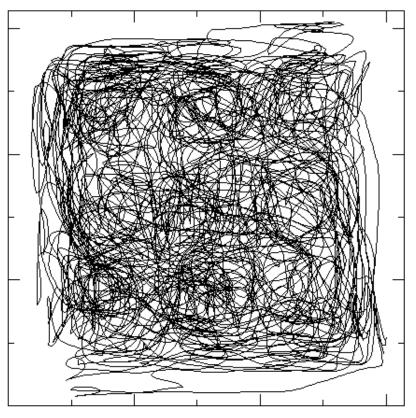
The LOUIS manual

Or, an account of how to use Mike's attempt to write an entirely new computer code that doesn't do quantum Monte Carlo

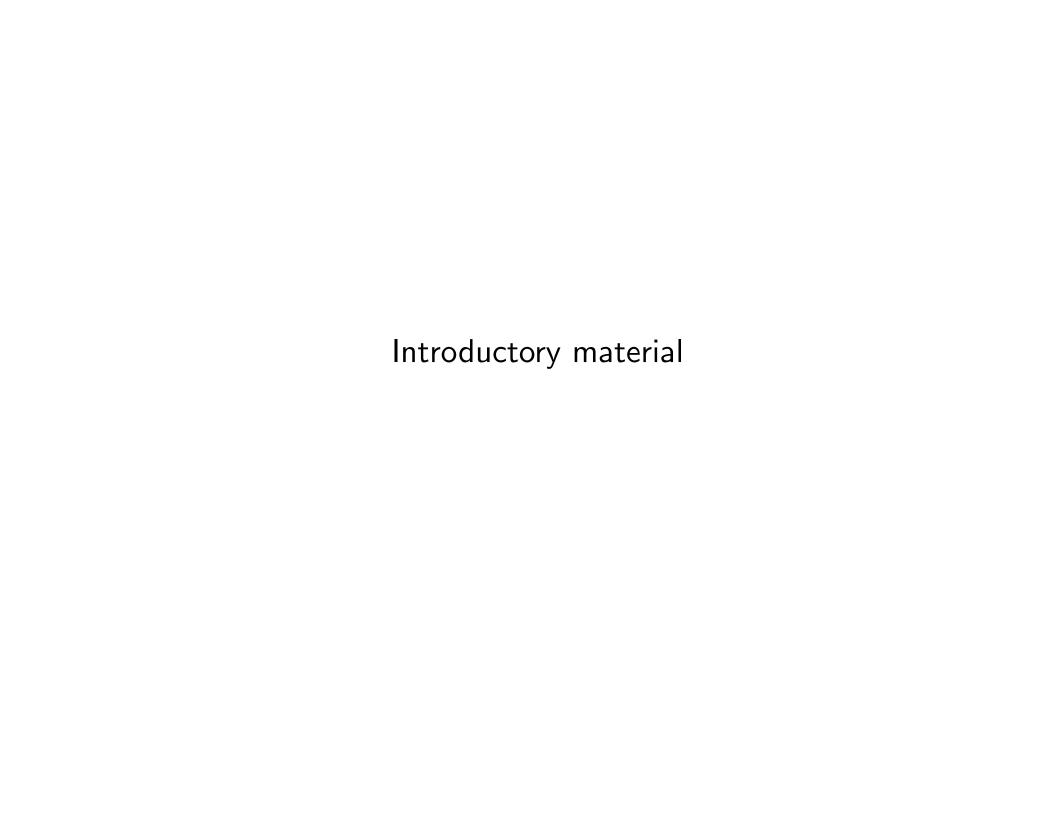
10th February 2010



Mike Towler

TCM Group, Cavendish Laboratory, University of Cambridge

 $\verb|www.tcm.phy.cam.ac.uk|/\sim mdt26 & and & \verb|www.vallico.net/tti/tti.htm||$



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 $\rho \to |\Psi|^2$ 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, $\mathrm{d}\bar{H}_{class}/\mathrm{d}t \leq 0$. 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 $d\Omega \to |\Psi|^2 d\mathbf{x}$ and ρ be the density of quantum particles.

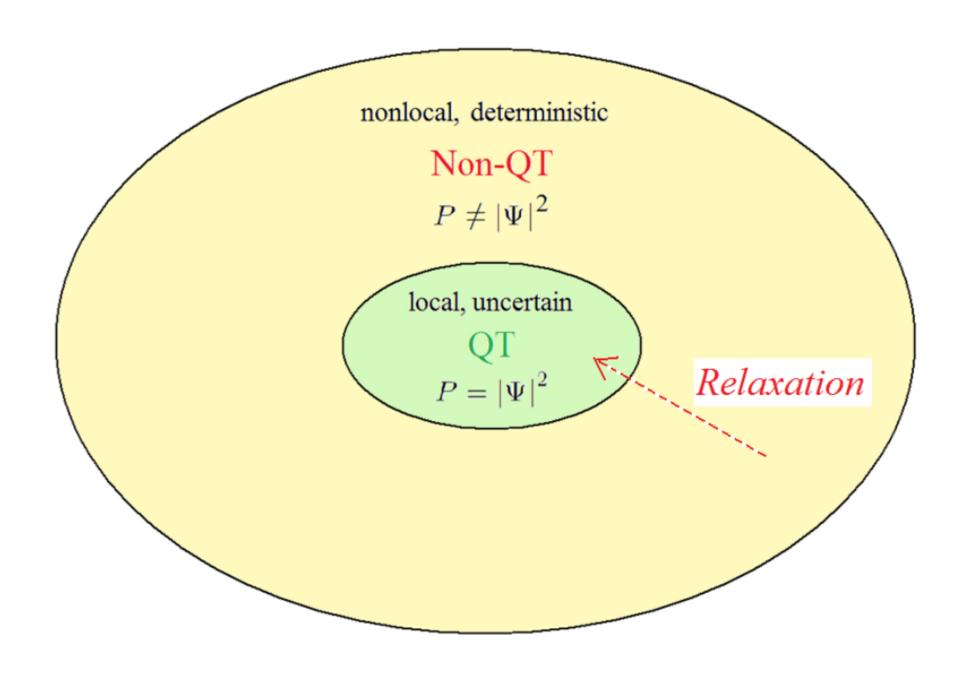
Subquantum H-theorem

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

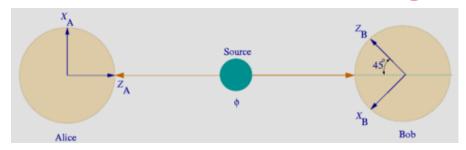
- For 'sufficiently complex' system assume have initial distribution $\rho(\mathbf{x},0)$ of configurations $\mathbf{x}(0)$ each guided by the same Ψ , with $\rho(\mathbf{x},0) \neq |\Psi(\mathbf{x},0)|^2$.
- By definition $\rho(\mathbf{x},t)$ satisfies continuity equation $\partial \rho/\partial t + \nabla \cdot (\dot{\mathbf{x}}\rho) = 0$, 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: $\mathrm{d}f/\mathrm{d}t = \partial f/\partial t + \dot{\mathbf{x}} \cdot \nabla f = 0$.
- 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. $\bar{\rho}=(1/\delta V)\int_{\delta V}\rho~\mathrm{d}\mathbf{x}$ etc.. For coarse-grained H have $\mathrm{d}\bar{H}/\mathrm{d}t\leq 0$; 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'.

Quantum theory is a special case of a much wider physics?



Possible experimental consequences: signal non-locality



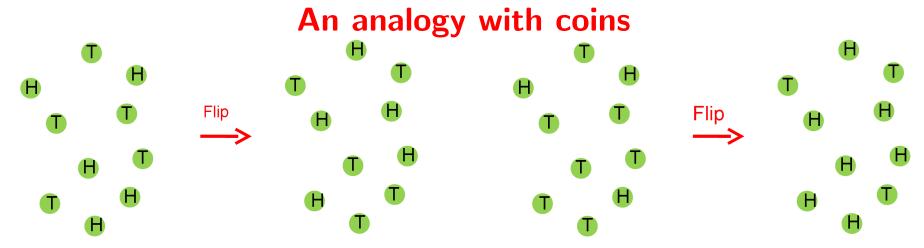
QM and experiment show violation of Bell's inequality (VBE) for events at space-like separations (implying non-locality). **How does this square with relativity?** No problem - remember, light speed is not a speed *limit*; it is the speed which remains *invariant* under certain (Lorentz) transformations of the reference frame. What constraints do VBE+QM imply? According to Maudlin, results unequivocal:

- VBE does not require superluminal matter or energy transport.
- VBE does *not* entail the possibility of superluminal signalling.
- VBE does require superluminal causal connections.
- VBE can be accomplished only if there is superluminal information transmission.

However, if you don't want to believe non-locality, what options do you have?

(1) Deny reality (then nothing can be non-local); (2) Believe many worlds interpretation (then everything happens, so you can't say there are non-local correlations); (3) Allow things to move backwards in time (Hopeless mix-up if present events depend on future and shape of future in part determined by present. Cramer's transactional interpretation not a solution.). Of all the apparent bizarrerie, believing that influences (in the above sense) travel very fast seems more appealing.

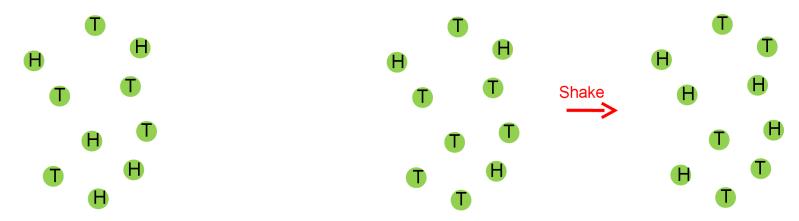
Valentini showed superluminal signalling becomes possible under conditions of *quantum non-equilibrium*, and that trajectory theories then have testable predictions: signal non-locality.



ratio of heads:tails remains 50:50

ratio of heads:tails changes from 30:70 to 70:30

Overall effect vanishes or 'cancels out' in special state where the coins have a 50:50 distribution.



Imagine further that coins are always found to have the 50:50 distribution. Why?

'Shaking' causes relaxation to an 'even' or 'equilibrium' distribution.

Similar with entanglement in quantum theory. Overall effect vanishes or 'cancels out' in the special state of 'quantum equilibrium' but not otherwise. Nonequilibrium particles could be used to send nonlocal signals, or to do 'subquantum' measurements on ordinary particles.

When did this shaking process happen? Presumably a long time ago, in the very early universe soon after the Big Bang.

Modelling the approach to equilibrium

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

In this paper, Valentini and Westman show using explicit numerical simulations that $ho \to |\Psi|^2$ 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 the 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 $d\mathbf{q}/dt = \mathrm{Im} \, \nabla \ln \Psi = \nabla S$ defines velocity field (\dot{x},\dot{y}) which determines evolution of ρ via continuity equation:

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

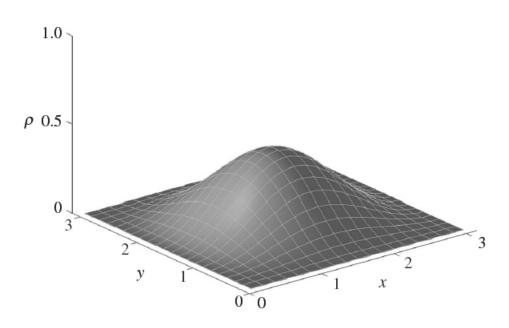
 \bullet Box has sides of length π with infinite barriers. The energy eigenfunctions are

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

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

Dynamical origin of quantum probabilities

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



 $|\psi|^2 = 0.5$ 0 y 1.0 0 3 y 1 1 x 3

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} :

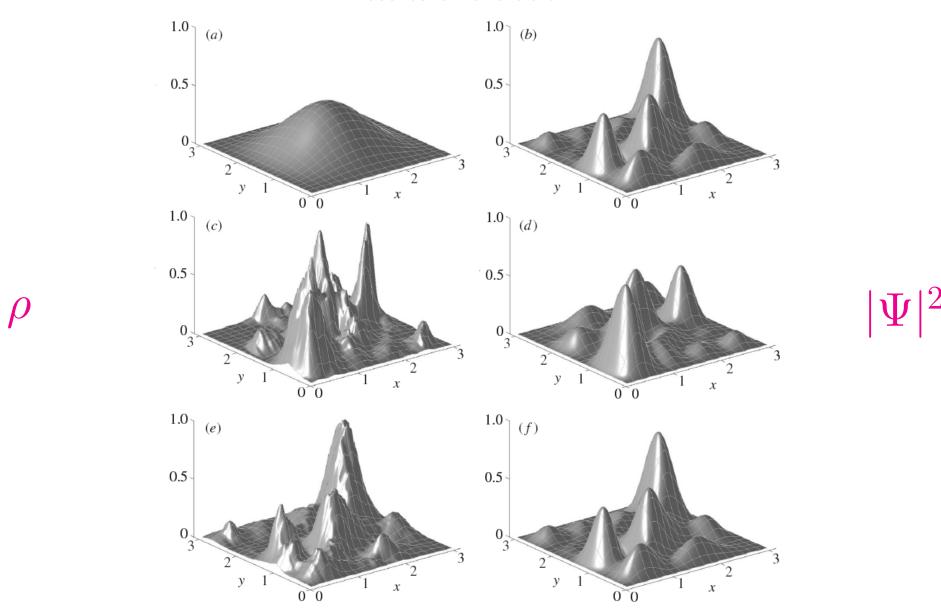
$$\Psi(x, y, 0) = \sum_{m, n=1}^{4} \frac{1}{4} \phi_{mn}(x, y) \exp(i\theta_{mn})$$

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

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

•

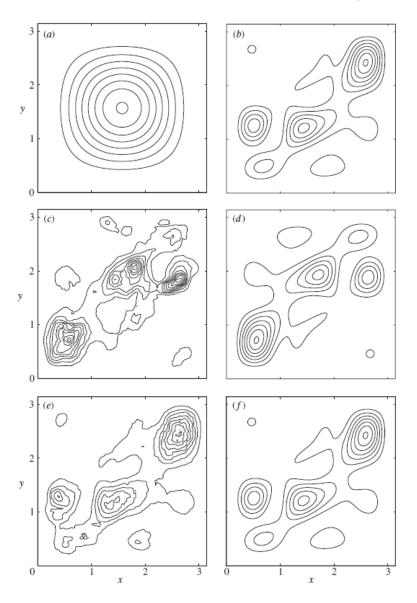
Results of evolution



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!

Results of evolution: contour plots



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.

 ρ

 $|\Psi|^2$

.

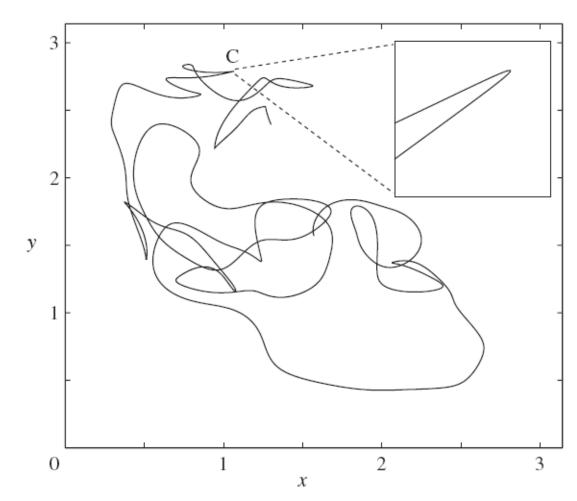
Character of the trajectories

Particle velocity components at t:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \mathrm{Im} \frac{1}{\Psi} \frac{\partial \Psi}{\partial x}$$
$$\frac{\mathrm{d}y}{\mathrm{d}t} = \mathrm{Im} \frac{1}{\Psi} \frac{\partial \Psi}{\partial y}$$

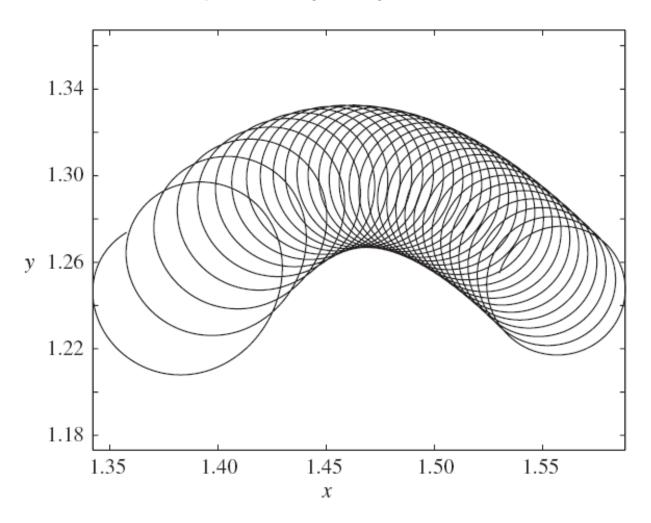
Calculate trajectory x(t), y(t) by numerical integration of above. Typical trajectory shown here - in general they are rather irregular.

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 $S = \operatorname{Im} \ln \Psi$ 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 .

Close-up of a trajectory near a node



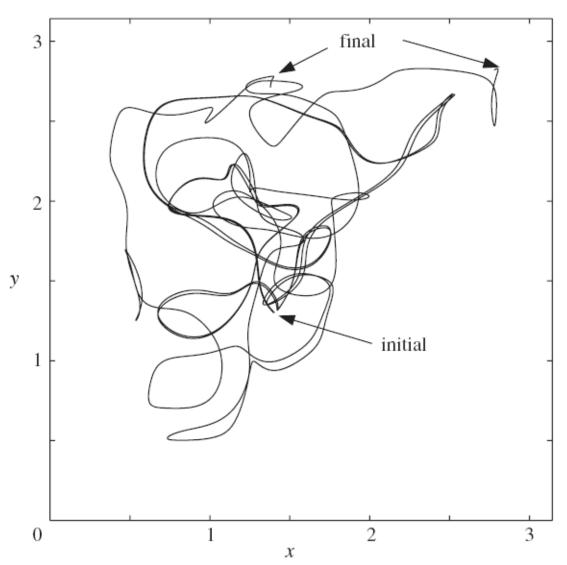
Motion rapid in regions where $|\Psi|$ is small. Above close-up of trajectory near nodal or quasi-nodal point where $|\Psi|$ very small (but not known to be strictly zero). Spatial region shown *ca.* 0.3% of whole box. Particle follows rapid circular motion around point moving from right to left - and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

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.

Additional simulations by Samuel Colin and Ward Struyve

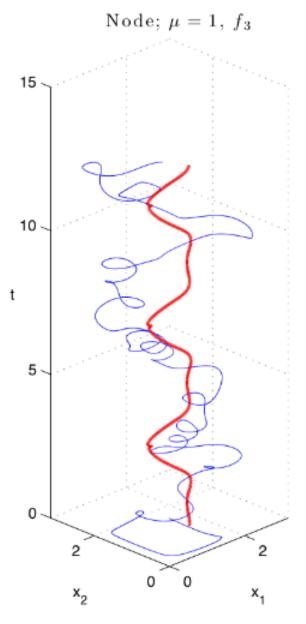
'Quantum non-equilibrium and relaxation to equilibrium for a class of de Broglie-Bohm-type theories', arXiv:0911.2823 (2009)

Repeat same 2D calculations while considering wider class of trajectory equations with alternative velocity fields which keep $|\Psi|^2$ invariant. Given $\mathbf{v} = \mathbf{j}/\rho = \nabla S/m$, can clearly add divergence-free term to current, i.e. $\mathbf{j} = \mathbf{j}_s + \mathbf{a}$ where $\nabla \cdot \mathbf{a} = 0$. Usually assumed \mathbf{a} is zero (appropriate for spinless Schrödinger particles). For particles with spin, Lorentz covariance sufficient to determine relativistic particle law of motion uniquely. Assumption that non-relativistic guidance equation is a limit of the relativistic (Dirac) one then uniquely fixes that law too:

$$\mathbf{v} = \frac{\nabla S}{m} + \frac{\nabla \log \rho \times \mathbf{s}}{m}$$
 where $\mathbf{s} = \frac{\hbar}{2} \chi^* \sigma \chi$

Spin thus a property of the wave field (the polarization-dependent part of its angular momentum) not of the particle. The spin affects the particle trajectory through a unique extra divergence-free contribution to the spin-independent Schrödinger momentum field.

- C+S found relaxation time depends substantially on form of guidance equation. In the regular Schrödinger theory the nodes are the only source of vorticity; the additional velocity field from the spin yields vorticity even away from nodes. Increased vorticity leads to greater chaotic behaviour and decreased relaxation times.
- Large percentages of trajectories could not be calculated particularly those that started near nodes. Significant loss in accuracy in computing e.g. *H* function and relaxation times.



The code - what it's supposed to do

Assume 2D for simplicity. Start with some initial non-equilibrium particle density $\rho(x_1, x_2, 0)$ and some initial non-stationary wave field $\Psi(x_1, x_2, 0)$ (i.e. its absolute square is not constant in time). Calculate (coarse-grained) particle density $\bar{\rho}(x_1, x_2, t)$ at various t and compare its shape with that of the time-dependent wave field $\Psi(x_1, x_2, t)$. Expect particles to become distributed as square of the wave function over time. Monitor this 'approach to equilibrium' by computing the H-function.

How to evaluate the time-evolved density

Since $f = \rho/|\Psi|^2$ is constant along a trajectory, one can calculate the time-evolved density as:

$$\rho(x_1, x_2, t) = |\Psi(x_1, x_2, t)|^2 f(x_1(0), x_2(0), 0)$$

For neatness, accuracy, and pretty plotting we want the density to be on a regular grid at time t which is just what it won't be if we allow the trajectories to evolve from a regular starting grid of points. We therefore use a trick: we have a regular lattice of points defined on the cell at time t. We evolve these backwards in time using the de Broglie dynamics to random positions $x_1(0), x_2(0)$ at t = 0, at which points we evaluate the f function in the above formula. Hence $\rho(x_1, x_2, t)$ on a nice lattice.

How to evaluate the trajectories

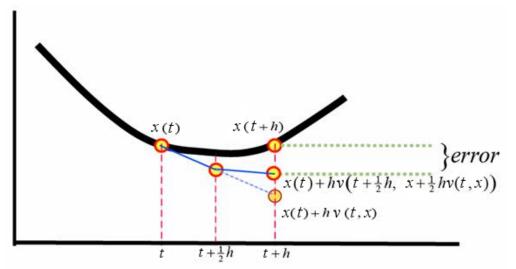
We need to integrate numerically the first-order ODE $\frac{d\mathbf{x}}{dt} = \mathbf{v} = \frac{\nabla S}{m} = \frac{1}{m} \text{Im} \frac{\nabla \Psi}{\Psi}$, that is we shall effectively do the following (though hopefully with slightly more sophistication):

$$\mathbf{x}(t + \Delta t) = \mathbf{x}(0) + \mathbf{v}\Delta t = \mathbf{x}(0) + \left(\operatorname{Im}\frac{\nabla \Psi}{\Psi}\right)\Delta t$$

Various possible algorithms e.g. Runge-Kutta, Bulirsch-Stoer, Verlet etc. Valentini *et al.* all used the *Runge-Kutta* method. We shall (at least initially) do the same.

The Runge-Kutta method applied to calculating trajectories

- Literal implementation of $\mathbf{x}(t+\Delta t) = \mathbf{x}(0) + \frac{\mathbf{d}\mathbf{x}}{\mathbf{d}t}\Delta t$ gives the not-very-practical *Euler's method*. **Runge-Kutta** is cleverer, but it still comes down to adding small increments to your function given by derivatives $(\frac{\mathbf{d}\mathbf{x}}{\mathbf{d}t} = \text{velocity }\mathbf{v} \text{ in this case})$ multiplied by stepsizes (here, in time $\Delta t = h$).
- Runge-Kutta methods propagate a solution over an interval by combining the information from several Euler-style steps (each involving one evaluation of the derivative) and then using the information obtained to match a Taylor series expansion up to some higher order. The picture shows a 2nd-order algorithm (we actually use a fancy 5th-order one).



All you need remember is the general form of a 5th-order Runge-Kutta formula:

$$k_{1} = h\mathbf{v}(t_{n}, x_{n})$$

$$k_{2} = h\mathbf{v}(t_{n} + a_{2}h, x_{n} + b_{21}k_{1})$$

$$\cdots$$

$$k_{6} = h\mathbf{v}(t_{n} + a_{6}h, x_{n} + b_{61}k_{1} + \cdots + b_{65}k_{5})$$

$$x_{n+1} = x_{n} + c_{1}k_{1} + c_{2}k_{2} + c_{3}k_{3} + c_{4}k_{4} + c_{5}k_{5} + c_{6}k_{6} + O(h^{6})$$

Cash-Karp Parameters for Embedded Runga-Kutta Method								
i	a_i	b_{ij}					c_i	c_i^*
1							$\frac{37}{378}$	$\frac{2825}{27648}$
2	$\frac{1}{5}$	$\frac{1}{5}$					0	0
3	$\frac{3}{10}$	$\frac{3}{40}$	$\frac{9}{40}$				$\frac{250}{621}$	$\frac{18575}{48384}$
4	$\frac{3}{5}$	$\frac{3}{10}$	$-\frac{9}{10}$	$\frac{6}{5}$			$\frac{125}{594}$	$\frac{13525}{55296}$
5	1	$-\frac{11}{54}$	$\frac{5}{2}$	$-\frac{70}{27}$	$\frac{35}{27}$		0	$\frac{277}{14336}$
6	$\frac{7}{8}$	$\frac{1631}{55296}$	$\frac{175}{512}$	$\frac{575}{13824}$	$\frac{44275}{110592}$	$\frac{253}{4096}$	$\frac{512}{1771}$	$\frac{1}{4}$
j =		1	2	3	4	5		

So, essentially, every time you take a little step in t you have to compute the velocity six times. To get the velocity in a certain direction x you need both Ψ and $\nabla_x \Psi$, and the velocity is a hideous expression involving the sum of (say) 16 modes each of which involves two sines and a complex exponential. We're going to spend a lot of time calculating velocities.

For reasons too boring to discuss, the estimate of the error is $\Delta = \sum_{i=1}^{6} (c_i - c_i^*) k_i$. If we can estimate the error, we can try to keep it within desired bounds. If the error is too big we repeat the step with a smaller stepsize h: adaptive stepsize control.

As a further check, after computing the **entire trajectory**, we redo it with a smaller value for the desired maximum error. If the final positions of the two trajectories differ by more than some small amount, then we redo the whole thing with an even tighter tolerance. If we reduce the maximum desired error to some crazily small value and still two successive trajectories don't end up in the same place (or we exceed a large maximum number of RK steps), then we say the trajectory has **failed** and we discount it in our calculations of densities etc.. Dr. X has a big problem with this.

The birth of LOUIS

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

Comparison with Dr. X code.

- A lot faster.
- Gives the right answer (hopefully). Has correct sign and order of indices in phases.
- To change behaviour of calculation use flexible-format 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 advanced portability (support for almost every architecture and compiler built in).
- Various modes of operation
 - single trajectory (forwards or backwards in time).
 - density
 - density + H function + relaxation time.
- Added timing routines
- Uses significantly less memory.
- Velocity formulae selectable in input (e.g. ordinary deBB or inclusion of 'spin term').
- Alternative integrator (Bulirsch-Stoer) for consistency checking (selectable in input).
- Selectable wave function types without compromising speed.
- Random phase generator.
- Built-in support for BOINC (nerd screensaver volunteer computing).
- Distribution contains script 'plot_louis' to integrate the code with GNUPLOT (for pictures and movies).

Things to do

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



LOUIS: some ideas about what to do with it (AV)

Relaxation time au

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.

(Part III student Nick Russell to do this.)

Phenomenological equation for $ar{H}$

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).

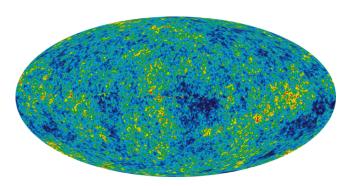
LOUIS: some more ideas about what to do with it (AV)

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!

