbf{x}$. Continuity equation and $df/dt = 0$ imply $dH/dt = 0$ i.e. exact fine-grained H constant as in classical case.
- Divide config space into cells of volume δV and define coarse grained-quantities e.g. $\bar{\rho} = (1/\delta V) \int_{\delta V} \rho \, d\mathbf{x}$ etc.. For coarse-grained H have $d\bar{H}/dt \leq 0$; necessary and sufficient condition for \bar{H} to have minimum value is $\rho = |\Psi|^2 \Rightarrow$ *equilibrium*. Decrease of \bar{H} corresponds to a 'stirring' of the two 'fluids' ρ and $|\Psi|^2$ by the same velocity field $\dot{\mathbf{x}}$ (since satisfy same continuity equation), making ρ and $|\Psi|^2$ less distinguishable on a coarse-grained level.

See literature for e.g. defining quantum equilibrium of *subsystems*, and defining 'relaxation times'.

The birth of LOUIS

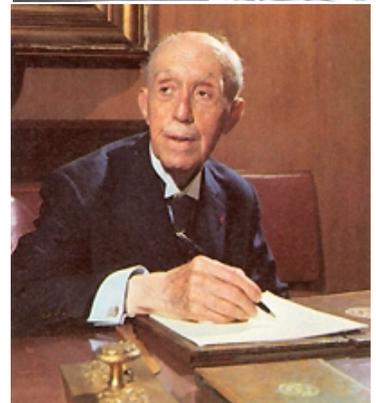
A new code to do quantum trajectory calculations and study the approach to quantum equilibrium

Comparison with previous code by 'Dr. X'.

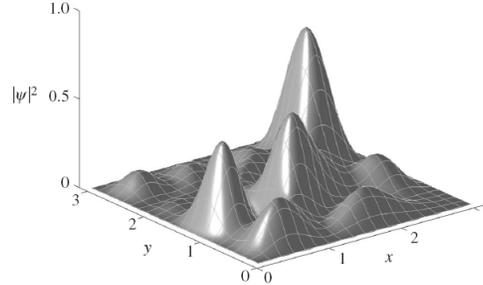
- Heavier.
- A lot faster ($\times 120!$). Allows us to do *much* bigger calculations.
- Gives the right answer. Numerics done correctly so 'bad trajectories' greatly reduced t .
- Change behaviour of calculation use CASINO/CASTEP-style input file rather than changing the source code. Introduced lots of internal error checking.
- General geometry.
- 1D, 2D, 3D calculations, not just 2D.
- Parallelized properly with MPI.
- Automated compilation with a proper Makefile and CASINO-style architecture selection. Use compiler optimization flags!
- Various modes of operation
 - single trajectory (forwards or backwards in time).
 - density
 - density + H function + relaxation time.
- Added timing routines
- Uses significantly less memory ('allocate statement').
- Velocity formulae selectable in input (e.g. ordinary deBB or inclusion of 'spin term').
- Add alternative integrators (Verlet, Bulirsch-Stoer) - should be faster and more accurate? Good consistency check.
- Random phase generator.

Things to do

- General wave functions (no analytic formula). Would require numerical integration of the Schrödinger equation.
- Multiple particles.



Example test case: particle in a 2D box



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

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

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

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

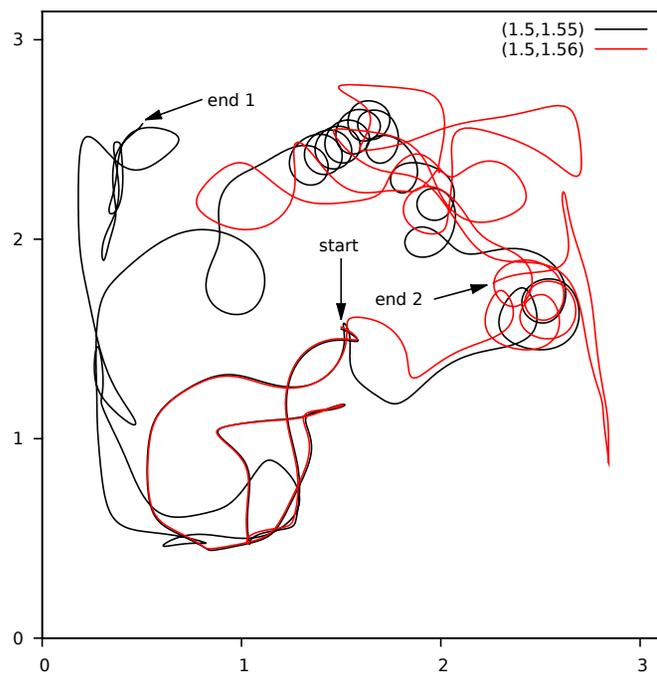
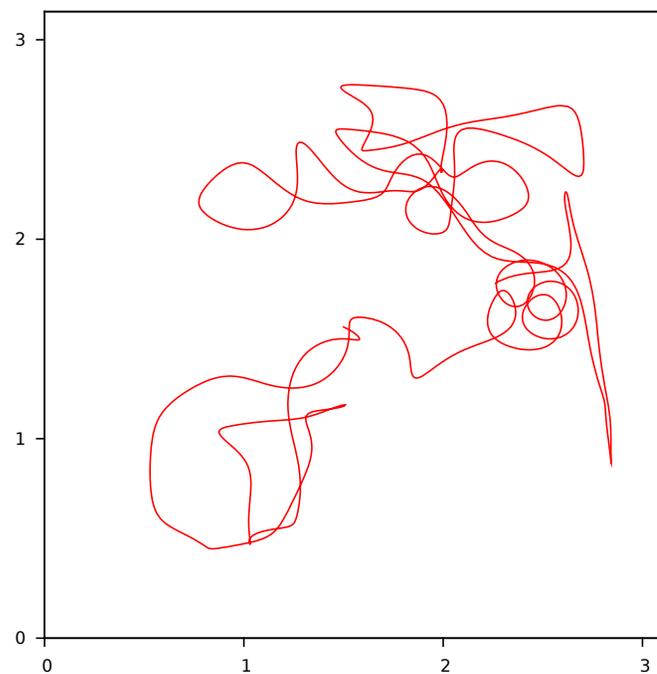
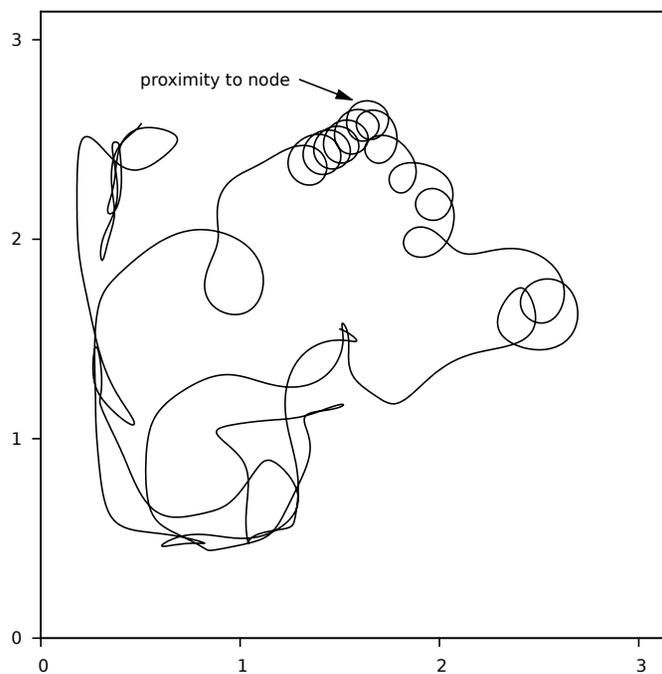
with energy eigenvalues $E_{mn} = \frac{1}{2}(m^2 + n^2)$, where $m, n = 1, 2, 3, \dots$

- Initial *non-stationary* Ψ is superposition of first N modes ($m, n = 1, 2, 3, 4, \dots$) with equal amplitudes but randomly chosen phases θ_{mn} . Note Ψ periodic in time with period 4π (since $4\pi E_{mn}$ is always an integer multiple of 2π).

$$\Psi(x, y, 0) = \sum_{m,n=1}^{\sqrt{N}} \frac{1}{\sqrt{N}} \phi_{mn}(x, y) e^{i\theta_{mn}} \quad \Psi(x, y, t) = \sum_{m,n=1}^{\sqrt{N}} \frac{1}{\sqrt{N}} \phi_{mn}(x, y) e^{i(\theta_{mn} - E_{mn}t)}$$

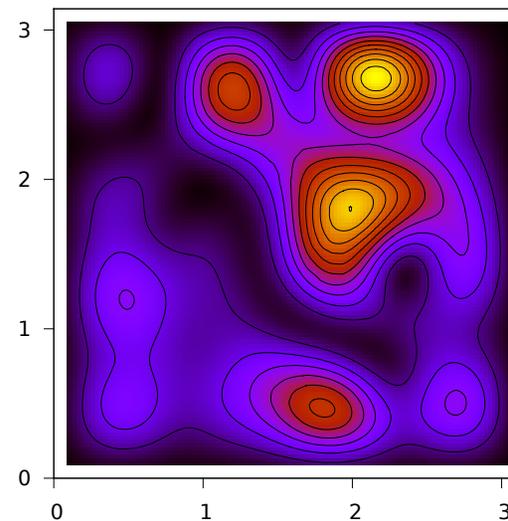
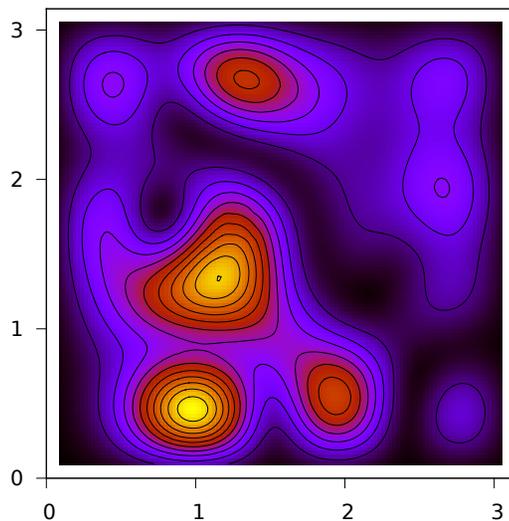
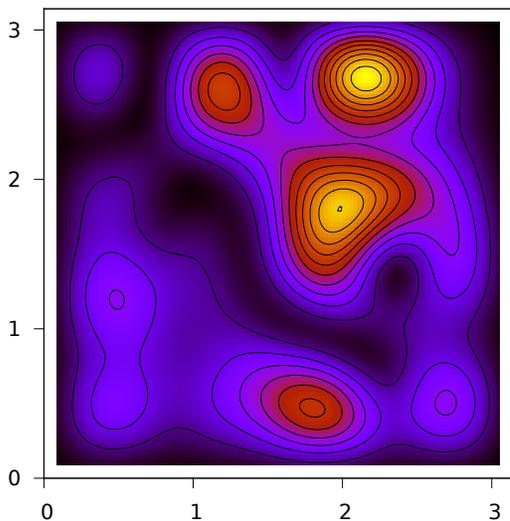
We have done these calculations with $N=4, 9, 16, 25, 36, 49, 64$ modes [previously only 16 (Valentini, Westman 2005), or 4 (Colin, Struyve 2010)]

Examples of trajectories

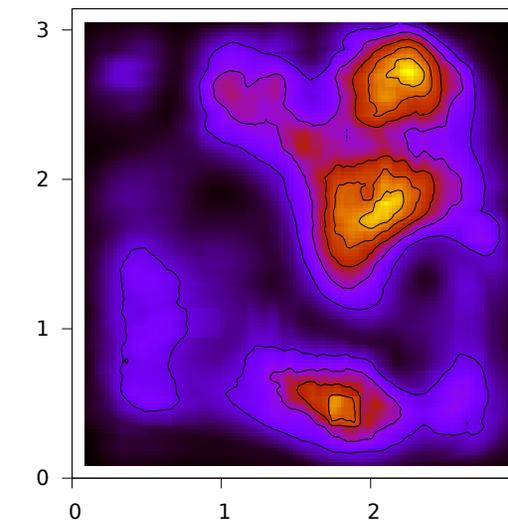
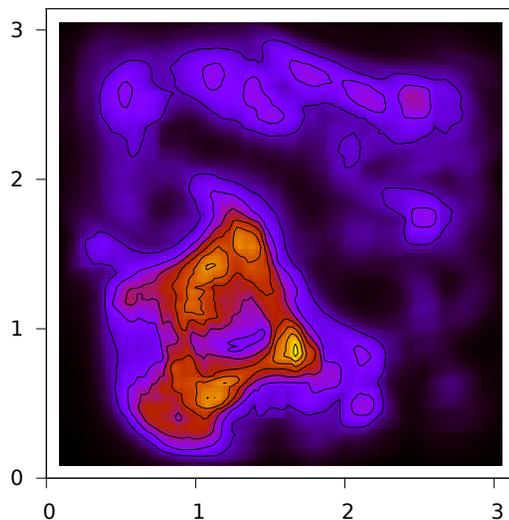
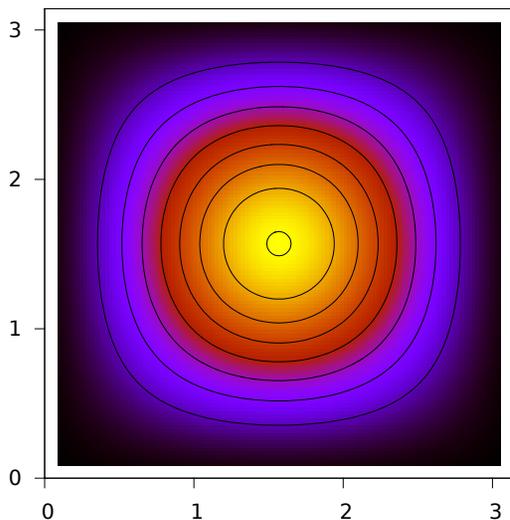


Dynamical relaxation to quantum equilibrium

ψ^2



ρ

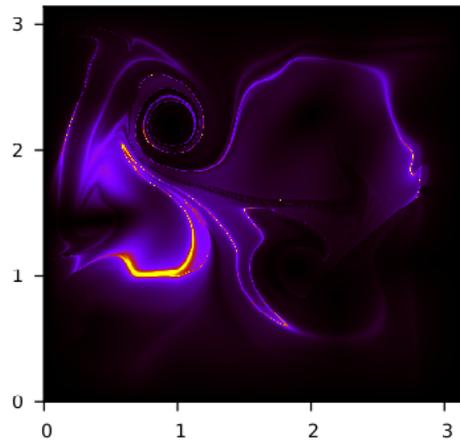


(a) $t=0$

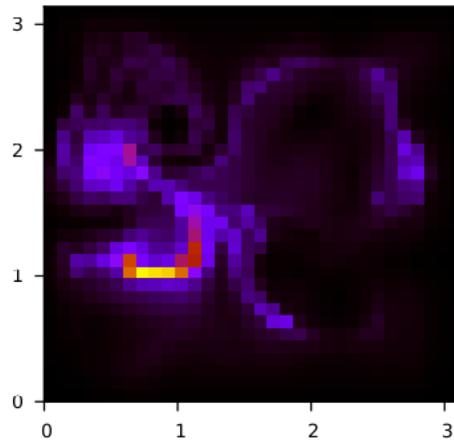
(b) $t=2\pi$

(c) $t=4\pi$

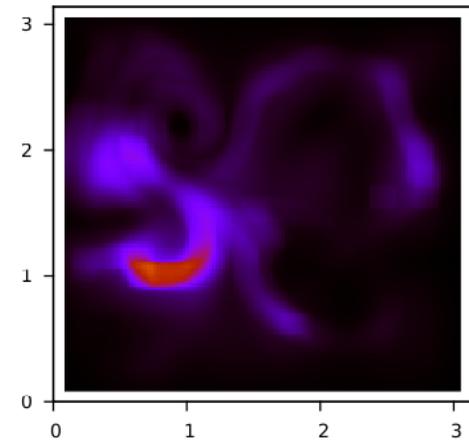
Effects of coarse-graining



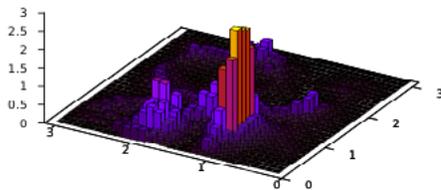
(a) fine-grained



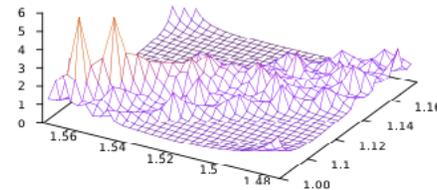
(b) coarse-grained, $\varepsilon = 32$



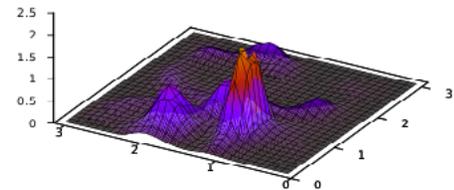
(c) smoothed



(d) $\varepsilon = 32$



(e) single coarse-graining cell



(f) smoothing applied

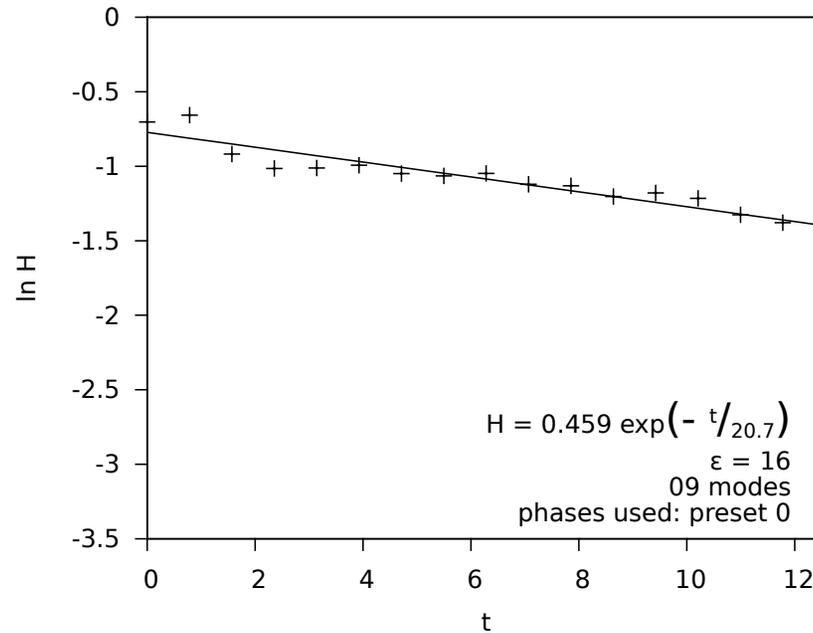
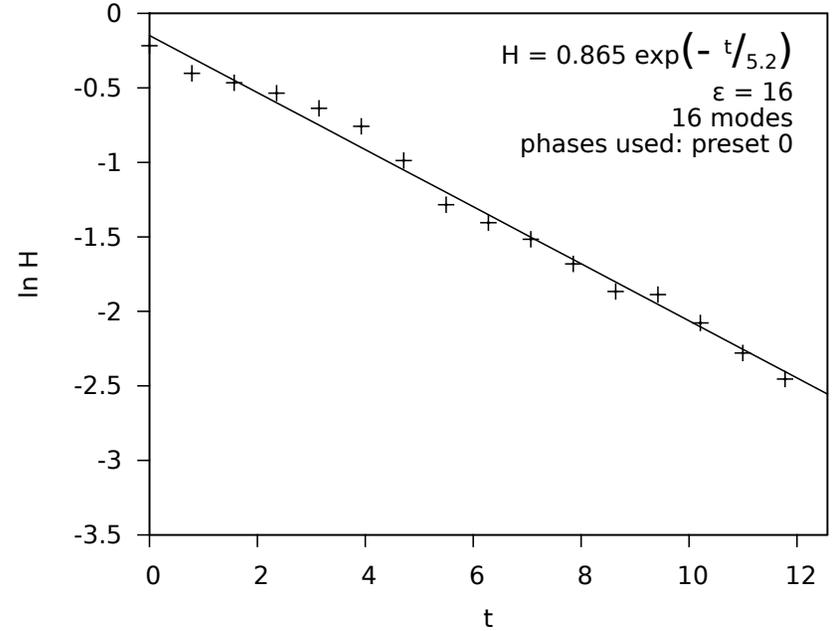
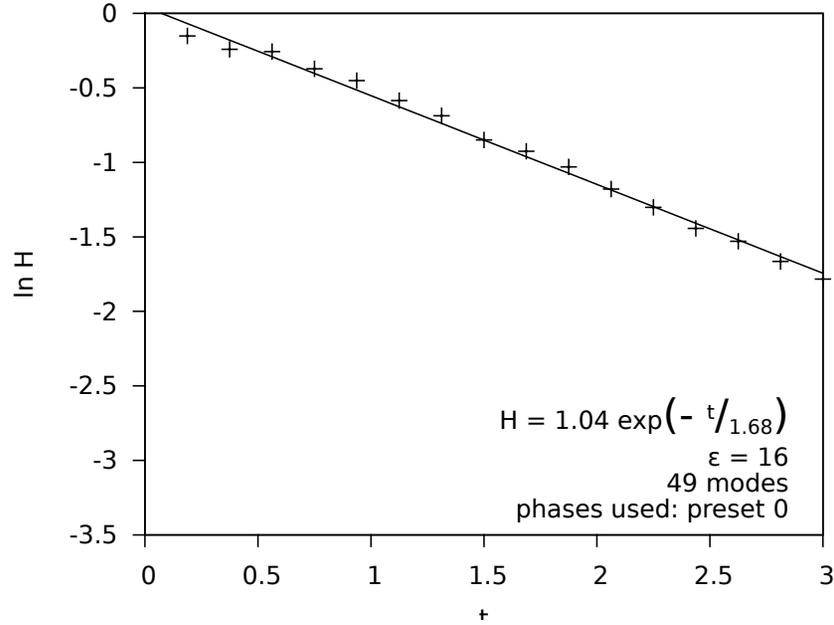
Effects of coarse-graining for a 16-mode system at $t = \frac{\pi}{2}$.

(d) ρ after coarse-graining of length 32 has been applied.

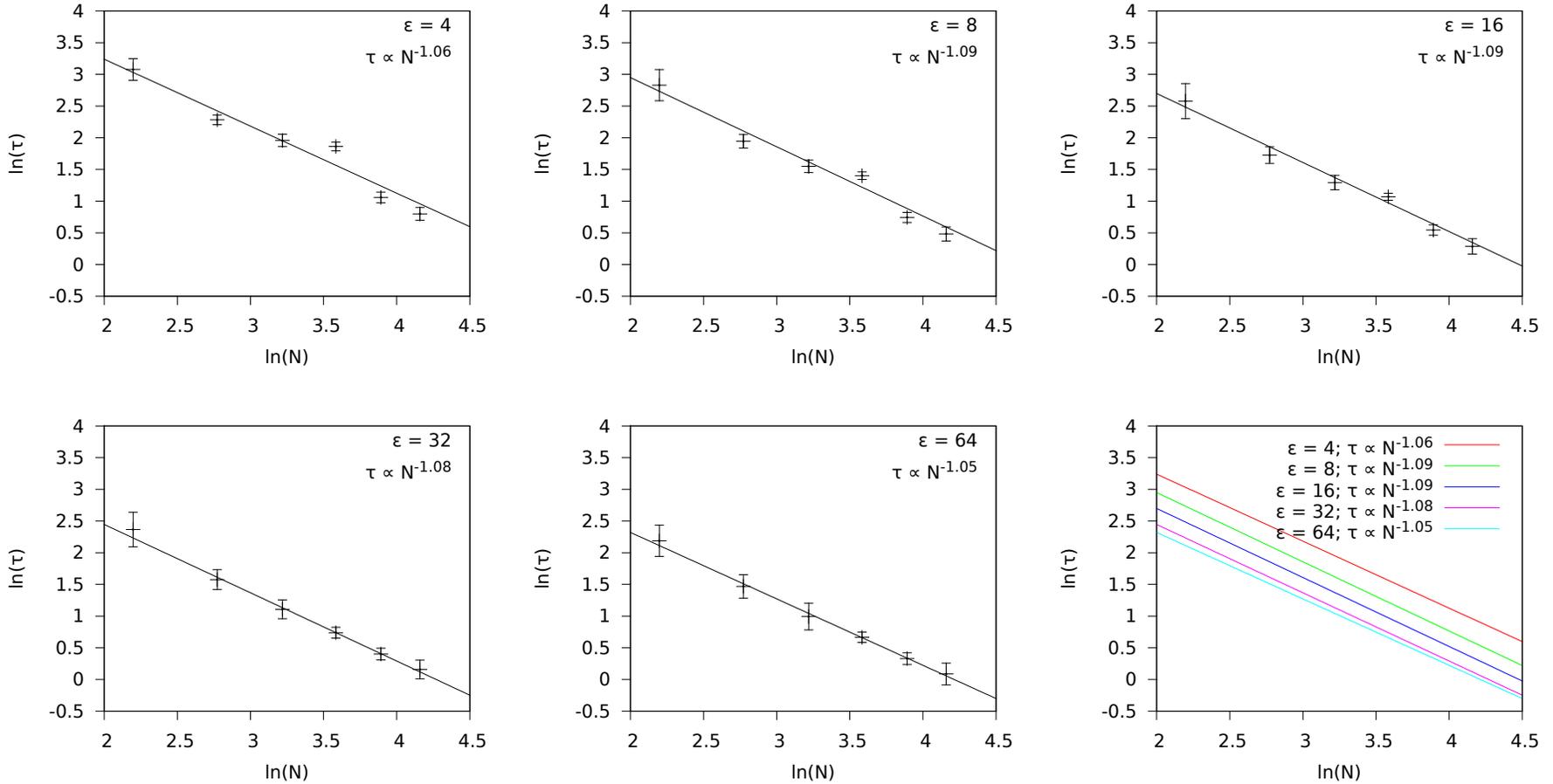
(e) Close-up on a single coarse-graining cell at the level of individual lattice points, showing the irregular nature of the underlying distribution.

(f) Effect of coarse-graining using overlapping cells, giving a smoothed distribution more suitable for visualization.

Exponential decay of the quantum H-function



Power law fit for τ vs. N



- It can be seen that for all coarse-graining lengths there is a roughly constant power law with index around -1, in contrast to theoretical predictions of -3 (Valentini) (ΔE is the energy spread of the wave function and is proportional to N^2):

$$\tau \approx \frac{\hbar^2}{\epsilon m^{\frac{1}{2}} (\Delta E)^{\frac{3}{2}}}$$

Nodes

- Divergent velocity field in the vicinity of nodes drive the relaxation process - their initial distribution is very important in determining the relaxation rate. Varying the initial phases used in the wave function will change the position of the nodes.
- In large superpositions (large N) there are many nodes and their distribution may be approximated as uniform, so the average effect is similar for different sets of initial phases. With small superposition of e.g. 4 modes, this approximation will no longer be valid; there may e.g. be only 1 node and its initial position will have a much larger effect on the subsequent relaxation (it takes a lot longer and τ has big errorbar).
- Valentini's original prediction for the dependence of the relaxation time on the number of modes (N^{-3} power law) turns out to be wrong because it assumes that the velocity field varies little over the length of a coarse-graining cell. Especially with large numbers of modes in the superposition, this is not true.
- One can justify the observed N^{-1} scaling theoretically by defining a system to have relaxed when the mean displacement of a degree of freedom is greater than its quantum spread (see derivation in Russell, Towler, Valentini paper).

Questions about nodal structure

- How many nodes are there in the 2D box? Is there a simple relationship between this and the number of modes in the superposition?
- In 2D, do the nodal points appear and disappear, or do they have a permanent existence? If not constant, what is the mean density of points in the plane?
- In 3D, do the nodal lines form loops or are they strings with ends? Can they be knotted?
- If the length in 3D varies, what is the mean length?
- How fast do the nodes move?
- Does pair-correlation for moving nodes depend on sense of vorticity of the surrounding current?

See work of Michael Berry: '*Phase singularities in isotropic random waves*'

'Phase singularities, that is, dislocations of wavefronts - also called optical vortices - are lines in space, or points in the plane, where the phase of the complex scalar wave $\Psi(\mathbf{r}, t) = \rho(\mathbf{r}, t) \exp[i\chi(\mathbf{r}, t)]$ is undefined. For the generic smooth Ψ we are interested in, dislocations are also loci of vanishing ρ : in light, they are lines of darkness; in sound, threads of silence. Interest in optical dislocations has recently revived, largely as a result of experiments with laser fields. In low-temperature physics, Ψ could represent the complex order parameter associated with quantum flux lines in a superconductor or quantized vortices in a superfluid.'

Calculates (1) mean length of dislocation line per unit volume, (2) mean density of dislocation points in the plane, (3) eccentricity of the ellipse describing the anisotropic squeezing of phase lines close to dislocation cores, (4) distribution of curvature of dislocation lines in space, (5) distribution of transverse speeds of moving dislocations, (6) position correlations of pairs of dislocations in the plane, with and without their 'topological charge'.

LOUIS: some ideas about what to do with it

Relaxation time τ

The relaxation time τ is the time over which \bar{H} decreases (recall that $\bar{H} = 0$ then ρ and $|\Psi|^2$ are the same). Predicted theoretically to be inversely proportional to both the coarse-graining length ϵ and to $\Delta E^{\frac{3}{2}}$, where ΔE is the variance of the energy. Use LOUIS to study how τ varies with the number of modes/mean energy/energy variance numerically.

Do we get scaling by a simple power of energy variance? Or of mean energy? Is there a general, fairly robust scaling law, over some broad range of conditions? Would be useful to know, e.g. in cosmology.

Phenomenological equation for \bar{H}

Previous studies have found an approximately exponential decay of \bar{H} with time. Can simulations suggest a phenomenological equation for \bar{H} analogous to the Boltzmann equation? Presumably this behaviour could be derived by supplementing the underlying dynamics with some sort of phenomenological Markovian assumption, analogous to the classical hypothesis of molecular chaos at every instant.

Nodal studies

Is there a tendency for neighbouring trajectories to diverge especially rapidly when they pass near a node. Is the number of *nodes* a better measure of the relaxation rate? There might be a simple relationship in the limit of a large number of nodes (think of the nodes moving around in the box like a gas of moving particles, except each node is like an 'electric mixer' stirring up the ρ and $|\Psi|^2$ 'fluid' densities).

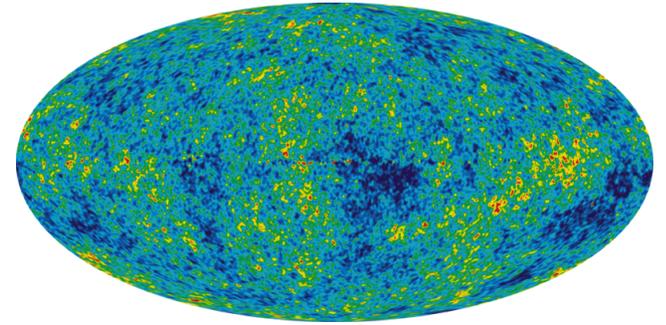
LOUIS: some more ideas about what to do with it

Effect of small perturbations

Can small perturbations drive relaxation over long timescales? E.g. take $\Psi(0)$ equal to the ground state plus excited modes with *tiny amplitude*. Then, $|\Psi|^2$ at all later times is close to the ground-state wavefunction-squared. Without the perturbations, an initial nonequilibrium ρ would remain static and always far from equilibrium. With the perturbations, can the trajectories eventually wander far enough to drive relaxation, or is the distance travelled forever too small? This would obviate the need for coarse-graining (necessary for isolated systems).

Look at expanding space

Valentini showed, for a scalar field on expanding space, relaxation to equilibrium is expected to be suppressed for a specific range of modes (long wavelength!). Possible consequence: a correction to predictions for the temperature fluctuations of the cosmic microwave background in the context of inflation theory.



Idea: generalize LOUIS so input is an initial nonequilibrium state for a given cosmology, and output is then a prediction of where nonequilibrium will be found later on. Expanding flat space is a good model of the early universe, and because of the expected asymptotic freedom all particles are effectively massless and 'relativistic' at high T , so using a free scalar field to model 'matter' isn't a bad start. One might reasonably take the initial quantum state to be a mixed thermal ensemble of wave functions (Which basis to use for decomposing the density operator? There are some proposals..). The calculation can then be run separately for each pure sub-ensemble. LOUIS does this, going through all the different pure sub-ensembles, until it finds one that doesn't relax. That would give a prediction for non-equilibrium today!

Mike's first pilot-wave theory paper

Dynamical relaxation to quantum equilibrium in de Broglie-Bohm theory

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(Dated: July 15, 2010)

Abstract

A computational approach is taken to studying pilot wave theory: a hidden variables theory that considers trajectories of non-relativistic quantum particles, and allows probability density functions that differ from the equilibrium distribution, $|\Psi|^2$. The evolution of an initially non-equilibrium distribution is calculated numerically for a particle in a two-dimensional infinite square potential well, moving under a wave function composed of a finite out-of-phase superposition of N energy eigenstates. The proximity to equilibrium is parametrised by the coarse-grained quantum H-function, \bar{H} , and in agreement with a study by Valentini and Westman, \bar{H} is found to decrease roughly exponentially, representing a relaxation to equilibrium. The timescale, τ , for this relaxation is calculated for various values of N and ε , the length scale of the coarse-graining; and its dependence on these two quantities is compared to a theoretical prediction. A power law, $\tau \propto N^{-1}$ is found to be fairly robust under different ε and a theoretical analysis is presented to explain this scaling. Although a weak dependence of τ on ε is observed, it does not appear to follow any straightforward scaling.

21st-century directions in de Broglie-Bohm theory and beyond

“A quantum foundations discussion workshop on the de Broglie-Bohm formulation of quantum mechanics and related topics is to take place in late August/early September 2010 at the Apuan Alps Centre for Physics, a 15th-century Tuscan former monastery in the mountains near the beautiful Italian city of Lucca. It is hoped that the meeting will be of great interest to anyone stimulated by the work of physicists Louis de Broglie and David Bohm, and by the directions their ideas have followed through the work of many people over more than eighty years. The meeting is being organized by Cambridge University physicist Dr. Mike Towler, who owns and runs the monastery, and Prof. Antony Valentini of Imperial College, London and Clemson University in South Carolina. In its six years of operation, the monastery has become well-known as a unique communal venue where the community spirit and magnificent location have inspired a series of memorable meetings; we very much hope this workshop will continue this tradition.”

LIST OF PARTICIPANTS (72!)

ACCEPTED INVITATION: Guido Bacciagaluppi, Herman Batelaan, Dionigi Benincasa, Andrew Bennett, Jeffrey Bub, Howard Burton, Jeremy Butterfield, Samuel Colin, Murray Daw, Chris Dewdney, Maaneli Derakhshani, Maurice de Gosson, Jonathan Halliwell, Lucien Hardy, Richard Havery, Basil Hiley, Pui Ip, Adrian Kent, Tim Maudlin, Alberto Montana, Wayne Myrvold, Hrvoje Nikolic, F. David Peat, Patrick Peter, Nelson Pinto-Neto, Paavo Pylkkänen, Peter Riggs, Simon Saunders, Maximilian Schlosshauer, Ilja Schmelzer, Lee Smolin, Rafael Sorkin, Ward Struyve, Mike Towler, Jos Uffink, Lev Vaidman, Antony Valentini, David Wallace, Georg Wikman, Howard Wiseman, James Yearsley

ACCEPTED BUT WITHDRAWN: Roger Penrose, Carlo Rovelli

NEVER INVITED AND DEFINITELY NOT COMING: Jack Sarfatti, Brian Josephson