# Hamilton Jacobi Theory as an arena to study the conceptual problems surrounding the quantum state

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# Key message

"If we look into Hamilton Jacobi theory closely, we will gain certain insights about the conceptual problems surrounding the quantum state."

# Structure

- Introducing Hamilton Jacobi Theory
- S, Psi and configuration space
- Operators, expectation values, eigenvalue equations

# Preliminaries

- Hamilton's principle is restricted to motion between fixed end-points

$$\mathcal{S} = \int_{q_1,t_1}^{q_2,t_2} \mathcal{L}(q, \dot{q}, t) dt$$

- Hamilton wanted a way to write down a theory that is free from this restriction of fixed end-points

# Hamilton-Jacobi Theory

- Hamilton-Jacobi Equation:

$$\frac{\partial \mathcal{S}}{\partial t} + \mathcal{H} = 0 \qquad \mathcal{H} = \mathcal{T} + V = \frac{1}{2m}\left(\frac{\partial \mathcal{S}}{\partial q_i}\right)^2 + V(q_i)$$

i = 1,2,…n, where n = # degrees of freedom

# Jacobi's procedure

$$\frac{\partial \mathcal{S}}{\partial t} + \mathcal{H} = 0$$

1. Solve for S (Any will do)
2. Define Integration constants as $a_i$
3. Define another set of constants by:

$$\frac{\partial \mathcal{S}}{\partial a_i} = b_i$$

4. Rearrange $\dfrac{\partial \mathcal{S}}{\partial a_i} = b_i$ to get exact motion

5. Find momentum by $\dfrac{\partial \mathcal{S}}{\partial q_i} = p_i$

# Free Particle 1

$$\frac{\partial \mathcal{S}}{\partial t} + \frac{1}{2m}\left(\frac{\partial \mathcal{S}}{\partial q}\right)^2 = 0$$

- Complete integral $\mathcal{S}(q,k,t) = \sqrt{2mk}q - kt + const$
- Equation of motion $\frac{\partial \mathcal{S}}{\partial k} = \sqrt{\frac{m}{2k}}q - t = \beta$

$$q = \sqrt{\frac{2E}{m}}(\beta + t)$$

- Constant momentum $\frac{\partial \mathcal{S}}{\partial q} = \sqrt{2mE} = p$

$$q = \sqrt{\frac{2mE}{m^2}}(\beta + t) = \frac{p}{m}(\beta + t) = vt + q_0$$

# Free Particle 2

- Another solution $$\mathcal{S}(q,t;q_0,0) = \frac{m}{2t}(q-q_0)^2$$

- Equation of motion $$\frac{\partial \mathcal{S}}{\partial q_0} = -\beta = -m\frac{q-q_0}{t}$$

$$q = q_0 + \frac{\beta}{m}t$$

- Momentum $$\frac{\partial \mathcal{S}}{\partial q} = p = m \times \frac{(q-q_0)}{t-0}$$

$$q = q_0 + vt$$

# Important points

- We have solution to the dynamical problem without the restriction of fixed initial conditions
- HJ procedure turns a purely mathematical problem (solving a PDE) into a useful physical theory

# S in configuration space

- S in general function of configuration space
- Claim: S suffers similar problem as the wavefunction
- Premise 1: S ‘lives’ and ‘evolves’ in configuration space
- Premise 2: S is involved in the physical law and the determination of relevant physical quantities
- Therefore S must be in some sense a real entity

# Caveat

- The physical effect of S can’t be ‘observed’ as in the wavefunction (cf double slit)
- There can be multiple solutions of S to the HJ equation
- -> this argument do not intend to argue that the metaphysical status of S must be the same as the quantum state

# Important message

- But this argument does intend to argue the following:

"the conceptual difficulty surrounding the wavefunction being a function on the configuration space arises due to its theoretical role as the entity that is determined by the physical law of the theory. It is a consequence of this role that forces us to consider the reality of the wavefunction seriously. This is also the reason why even though Hamilton Jacobi theory is thoroughly classical, a similar conceptual difficulty can arise for the S function. If it were relegated to a less important role, this conceptual difficulties will at least be less severe."

- Introducing Hamilton Jacobi Theory
- Configuration Space realism
- Operators, expectation values, eigenvalue equations

# Schrodinger’s first communication

Quantisation as a Problem of Proper Values (Part I)

(*Annalen der Physik* (4), vol. 79, 1926)

# Schrödinger's first communication

Here we now put for $S$ a new unknown $\psi$ such that it will appear as a *product* of related functions of the single co-ordinates, *i.e.* we put

(2) $$S = K \log \psi.$$

The constant $K$ must be introduced from considerations of dimensions; it has those of *action*. Hence we get

(1′) $$H\left(q, \frac{K}{\psi}\frac{\partial \psi}{\partial q}\right) = E.$$

this holds even when mass-variation is not neglected.) We now seek a function $\psi$, such that for any arbitrary variation of it the integral of the said quadratic form, taken over the whole co-ordinate space,[1] is stationary, $\psi$ being everywhere real, single-valued, finite, and continuously differentiable up to the second order. *The quantum conditions are replaced by this variation problem.*

Our variation problem then reads

(3) $$\delta J = \delta \iiint dx\, dy\, dz \left[ \left(\frac{\partial \psi}{\partial x}\right)^2 + \left(\frac{\partial \psi}{\partial y}\right)^2 + \left(\frac{\partial \psi}{\partial z}\right)^2 - \frac{2m}{K^2}\left(E + \frac{e^2}{r}\right)\psi^2 \right] = 0,$$

# Crucial relation

- $S = K \log \psi.$ is crucial to understand `operators', 'expectation values', 'eigenvalue equations'

$$\frac{\partial \mathcal{S}}{\partial q_i} = \frac{K}{\psi}\frac{\partial \psi}{\partial q_i}, \qquad \frac{\partial \mathcal{S}}{\partial t} = \frac{K}{\psi}\frac{\partial \psi}{\partial t}$$

$$\frac{\partial \psi}{\partial q_i} = \frac{\psi}{K}\frac{\partial \mathcal{S}}{\partial q_i}, \qquad \frac{\partial \psi}{\partial t} = \frac{\psi}{K}\frac{\partial \mathcal{S}}{\partial t}$$

# Key quantities

- To form statistical averages using HJ theory

$$d_{pi} = \rho \times p_i = \rho \left( \frac{\partial \mathcal{S}}{\partial q_i} \right) = \rho \left( \frac{K}{\psi} \frac{\partial \psi}{\partial q_i} \right)$$

$$\langle p_i \rangle = \iiint dx dy dz d_{pi} = \iiint dx dy dz \left( \rho \left( \frac{K}{\psi} \frac{\partial \psi}{\partial q_i} \right) \right)$$

# What happens if…

$$K = -i\hbar \qquad \rho = |\psi|^2$$

- Momentum density

$$d_{pi} = \rho\left(-\frac{i\hbar}{\psi}\frac{\partial\psi}{\partial q_i}\right) = \psi^*\left(-i\hbar\frac{\partial}{\partial q_i}\right)\psi = \psi^*\hat{p}\psi$$

- Momentum average

$$\langle p_i\rangle = \iiint dxdydz(d_{pi}) = \iiint dxdydz\left(\psi^*\left(-i\hbar\frac{\partial}{\partial q_i}\right)\psi\right) = \iiint dxdydz\,(\psi^*\hat{p}_i\psi)$$

- Momentum eigenvalue equation

$$p = \frac{\partial S}{\partial q_i} = \frac{i\hbar}{\psi}\frac{\partial\psi}{\partial q_i} \Rightarrow \hat{p}\psi = p\psi$$

# Variational integral

$$\delta\langle\mathcal{H}-E\rangle=0\Rightarrow\delta\iiint\rho(\mathcal{H}-E)dxdydz=0$$

- Substitute the right expressions

$$\delta\iiint dxdydz\rho\left(\frac{1}{2m}\left[\left(\frac{\partial\mathcal{S}}{\partial x}\right)^2+\left(\frac{\partial\mathcal{S}}{\partial y}\right)^2+\left(\frac{\partial\mathcal{S}}{\partial z}\right)^2\right]+V-E\right)=0$$

- Use the relation between S and ψ: Schroedinger's integral!

$$\delta J=\delta\iiint dxdydz\left[\left(\frac{\partial\psi}{\partial x}\right)^2+\left(\frac{\partial\psi}{\partial y}\right)^2+\left(\frac{\partial\psi}{\partial z}\right)^2-\frac{2m}{K^2}\left(E+\frac{e^2}{r}\right)\psi^2\right]=0$$

# What is this all about?

- A cheat

-> ψ complex, S real and so not in 1-to-1 relation with S

# Lessons

- Momentum ‘operators’ and ‘expectation values’ and eigenvalue equation not arbitrary, but related to HJ theory
- The Schrödinger equation is the condition for the variational integral to obtain a stationary value. This variational integral has an obvious interpretation: in the case of a minimum, the Schrödinger equation and the boundary conditions together ensures that the average difference between the Hamiltonian and the energy is at a minimum for the physical system.

# Conclusion