Pilot-wave theory, Bohmian metaphysics, and the foundations of quantum mechanics

Lecture 2

Pilot waves and the classical limit. Derivation and justification of the theory.

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Acknowledgement

The material in this lecture is largely a summary of standard works (books and articles) by Peter Holland, David Bohm, Basily Hiley, Detlef Dürr, Stefan Teufel, Antony Valentini, Sheldon Goldstein, Jeremy Butterfield, Gary Bowman, H. Nikolic, Michael Kiessling, Maurice de Gosson and possibly others. A list of works consulted in the preparation of these slides and other relevant reading material is available on the course web site.

MDT
Where we ended up last week..

Pilot-wave theory self-consistent, intuitive, agrees with all QM predictive-observational data but typical response [Encyclopedia Britannica 2007] not encouraging:

“Attempts have been made by Broglie, David Bohm, and others to construct theories based on hidden variables, but the theories are very complicated and contrived. For example, the electron would definitely have to go through only one slit in the two-slit experiment. To explain that interference occurs only when the other slit is open, it is necessary to postulate a special force on the electron which exists only when that slit is open. Such artificial additions make hidden variable theories unattractive, and there is little support for them among physicists”.

But there is hope! In fact the above misrepresents pilot-wave theory in several ways:

- Saying ‘electron [goes] through only one slit’ merely endows theory with a clear ontology (what exists?) - something missing from the standard theory - and is hardly a basis for complaint.
- Manifestly not ‘very complicated’ or ‘contrived’. Schrödinger equation is as usual. Velocity field for particle trajectories is usual probability current density vector over density. So from established mathematical ingredients of the standard theory the pilot-wave approach just tries to make sense of the orthodox talk about ‘particles’. Hardly contrived to then contemplate them having positions.
- Does not ‘postulate special force on electron which exists only when [both slits] open’ to ‘explain that interference occurs’. Just say electron guided by velocity field implicit in solution to Schrödinger’s equation. $\Psi$ develops interference only when both slits are open, with obvious consequences for how $\Psi$ guides the electron.

“If we cannot disprove Bohm, then we must agree to ignore him.” [J.R. Oppenheimer]
Today’s questions

(1) *How do we justify or even ‘derive’ pilot-wave approach mathematically?*

(2) *How is pilot-wave approach related to classical physics?*

- Unfortunate common criticism: hidden variables approaches like pilot-wave theory just *‘an attempt to return to classical physics’*. In fact it invokes a concept not anticipated in classical physics - that of a ‘state’ of a mechanical system that lies beyond the material points. Role of trajectory is to bring out this new concept so sharply that it can’t be ignored.

- This essentially non-classical programme differs from Niels Bohr who strove to leave classical concepts intact as far as possible by restricting their applicability.
The classical and quantum worlds

How does classical world emerge from quantum one?

Classical world: the world of objects of familiar experience that obey Newtonian laws.

- **Standard QM**: only wave function or results of measurements exist, so answer to question is difficult. Validity of classical concepts *presupposed*, since only in terms of these can one unambiguously communicate experimental results in quantum domain. *Correspondence principle* then demonstrates consistency of quantum theory with this presupposition.

Standard QM is not a precise microscopic theory as the division between the microscopic and macroscopic world is not made precise. Can therefore say that QM does not contain the means for describing the classical world in any approximate sense. Need to go beyond standard QM. Two possibilities known for amending QM: either wave function is not all there is (→ *hidden variables*) or Schrödinger’s equation is wrong (→ *objective collapse* - GRW etc.).

- **Pilot-wave theory**: Like classical mechanics, this is a theory about real objects and therefore we expect it can be used to formulate the problem of the classical limit within QM. Today we shall see - amongst other things - how this might be done.
The classical limit in standard QM

Correspondence principle: vague notion stating that, in effect, the behaviour of quantum systems reproduces classical physics under suitable conditions (e.g. in limit of large size or large quantum numbers or as \(\hbar \to 0\) - whatever that means).

With Schrödinger equation interpreted probabilistically, Ehrenfest showed Newton’s laws hold on average, in that the quantum statistical expectation value of position and momentum operators obey Newton’s laws (if \(V\) varies slowly over wave packet):

\[
\frac{d}{dt} \langle A \rangle = \frac{1}{i\hbar} \langle [A, H] \rangle + \langle \frac{\partial A}{\partial t} \rangle \quad \Rightarrow \quad \text{e.g.} \quad \frac{d}{dt} \langle p \rangle = \langle -\nabla V(x,t) \rangle = \langle F \rangle
\]

Which operators correspond to physical quantities or measurements? Correspondence principle limits the choices to those that reproduce CM in the limit.

As standard QM only reproduces CM statistically and because statistical interpretation only gives probabilities of different classical outcomes, Bohr argued that CM does not emerge from QM in the same way that e.g. CM emerges as approximation of special relativity at small \(v\). He argued that CM exists independently of QM and cannot be derived from it - it is inappropriate to understand observer experiences using purely QM notions like wave functions as different states of experience of an observer are defined classically and do not have a QM analog.
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:

\[ F_i(q_1, q_2, \ldots, q_N) = m_i \ddot{q}_i \]  
Newtonian mechanics

\[ \dot{q} = \frac{\partial H}{\partial p}(q, p) \quad \dot{p} = -\frac{\partial H}{\partial q}(q, p) \]  
Hamiltonian dynamics  \rightarrow  \text{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).

\[ \delta \int_{t_0}^{t_1} L(q(t), \dot{q}(t)) \, dt = 0 \]  
Lagrangian dynamics  \rightarrow  \text{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).

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

Solve a single 1st-order PDE in which the unknown function does not occur explicitly.
What have Hamilton and Jacobi got to do with Schrödinger?

Consider classical particle - the position of which is not known with certainty. We must deal with statistical ensemble in which only probability density $\rho(x, t)$ is known.

- Probability must be conserved, i.e. $\int \rho d^3x = 1$ for each $t$. Therefore must satisfy continuity equation $\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v})$ where $\mathbf{v}(x, t)$ is the velocity of the particle.

- In Hamilton-Jacobi formulation of CM, velocity given by $\mathbf{v}(x, t) = \frac{\nabla S(x, t)}{m}$ where $S(x, t)$ is a solution of the Hamilton-Jacobi equation, $-\frac{\partial S}{\partial t} = \frac{(\nabla S)^2}{2m} + V$.

- Can write the two green equations in more elegant form as single complex equation. Introduce a complex function $\Psi = \sqrt{\rho} e^{iS}$ where $\hbar$ is arbitrary constant with dimension of action so exponent is dimensionless. Then, the two equations are equivalent to

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

This is the time-dependent Schrödinger equation with extra term $Q$, and $|\psi(x, t)|^2$ has same interpretation as in QM: a probability density of particle positions.

Analogy with classical stat mech? We shall understand this in more detail presently..
Hamiltonian dynamics

Introduce *phase space* variables

\((q, p) = (q_1, \ldots, q_N, p_1, \ldots, p_N)\).

Hamiton’s evolution equations are

\[
\dot{q} = \frac{\partial H}{\partial p}(q, p) \quad \dot{p} = -\frac{\partial H}{\partial q}(q, p)
\]

with the Hamiltonian function defined as

\[
H(q, p) = \frac{1}{2} \sum_{i=1}^{N} \frac{p_i^2}{m_i} + V(q_1, \ldots, q_N).
\]

Differential equation a relation between *flow* and (time-dependent) *vector field*. Flow is the mapping along *integral curves* for vector field i.e. curves whose tangent vector (time derivative) at each point along curve is vector field itself at that point. Intuitively, integral curve traces out path in phase space that imaginary particle moving in vector field would follow. Vector field encodes the physical law.

Vector field generated by function \(H\) on phase space: \(v^H(q, p) = \left( \begin{array}{c} \frac{\partial H}{\partial p} \\ -\frac{\partial H}{\partial q} \end{array} \right)\).

Hamiltonian dynamics then given simply by \(\left( \begin{array}{c} \dot{q} \\ \dot{p} \end{array} \right) = v^H(q, p)\).

For fixed \(H\)-hypersurfaces (fixed energy, taking \(H\) time-independent), the trajectories remain within the hypersurface, in accordance with energy conservation.
Properties of Hamiltonian flow

Fundamental properties are:

1. **Conservation of energy** - the value of the Hamiltonian function does not change along trajectories.

   Implies that if Poisson bracket \( \{f, H\} = 0 \) then \( f \) is a constant of the motion (where \( f \) is any function on phase space, and \( \{f, H\} = \frac{\partial f}{\partial t} = \frac{\partial f}{\partial q} \dot{q} + \frac{\partial f}{\partial p} \dot{p} = \frac{\partial f}{\partial q} \frac{\partial H}{\partial p} - \frac{\partial f}{\partial p} \frac{\partial H}{\partial q} \)).

2. **Conservation of volume** - Flow lines have neither sources nor sinks, i.e. the vector field is divergence free (an ‘incompressible fluid’).

   Any phase space subset getting transported via Hamiltonian flow remains unchanged. This is essentially **Liouville’s theorem** - basis of classical statistical mechanics.
Analogy of mechanics and optics

Can we find an analogy of mechanics with wave optics and/or its short-wavelength limit - geometrical optics?

Geometrical optics views light as having a corpuscular nature; its propagation can be defined in terms of rays, which are the trajectories of these corpuscles. Interference and other pure wave phenomena are neglected. Involves Fermat’s extremal principle and Huygens’ principle according to which light rays/corpuscles take the path of shortest time and moreover they follow the normals of wave fronts.

Yes, we can!

- Extremal principle replacing Fermat’s is least action principle of Lagrangian dynamics.
- Equivalent of Huygens’ principle involves definition of waves which guide mechanical trajectories - leads to Hamilton-Jacobi theory.

Then natural to speculate that classical mechanics might describe the short-wavelength regime of a wave mechanics (which is just what de Broglie and Schrödinger did!).
Lagrangian dynamics

• Mechanical trajectories between \( t_0, a \) and \( t_1, b \) given by extremals of the action \( S \)

\[
S = \int_{t_0}^{t_1} L(q, \dot{q}, t) \, dt
\]

• Standard calculus of variations treatment gives 2nd-order Euler-Lagrange equations.

\[
\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0
\]

For Newtonian mechanics, Lagrangian \( L(q, \dot{q}) = \frac{1}{2} \dot{q} \cdot m \dot{q} - V(q) \) which yields the Newtonian equations as Euler-Lagrange equations.

• Lagrange function and Hamiltonian function are Legendre transforms of one another (essentially reparametrizing a function in terms of its slope). Replace \((q, p)\) by \((q, \dot{q})\) using the implicitly-given function \( \dot{q} = \frac{\partial H(q, p)}{\partial p} \) where the equation is solved by \( p \) as a function of \( \dot{q} \), i.e. \( H(q_i, p_i, t) = \sum_i p_i \dot{q}_i - L(q_i, \dot{q}_i, t) \).
Hamilton-Jacobi theory

“Don’t worry, young man: in mathematics, none of us really understands any idea - we just get used to them”

John von Neumann, after explaining (no doubt very quickly!) the method of characteristics (i.e. Hamilton-Jacobi theory) to a young physicist, as a way to solve his problem; to which the physicist had replied: “Thank you very much; but I’m afraid I still don’t understand this method.”

\[-\frac{\partial S}{\partial t} = H \left( q, \frac{\partial S}{\partial q}, t \right) = \frac{(\nabla S)^2}{2m} + V\]

In mechanics, HJT represents particle motion as a wave motion.

• Is action $S$ in Lagrange formulation same as $S$ (‘Hamilton’s principal function’) in the Hamilton-Jacobi equation?

Nearly. $S$ is related to the usual action $S$ by fixing initial time $t_1$ and endpoint $q_1$ and allowing upper limits $t_2$ and second endpoint $q_2$ to vary; these variables are the arguments of the $S$ function. In other words, Hamilton’s principal function $S$ is indefinite integral of the Lagrangian with respect to time. The action $S$ is a particular definite integral for fixed endpoints.
Properties of the $S$ field
From the calculus of variations to the Hamilton-Jacobi equation

We will no longer consider just a single line integral $\int L \, dt$, but a whole field of solutions i.e. line integrals along all curves of a space-filling congruence, defined thus:

- Define family of hypersurfaces $S(q_i, t) = \sigma$ covering region of interest (i.e. single unique hypersurface runs through each point). $S$ is twice continuously differentiable.

- Define family of curves $C$ given by $q_i = q_i(t)$ that intersect each hypersurface once (and are nowhere tangent to them). Then $\sigma$ is function of $t$ along $C$, and

\[
\Delta = \frac{d\sigma}{dt} = \sum_i \frac{\partial S}{\partial q_i} \dot{q}_i + \frac{\partial S}{\partial t} \quad (\Delta \neq 0).
\]

- Tangential displacement along $C$ from $(q_i, t)$ to $(q_i + dq_i, t + dt)$ induces an increment $d\sigma$ in $\sigma$, and an increment $dI = L(q_i, \dot{q}_i, t)dt$ in $I = \int L \, dt$.

- Now connect to calculus of variations: what curve $\dot{q}_i$ makes $dI/d\sigma$ a minimum? (for fixed $d\sigma$). Given $dI/d\sigma = L/\Delta$, we require

\[
\frac{\partial}{\partial \dot{q}_i} \left( \frac{dI}{d\sigma} \right) = 0, \quad i = 1, \ldots, n \quad \Rightarrow \quad \frac{\partial L}{\partial \dot{q}_i} = \frac{L}{\Delta} \frac{\partial S}{\partial q_i}
\]

- Curve satisfying above RHS is the one you want. Such a curve said to be in the direction of the geodesic gradient determined by the family of surfaces.
Properties of the $S$ field II

From the calculus of variations to the Hamilton-Jacobi equation

• Extra condition on surfaces implies minima of $dI/d\sigma$ defined by geodesic gradient equation below are also minima of $dI/dt$ i.e. extremals of the variational problem.

$$\frac{\partial L}{\partial \dot{q}_i} = \frac{L}{\Delta} \frac{\partial S}{\partial q_i}$$

• Two equivalent forms of this condition (recall $\Delta = d\sigma/dt$):
  
  (i) $L/\Delta = dI/d\sigma$ is constant on each surface, or
  
  (ii) $S$ solves the Hamilton-Jacobi equation (see next slide).

• Condition (i) implies we can reparametrize the family of surfaces such that $L = \Delta$ everywhere, in which case

  (iii) the geodesic gradient now given by $\partial L/\partial \dot{q}_i = p_i = \partial S/\partial q_i$, and

  (iv) Each point has unique curve passing through it (set of curves = ‘congruence’).

  (v) increment $dI$ in $\int L\,dt$ along curve of the family obeys $dI = L\,dt = \Delta\,dt = d\sigma$.

• Integral of $dI$ along curve from any point $P_1$ on surface $S(q_i, t) = \sigma_1$ to a point $P_2$ on same curve on $S(q_i, t) = \sigma_2$ is same for any $P_1$ i.e. $\int_{P_1}^{P_2} L\,dt = \int_{P_1}^{P_2} dS = \sigma_2 - \sigma_1$. 
Properties of the $S$ field III

From the calculus of variations to the Hamilton-Jacobi equation

$L = \Delta$ and the definition of $\Delta$ as a total derivative give

$$L(q_i, \dot{q}_i, t) = \Delta = \frac{d\sigma}{dt} = \sum_i \frac{\partial S}{\partial q_i} \dot{q}_i + \frac{\partial S}{\partial t},$$

where $\dot{q}_i$ refers to direction of geodesic gradient, i.e. $\dot{q}_i = \dot{q}_i(q_i, \partial S/\partial q_i, t)$. Thus

$$-\frac{\partial S}{\partial t} = \sum_i \frac{\partial S}{\partial q_i}(q_i, \partial S/\partial q_i, t) - L(q_i, \dot{q}_i(q_i, \partial S/\partial q_i, t), t)$$

RHS Legendre transform of Lagrangian i.e. Hamiltonian (with $p_i$ replaced by $\partial S/\partial q_i$)

$$\frac{\partial S}{\partial t} + H(q_i, \frac{\partial S}{\partial q_i}, t) = 0 \quad \text{Hamilton-Jacobi equation}$$

Connection with mechanics

The isosurfaces of the function $S(q_i, t)$ can be determined at any time $t$. The motion of an $S$-isosurface as a function of time is defined by the motions of the particles beginning at the points $q_i$ on the isosurface. The motion of such an isosurface can be thought of as a wave moving through $q$ space.
Hamilton-Jacobi theory and the calculus of variations

Choose region small enough so there is unique extremal curve \( C \) between any two points. Value of fundamental integral along \( C \) is well-defined fn. of endpoint coords.

\[
S(q_1,t_1; q_2,t_2) = \int_{t_1}^{t_2} L\ dt = \int_{t_1}^{t_2} \left( \sum_i p_i \dot{q}_i - H \right)\ dt = \int_{t_1}^{t_2} \left( \sum_i p_i dq_i - H dt \right)
\]

Make small arbitrary displacements at each endpoint. Using fact that integral is along an extremal, the variation in \( S \) is

\[
\delta S = \frac{\partial S}{\partial t_1} \delta t_1 + \frac{\partial S}{\partial t_2} \delta t_2 + \sum_i \frac{\partial S}{\partial q_{1i}} \delta q_{1i} + \sum_i \frac{\partial S}{\partial q_{2i}} \delta q_{2i} = \left[ \sum_i p_i \delta q_i - H(q_j, p_j, t) \delta t \right]_{t_1}^{t_2}
\]

Independent displacements \( \implies \) can identify coeffs on both sides \( \implies \) HJ equation:

\[
\frac{\partial S}{\partial t_2} = -\left[ H(q_i, p_i, t) \right]_{t=t_2}, \quad \frac{\partial S}{\partial q_{2i}} = [p_i]_{t=t_2}
\]

\[
\frac{\partial S}{\partial t_1} = [H(q_i, p_i, t)]_{t=t_1}, \quad \frac{\partial S}{\partial q_{1i}} = -[p_i]_{t=t_1}
\]

Interesting! If know \( S \) can get all extremals (possible motions) of the system without solving any differential equations (no integrations just differentiation and elimination).
Hamilton-Jacobi theory and canonical transformations

HJ theory normally presented as follows, rather than via calculus of variations

• In Hamiltonian formulation of CM, can replace \( q_i, p_i \) by new set of \( 2n \) independent variables \( Q_i, P_i \) - with new Hamiltonian \( K(Q, P, t) \) - through coordinate transformation in phase space. New set of coords is canonical if Hamilton’s equations retain their form under the transformation i.e. \( \dot{Q}_i = \frac{\partial K}{\partial P_i} \) and \( \dot{P}_i = -\frac{\partial K}{\partial Q_i} \).

• Both sets of variables must obey Hamilton’s principle

\[
\delta \int_{t_0}^{t_1} \left[ p_i \dot{q}_i - H(q, p, t) \right] dt = 0 \quad \delta \int_{t_0}^{t_1} \left[ P_i \dot{Q}_i - K(Q, P, t) \right] dt = 0
\]

where integrands differ by a total time derivative \( \frac{dF}{dt} \) of a ‘generating function’ (doesn’t affect location of extremals). Implies transformation equations:

\[
\frac{dF}{dt} = \frac{\partial F}{\partial t} + \frac{\partial F}{\partial q} \dot{q} + \frac{\partial F}{\partial Q} \dot{Q} \quad \implies \quad p_i = \frac{\partial F}{\partial q_i}, \quad P_i = -\frac{\partial F}{\partial Q_i}, \quad K = H + \frac{\partial F}{\partial t}
\]

• Turns out \( S \) is generating function of canonical transformation which makes new Hamiltonian \( K \) zero. Problem of motion solved since new coords constant along a trajectory. \( K = 0 \) if \( F \) satisfies \( H(q, p, t) + \frac{\partial F}{\partial t} = 0 \) i.e. it satisfies HJ equation:

\[
\frac{\partial S(q, Q, t)}{\partial t} + H \left( q, \frac{\partial S(q, Q, t)}{\partial q}, t \right) = 0
\]
Hamilton-Jacobi theory and the theory of characteristics

Characteristics of first-order PDE \( x \frac{\partial u}{\partial x} - 2y \frac{\partial u}{\partial y} = 0 \). Shaded region shows where solution to equation defined, given an imposed boundary condition at \( x = 1 \) between \( y = 0 \) and \( y = 1 \), shown as a bold vertical line.

If the boundary curve crosses any characteristics more than once then this can overdetermine the problem solution and generally results in there being no solution.

- The method of characteristics is a technique for solving PDEs. Idea is to reduce a PDE to a family of ODEs along which the solution can be integrated from some initial data given on a suitable hypersurface.

- For a first-order PDE, the method of characteristics defines curves (called characteristics) along which the PDE becomes an ODE. Once the ODE is found, it can be solved along the characteristic curves and transformed into a solution for the original PDE.

- In the case of classical mechanics, the mechanical paths are the characteristics of the Cauchy problem associated with the Hamilton-Jacobi equation. The \( S \) function generates a canonical transformation to coordinates and momenta that are constant along a trajectory. This establishes an equivalence between the \( 2n \) 1st-order Hamilton ODEs and the single 1st-order Hamilton-Jacobi PDE.
An example mechanical problem and the nonuniqueness of $S$

- Solution is complete integral of HJ 1st-order PDE (depends on $n$ constants $\alpha_i$). Such solutions not unique (different functional dependence of $S$ on $q_i, t, \alpha_i$). Extra set of constants $\beta_i$ implied by transformation equation for $P_i$ (recall $P_i = -\partial S/\partial Q_i$).
- $S$ connected with infinite set of potential trajectories pursued by ensemble of identical particles. Get this set by varying the constants $\beta_i$ for fixed $\alpha_i$.

**Example**: single free particle (for which HJ eqn is $\partial S/\partial t + (\nabla S)^2/2m = 0$)

**Solve by separation of variables**:

$$S(x, y, z, P_1, P_2, P_3, t) = \frac{1}{2m}(P_1^2 + P_2^2 + P_3^2)t + P_1x + P_2y + P_3z$$

- $\alpha_i$ is initial momentum vector $P_i$
- Trajectory $\partial S/\partial P_i = Q_i \Rightarrow$ uniform motion $-(P/m)t + x = Q$ or $x(t) = x_0 + vt$ starting at $x_0$, velocity $v$
- Ensemble: vary $x_0 \Rightarrow$ plane wave $S$

**Solve by integrating $L$ along trajectory**:

$$S(x, t; x_0, 0) = \frac{m}{2t}(x - x_0)^2$$

- $\alpha_i$ is initial position vector $x_{0i}$
- Trajectory $\partial S/\partial x_{0i} = -P_i \Rightarrow$ uniform motion $-m(x - x_0)/t = -P$ or $x(t) = x_0 + vt$ from $x_0$, range of momenta $P$
- Ensemble: vary $P \Rightarrow$ spherical $S$

Propagation of plane and spherical HJ wave surfaces which have common tangent at one point $x_0$. Both functions imply same motion for particle starting from $x_0$ with momentum $P$. Trajectory with momentum $P'$ generated by spherical wave but not plane wave.
Story so far

- Problem of dynamics as defined by Hamilton’s equations can be formulated in terms of a partial differential equation determining the evolution of a field $S(q, t)$.

- The role of the function $S(q, t)$ is to generate a (momentum) vector field on configuration space through the relation $p_i = \partial S/\partial q_i$. Integral curves along the field are possible trajectories of the $N$-particle system. For one body the basic law of motion is $\dot{x} = \nabla S/m$.

- $S$ is thus connected with an ensemble of identical systems rather than a single trajectory as in Lagrangian theory. It is in this way that the $S$ functions may be physically distinguished.

- For fixed $q_0, p_0$ all $S$ functions imply the same time development $q(t)$. This reflects the fact that the state of a material system is completely exhausted by specifying its position and momentum - the $S$ function plays no role in either defining the state or in determining the dynamics.
Analogy with optics

- Properties of $S$ only capture some of the features of genuine wave motion. Propagation of $S$ proceeds according to laws of geometrical optics; trajectory corresponds to a *light ray* and the Hamilton-Jacobi equation is the *eikonal equation*. However, any counterpart of principle of linear superposition is absent. Connection between canonical extremals and geodesically equidistant hypersurfaces underpins fact that both corpuscular and wave conceptions of light can account for the phenomena (reflection and refraction) described by geometric optics.

- **Huygens’ principle**: Consider characteristic function $S$ to define family of geodesic hyperspheres $S(q_1, t_1; q_2, t_2) = \sigma$ with fixed centre $P_1 = (q_1, t_1)$. Let $h_1, h_2$ be two hypersurfaces corresponding to constant values $\sigma_1, \sigma_2$ of $S$. Let $P_1$ be in $h_1$, and the canonical extremal $C$ through $P_1$ intersect $h_2$ in $P_2$ (which is in the geodesic sphere centred on $P_1$ with radius $\sigma_2 - \sigma_1$). Huygens’ principle then states the obvious that $h_2$ is the *envelope* of the set of geodesic spheres of radius $\sigma_2 - \sigma_1$ with centres on the surface $h_1$.

- **Fermat's principle**: states (roughly speaking) that a light ray between spatial points $P_1$ and $P_2$ travels by the path that makes stationary the time taken. Obvious consequence of Hamilton-Jacobi.
A heuristic derivation of the Schrödinger equation

De Broglie and Schrödinger proposed that $S$ represented a property of an individual system - not an ensemble of systems each fully described by its classical state $(q, p)$.

• Apply HJ theory to classical mechanical system. $S$ function defines for each time $t$ surfaces of constant $S$ in configuration space. By varying $t$ can calculate speed $u$ with which these ‘wave fronts’ propagate: $S(x, t) = c \rightarrow S(x, t + dt) = c$.

• With arbitrary $dx$ and $dt$ the $S$ function changes by $dS$ which we set to zero:

$$dS = \nabla S \cdot dx + \frac{\partial S}{\partial t} dt = |\nabla S| n \cdot dx + \frac{\partial S}{\partial t} dt = 0$$

Here $n = \nabla S/|\nabla S|$ is the unit vector perpendicular to surface $S = c$ at point $x$, and $n \cdot dx = ds$ is the component of $dx$ lying along normal to surface. Thus wave front speed at point $x$ is $u(x, t) = ds/dt = -(\partial S/\partial t)/|\nabla S|$ This implies relation between wave and particle velocities (since vector $|\nabla S|$ characterizes both).

• Use conservative system with energy $E$. Can integrate HJ equation $\partial S/\partial t + E = 0$ to give $S(x, E, t) = S^*(x, E) - Et$ where $S^*$ - called Hamilton’s characteristic function - is just the initial $S$ function. Then, since $p_i = \partial S^*/\partial q_i$, the wave speed is

$$u = \frac{E}{|\nabla S^*|} = \frac{E}{p}$$
A heuristic derivation of the Schrödinger equation II

• Now postulate that wave fronts are surfaces of constant phase of suitable time-dependent complex-valued function $\psi$ on the configuration space:

$$\psi = R(q_i, t) \exp (-2\pi i[\nu t - \phi(q_i)]) = R(q_i, t) \exp \left\{ \frac{i}{\hbar} [S^*(q_i) - Et] \right\}$$

with $R$ and $\phi$ real. Then $\nu t - \phi$ is the phase, and (apart from possible $t$-dependence of $R$) $\nu$ is the frequency associated with $\psi$.

• Then postulate there is some constant $\hbar$ (with $\hbar = h/2\pi$) such that $h [\nu t - \phi(q_i)] = Et - S^*(q_i)$. This must hold for all $q_i, t$ and so $E = h\nu$ and $S^*(q_i) = h\phi(q_i)$. Furthermore, $u = \lambda\nu = \frac{E}{p} \implies \lambda = \frac{h}{p}$.

• For $R$ indept of $q$; differentiation of $\psi$ wrt $q_i$ gives eigenvalue equation $\frac{\partial \psi}{\partial q_i} = \frac{i}{\hbar} \frac{\partial S^*}{\partial q_i} \psi$ (recalling $p_i = \partial S^*/\partial q_i$) $\implies$ association of operator $\hat{p}_i = \frac{\hbar}{i} \frac{\partial}{\partial q_i}$ with momentum. For $q_i$-dept $R$ postulate association of operator $\hat{H} = H(q_i, \hat{p}_i, t)$ with system energy.

• For $R$ indept of $t$; differentiation of $\psi$ wrt $t$ gives eigenvalue equation $i\hbar \frac{\partial \psi}{\partial t} = E\psi \implies$ association of operator $\hat{E} = i\hbar \frac{\partial}{\partial t}$ with system energy.

• If use postulated operators for general $R(q_i, t)$ (with $\hbar =$ Planck’s constant) we get:

Schrödinger equation $\hat{H}\psi = i\hbar \frac{\partial \psi}{\partial t}$
The quantum Hamilton-Jacobi equation

Substitute amplitude-phase decomposition (polar form) of the complex time-dependent wave function \( \Psi(x, t) = R(x, t) \exp(iS(x, t)/\hbar) \) into the time-dependent Schrödinger equation. Separate real and imaginary parts to get two coupled evolution equations, i.e., the continuity equation for \( \rho = R^2 \):

\[
\frac{\partial R^2}{\partial t} + \nabla \cdot \left( \frac{R^2 \nabla S}{m} \right) = 0
\]

and a modified (quantum) Hamilton-Jacobi equation for \( S \):

\[
-\frac{\partial S}{\partial t} = \frac{(\nabla S)^2}{2m} + V + Q
\]

where

\[
Q = -\frac{\hbar^2}{2m} \frac{\nabla^2 R}{R}.
\]

- Phase of quantum-mechanical wave function \( \Psi \) and Hamilton’s principal function \( S \) from classical mechanics obey same eqn in limit of vanishing quantum potential \( Q \).
- Postulate that not only is \( \Psi \) an objectively existing physical field but \( S \)-function is elevated from a passive to an active role.

\textbf{CM}: particle dynamics \( \implies \) evolution of field \( S \) in configuration space.

\textbf{QM}: Field dynamics of \( S \) (and other coupled fields) in configuration space \( \implies \) particle dynamics.
Pilot-wave theory: wave particle duality

• New conception of matter through synthesis of wave and particle characteristics. Matter has intrinsic field aspect, with mass points moving/interacting under influence of a new kind of ‘internal energy’ as well as the more familiar potentials of classical dynamics. ‘Internal potential’ is organizational or self-referential form of energy which brings about ‘inner tension’ in material system to which the mass points respond.

• Unlike classical physics local motion of a given particle depends on the quantum state of the entire system. This potentially introduces nonlocal effects. Wave function on configuration space binds the whole of reality into an ‘Undivided Wholeness in Flowing Movement’ (Bohm).

• Statistical predictions of QM are restated in terms of the deterministic motion of a particle whose initial position is statistically distributed, this ensemble distribution being in turn determined by $\psi$. This way, the mean values of quantum-mechanical observables are identified with the average values of a statistical ensemble of particles.
Pilot-wave theory: the dynamics of particles

• Postulate *phase of wave function* as generator of trajectories of particles through \( p = \nabla S \). Solution thus requires specifications of initial positions. Gives single valued trajectory field (‘congruence’) for particles.

• Additional postulate cannot be derived from wave function, but this is expected. Cannot logically deduce model of substantial matter and its motion from algorithm which has no such concepts at all (i.e. makes no statements as to what matter is.).

• Deduce postulate reasonable because (1) velocity field is just usual probability current density vector over density i.e. particles follow stream lines of probability flow (hydrodynamic analogy) so it is already in the theory, (2) analogy with classical Hamilton-Jacobi theory, (3) it agrees with experiment, (4) symmetry considerations [J. Stat. Phys. 67, 843 (1992) p.852]. Basically if particles exist and \( \Psi^2 \) is their time-dependent probability distribution then this *is what they would do by definition*.

• Probability given by \( R^2 \). Now means probability that the particle is at a precise location at time \( t \), rather than probability of finding it there in a suitable measurement. Justified since particles not so distributed become so under pilot-wave evolution.

• \( R \) (amplitude of physically real field \( \psi \)) gives probability amplitude, and hence \( R^2 \) gives the particle distribution in the sense of statistical ensembles. Continuity equation involving \( R \) is statement of conservation of probability flow.
De Broglie formulation (1927)

In nonrelativistic quantum theory of system of \( N \) particles with positions \( x_i(i = 1, \ldots, N) \) it is now generally agreed that, with appropriate initial conditions, quantum physics may be accounted for by deterministic dynamics defined by two differential equations, the Schrödinger equation:

\[
i\hbar \frac{\partial \Psi}{\partial t} = \sum_{i=1}^{N} -\frac{\hbar^2}{2m_i} \nabla_i^2 \Psi + V \Psi
\]

for a ‘pilot wave’ \( \Psi(x_1, x_2, \ldots, x_N, t) \) in configuration space, and the de Broglie guidance equation

\[
m_i \frac{dx_i}{dt} = \nabla_i S
\]

for particles trajectories \( x_i(t) \). Phase \( S(x_1, x_2, \ldots, x_N, t) \) defined by \( S = \hbar \text{Im} \ln \Psi \) of wave function in complex polar form \( \Psi = |\Psi| \exp[iS/\hbar] \). Easy to show \( \nabla S \) is equivalent to probability current \( j \) over \( |\Psi|^2 \). The particles are thus ‘pushed along’ by the wave along trajectories perpendicular to surfaces of constant phase.
Bohm’s pseudo-Newtonian reformulation (1952)

Bohm’s 1952 presentation: take first time derivative of guidance equation $m\ddot{x} = \nabla S$
then use TDSE to get second-order theory analagous to Newton’s second law:

$$\frac{\partial}{\partial t} \nabla_i S(x, t) = \nabla_i \frac{\partial}{\partial t} \hbar \Im \ln \Psi = \nabla_i \Im \left[ \frac{\hbar}{\Psi} \frac{\partial}{\partial t} \Psi \right] =$$

$$\nabla_i \Im \left[ \frac{i}{\Psi} \left( \frac{\hbar^2}{2m_i} \nabla_i^2 \Psi - V\Psi \right) \right] = -\nabla_i \left[ \frac{1}{\Psi} \left( -\frac{\hbar^2}{2m_i} \nabla_i^2 \Psi + V\Psi \right) \right] = -\nabla_i [V + Q]$$

$$\implies m_i \dddot{x}_i = -\nabla_i (V + Q) \text{ where quantum potential } Q = -\sum_i \frac{\hbar^2}{2m_i} \frac{\nabla_i^2 |\Psi|^2}{|\Psi|}.$$  

May give casual readers impression that Bohm trying to derive quantum mechanics from Newtonian point mechanics by postulating new special forces derived from new potential, the quantum potential. Not so of course but people often confused by this.

Presence of $Q$ (or, equivalently, ‘pushing’ by pilot wave) radically modifies trajectory obtained with usual $V$, e.g. particle can be accelerated even if $V = 0$. Conversely $Q$ may cancel $V$, yielding no acceleration even if expected on classical grounds.
Where is the classical limit?

- Conceptually, 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. How does state or context dependence characteristic of quantum domain turn into state independence at classical level? When do the trajectories look Newtonian? Compare quantum and classical HJ equations:

\[ -\frac{\partial S}{\partial t} = \frac{(\nabla S)^2}{2m} + V - \frac{\hbar^2}{2m} \nabla^2 R \quad \text{vs.} \quad -\frac{\partial S_{cl}}{\partial t} = \frac{(\nabla S_{cl})^2}{2m} + V \]

- Require \( Q = 0 \) to get classical dynamics exactly. Since force on particle depends on gradient of \( Q \) - recall \( m_i \ddot{x}_i = -\nabla_i (V + Q) \) - we also require \( F_Q = -\nabla Q = 0 \).

- However classical limit is more subtle than this: \( Q \) is not a physical parameter but, through \( R \), a state-dependent function. Though limits like \( m \rightarrow \infty \) or \( \hbar \rightarrow 0 \) may be required to satisfy \( Q \rightarrow 0 \), these will be in addition to a proper choice of state.

- Problem is that as the classical world is approached, we do not know the physical criteria that will unambiguously make the quantum potential vanish and lead to classical trajectories, irrespective of how the classical limit is defined.
Comparison of classical and quantum trajectories

Central point: Behaviour of pure-state ensemble of pilot-wave trajectories is fundamentally different from that of an ensemble of classical trajectories.

- If two classical trajectories ever have identical $x$ and $p$, then they must always have identical $x$ and $p$; they must be the same trajectory.

- Different classical trajectories can share the same $x$ at some time, and therefore they can cross in configuration space. A unique trajectory is defined only when a point in phase space is specified.

Consider ensemble of pilot-wave trajectories described by pure quantum state $\psi$. Momenta from $p = \nabla S$ and $S$ determined by $\psi$.

- Since $S$ is single-valued function of $x$, specification of $x$ (and the time) uniquely determines $p$ for each trajectory in the ensemble. If at any time two trajectories share same $x$, must also share same $p$ and must therefore be same trajectory. Pure state pilot-wave trajectories cannot cross in configuration space, nor can they cross nodal lines (zeroes of complex $\psi$) or surfaces (zeroes of real $\psi$).

- This is an additional difficulty in obtaining classical dynamics from pilot-wave dynamics. Note that if you use mixed states then the trajectories can cross in configuration space, but then this no longer describes an individual system.
Einstein’s critique

“I have written a little nursery song about physics, which has startled Bohm and de Broglie a little. It is meant to demonstrate the indispensability of your statistical interpretation of quantum mechanics."

[Einstein, letter to Max Born (1953)]

Sphere of mass $m$, diameter 1mm, constant $E$, trapped between perfectly reflecting walls 1m apart. Usual particle-in-a-box stationary state $\psi_n(x, t) = (2/a)^{1/2} \sin(k_n x)e^{iE_nt/\hbar}$ should represent possible description of physical state in ‘macroscopic limit’ of this function ($x$ being COM coordinate).

**Objection to standard QM:** In limit - if $\psi$ all there is - particle not assigned definite properties like quasi-localization round a point, which it obviously has independently of measurement or observers.

*Quite true:* Cannot deduce classical theory of matter from a statistical theory of observation i.e. from any solution of Schrödinger equation in any limit, even well-localized ones (packets) that approximately remain so over time. Must supplement pure theory of linear fields by physical postulate (like in pilot-wave theory) or can’t claim material object at definite $x$ independent of measurement as in CM.

**Objection to Bohm/de Broglie:** In macrolimit should recover classical motion from guidance equation yet $v = 0$ always true independently of quantum number. Thus pilot-wave treatment of individual process cannot be accurate description of reality, hence QM must refer to ensembles.

*Not true:* Assuming CM emerges in pilot-wave macro-limit for all valid QM states is wrong - good example! Ensemble interpretation not same as CM: in macro-limit $\psi_n$ many static nodes where $x$-measurement never finds particle - no classical to-and-fro uniform motion. Einstein implies QM fails not particular interpretation! How static pilot-wave result compatible with $p$ measurement? If not watching particle move, $t \to \infty$ time-of-flight gives classical $p$ (Lecture 1). If particle really moving $\psi$ is wave packet (continually spreads then reforms) and pilot-wave trajectory approaches classical limit.
Is $Q \to 0$, $F_Q \to 0$ a good correspondence principle?

1. **Free particle motion in $x$ direction**: Consider free-particle momentum eigenstate $\psi^+ = A \exp i(kx - Et/\hbar)$. Corresponds to ensemble of free-particle trajectories with identical momenta $\hbar k$, and with initial positions uniformly distributed from $x = -\infty$ to $x = +\infty$. Both $Q$ and $F_Q$ vanish so pilot-wave trajectories classical.

2. **Free particle motion in $x$ and $-x$ directions**: How to obtain ensemble of particles uniformly distributed along $x$-axis with equal weighting of momenta $+\hbar k$ and $-\hbar k$? Try superposing $\psi^+$ and $\psi^- = A \exp i(-kx - Et/\hbar)$. Get $\psi = B \cos(kx)e^{-iEt/\hbar}$ which has $\nabla S = 0$ so every pilot-wave trajectory is motionless! Thus zero $Q$ and $F_Q$ not sufficient for realization of classical limit in pilot-wave theory.

3. **Coherent states in the 1-D quantum harmonic oscillator**: Probability distribution is Gaussian of constant width (like the $n = 0$ state) whose peak follows the classical trajectory.

$$Q = -\frac{m\omega^2}{2}(x - a \cos(\omega t))^2 + \frac{\hbar \omega}{2} \quad \text{and} \quad F_Q = m\omega^2(x - a \cos(\omega t))$$

No trajectory can satisfy both $Q = 0$ and $F_Q = 0$. However, since pilot-wave trajectories are ‘dragged along’ by the wave packet, we can still claim that this is a classical state - a claim not now based on satisfaction of conditions on $Q$ and $F_Q$ but only on narrowness of the state and fact that peak follows classical trajectory.
Narrow packets

• Isolated particle ‘in wave packet’ of usual form for solving Schrödinger equation with $V = 0$:

$$
\psi(x, t) = \int e^{i(k \cdot x - \omega(k) t)} \hat{f}_{k_0}(k) \, d^3k \quad \text{with} \quad \omega(k) = \frac{\hbar k^2}{2m}
$$

Group velocity $(\partial \omega / \partial k)(k_0) = \hbar k_0 / m$. Dispersion relation ensures wave spreads linearly with $t$ (can show larger mass implies smaller spreading rate).

• Consider packet over short enough $t$ so spreading negligible. Watch evolution of particle position $X(t) = \hbar/m \text{Im} \nabla \text{ln} \psi[X(x, t), t]$ as it moves with evolving packet. QEH/equivariance $\Rightarrow$ average $\langle X \rangle^\psi(t) = \int X(x, t)|\psi(x, 0)|^2 \, d^3x = \int x|\psi(x, t)|^2 \, d^3x$. Intuitively, non-spreading Schrödinger wave should move classically, and indeed:

$$
\frac{d}{dt}\langle X \rangle(t) = \int x \frac{\partial}{\partial t}|\psi(x, t)|^2 \, d^3x = -\int x \nabla \cdot J(x, t) \, d^3x = \int J(x, t) \, d^3x = \langle v(X(x, t)) \rangle
$$

Second derivative gives Newton’s equations in the mean - a version of *Ehrenfest’s theorem*:

$$
\frac{d^2}{dt^2}\langle X \rangle(t) = \int \left( \frac{\partial}{\partial t} J(x, t) \right) \, d^3x = \frac{1}{m} \langle -\nabla V(X) \rangle(t)
$$

For classical limit require $\langle -\nabla V(X) \rangle(t) = \nabla V(\langle X \rangle)(t)$ ie. want well-localized wave $\psi(x, t)$ with $\text{Var}(X) = \langle (X - \langle X \rangle)^2 \rangle \approx 0$. Can show width of $\Psi$ should obey $\text{Var}(X) \ll \sqrt{\frac{V'}{V \cdot m}}$.

• Effect of spreading in fact countered by interactions with environment (‘decoherence’ - Lecture 4). Packet remains localized due to effective collapse. *Decoherence* thus makes pilot-wave trajectory approximately classical. At this level argument dodgy but more rigorous maths possible.
Wide packets

Narrow packet evolution one way to do classical limit - if move classically then trajectories, being dragged along, do so too. More general answer from opposite: freely moving wave packet that spreads - $\psi$ scaled to be macroscopic in time and space. Dispersion produces ‘local plane waves’ that don’t interfere because of decoherence (each gets multiplied by wave function for environment). Left with one such wave guiding particle along classical trajectory. [Maths in Dürr and Teufel, Section 9.4].

Final remarks on classical limit

- Classical and quantum worlds connected in pilot-wave theory by virtue of an unambiguous relation between primitive notions of ‘state’ in the two theories. The quantum state is defined by $\psi(x, t)$ and $x(t)$ which evolve as a unit in a deterministic manner. When the former has no influence on the latter the classical and quantum states coincide.

- For most practical purposes, can say as follows: pilot-wave evolution approximately classical when relevant de Broglie wave length much smaller than scale on which potential energy varies. Under normal circumstances this is satisfied for center of mass motion of macroscopic object. Good criterion since relates property of state to property of dynamics. Note deviations from Newtonian behaviour unobservable on classical scale perfectly acceptable within classical limit argument.

- Three levels - (1) quantum trajectories, (2) classical trajectories, (3) what one sees (measures). These are non-overlapping sets! Not all valid quantum states have a classical limit. Not all classical trajectories give rise to what one sees. What one sees not necessarily what is happening. Sigh.

- Formal arguments about classical limit turn out to be subtle and difficult (analagous to studying deviations from thermodynamic behaviour of large but finite system about which not much is known). More rigorous mathematical results welcome.
Further reading

Interesting relevant material beyond the level of this course:

Articles


- ‘Quantum back-reaction and the particle law of motion’, P.R. Holland (2006)

Books


Links to the articles are provided on the course website.
Some quotes from Newton’s *Opticks* (first published 1704)

Newton’s corpuscular theory says that light corpuscles (‘Rays’) generate ‘Waves or Vibrations’ in an ‘Aethereal Medium’, like a stone thrown into water generates water waves. In addition, supposed that waves in turn affect motion of the corpuscles which ‘may be alternately accelerated and retarded by the Vibrations’.

In particular he thought that effect of medium on motion of corpuscles was responsible for interference and diffraction:

> “And doth not the gradual condensation of this Medium extend to some distance from the Bodies, and thereby cause the Inflexions of the Rays of Light, which pass by the edges of dense Bodies, at some distance from the Bodies?”

i.e. for diffraction to occur, motion of corpuscles must be affected at a distance by the diffracting body. Also, to account for coloured fringes in diffraction of white light by opaque bodies (Grimaldi), corpuscles would have to execute an oscillatory motion:

> “Are not the Rays of Light in passing by the edges of and sides of Bodies, bent several times backwards and forwards, with a motion like that of an Eel? And do not the three Fringes of colour’d Light above mention’d arise from three such bendings?”

> ‘Science still awaits the mathematical theory of the eel.’ (David Park book 1997)
**Rest of course**

Lecture 1: 21st January 2009
*An introduction to pilot-wave theory*

Lecture 2: 28th January 2009
*Pilot waves and the classical limit. Derivation and justification of the theory*

Lecture 3: 4th February 2009
*Elementary wave mechanics and pilot waves, with nice examples*

Lecture 4: 11th February 2009
*The theory of measurement and the origin of randomness*

Lecture 5: 18th February 2009
*Nonlocality, relativistic spacetime, and quantum equilibrium*

Lecture 6: 25th February 2009
*Calculating things with quantum trajectories*

Lecture 7: 4th March 2009
*Not even wrong. Why does nobody like pilot-wave theory?*

Lecture 8: 11th March 2009
*Bohmian metaphysics : the implicate order and other arcana*

Followed by a GENERAL DISCUSSION.

Slides/references on web site: [www.tcm.phy.cam.ac.uk/~mdt26/pilot_waves.html](http://www.tcm.phy.cam.ac.uk/~mdt26/pilot_waves.html)