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Action $S \lessgtr \hbar$. $[\hat{x},\, \hat{p}] = \mathrm{i}\hbar$. Classical analogue $[x,\, p]_{\mathrm{PB}} = 0$. Almost any statement you make quantum mechanically has a classical analogue.

Bohr's model of hydrogen atom

Hypotheses

1. atoms can only assume discrete energy levels E_n, $n = 1, 2, 3, \ldots$
2. in allowed states, atoms do not radiate.
3. radiation during transitions $\hbar\omega = E_n - E_m$.

Circumference $S/\lambda = n$.

More generally

$$\int \frac{\mathrm{d}s}{\lambda} = n$$

De Broglie's relation $p = h/\lambda$.

$$\frac{1}{h}\int p\,\mathrm{d}s = n$$

For a circle, $\mathrm{d}s = r\,\mathrm{d}\varphi$:

$$\frac{2\pi}{h} p_\varphi = n$$

$$\boxed{p_\varphi = n\,\hbar}$$

Pauli tried to do this in his Ph.D. thesis to the hydrogen molecular ion, and it came out all wrong. He found it to be unstable, and it is known to exist. Here we worked with a periodic path, and for most systems there are no periodic paths. The connection between classical and quantum mechanics is the phase.

Schrödinger equation for a free particle

$$\mathrm{i}\hbar\frac{\partial\Psi}{\mathrm{d}t} = -\frac{\hbar^2}{2m}\,\partial_x^2\Psi, \quad \hat{H} = \frac{\hat{p}^2}{2m}, \quad \hat{p} = \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}$$

Plane waves:

$$\Psi(x,t) \propto \mathrm{e}^{\mathrm{i}(kx - \omega t)}$$

$p = \hbar\,k = h/\lambda$.

Dispersion:

$$\hbar\omega = \frac{\hbar^2 k^2}{2\,m} = E = \frac{p^2}{2\,m}$$

$$\Psi(x,t) = A\exp\left\{\frac{\mathrm{i}}{\hbar}R\right\}$$

$$R = p\,x - E\,t = \int_0^t \mathrm{d}t'\left(p\frac{\mathrm{d}x}{\mathrm{d}t'} - H\right) = \int_0^t \mathrm{d}t'\,L(x,\dot{x}), \quad \dot{x} = \frac{\mathrm{d}x}{\mathrm{d}t'}$$

R is Hamilton's principal function.

Classical trajectories obey extremum principle $\delta R = 0$. Euler 1744.

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{x}}\right) - \frac{\partial L}{\partial x} = 0$$

The correspondence principle? $\Psi(x,t) = A\,\mathrm{e}^{\mathrm{i}R/\hbar}$. We want to determine the velocity with which this wave moves. Phase velocity

$$v_{\mathrm{ph}} = \frac{\omega}{k} = \frac{\hbar\,\omega}{\hbar\,k} = \frac{\frac{1}{2}\,m\,v^2}{m\,v} = \frac{v}{2}$$

Group velocity:

$$v_{\mathrm{gr}} = \frac{\mathrm{d}\omega}{\mathrm{d}k} = v$$

This does give rise to the classical velocity. Why is this the right thing to calculate? A plane wave is not what we want to consider when taking the classical limit, because it is not localised. We want to consider a wave packet:

$$\Psi(x,t) = \int \mathrm{d}k\,A(k)\,\mathrm{e}^{\mathrm{i}R/\hbar}$$

Assume that $A(k)$ is a slowly varying function, with a maximum at k_0. The condition for constructive interference:

$$0 \approx \frac{\mathrm{d}R}{\mathrm{d}k}$$

$$R = p\,x - E\,t = \hbar\,k\,x - \hbar\,\omega\,t$$

$$\left.\frac{\mathrm{d}R}{\mathrm{d}k}\right|_{k_0} = \hbar\left.\left(x - \frac{\mathrm{d}\omega}{\mathrm{d}k}\,t\right)\right|_{k_0}$$

$$v = \frac{x}{t} = \frac{\mathrm{d}\omega}{\mathrm{d}k}$$

Separation of variables:

$$\Psi(x,t) = \psi(x)\,\mathrm{e}^{-\mathrm{i}Et/\hbar}$$

$$\mathrm{i}\hbar\,\frac{\partial\Psi}{\partial t} = E\,\Psi$$

$$-\frac{\hbar^2}{2\,m}\,\frac{\partial^2}{\partial x^2}\psi(x) = E\,\psi(x)$$

We wrote $\Psi(x,t) = A\,\mathrm{e}^{\mathrm{i}R/\hbar}$. Then we known

$$\psi(x) = A\,\mathrm{e}^{-\mathrm{i}S/\hbar}, \quad \text{where } S = R + E\,t$$

S is called the Maupertuis action.

$$R = \int_0^t \mathrm{d}t'\,(p\dot{x} - H\,)$$

$$S = \int_0^t \mathrm{d}t'\,p\,\dot{x} = \int_{x_{\mathrm{init}}}^{x_{\mathrm{final}}} \mathrm{d}x\,p$$

$$H = \frac{p^2}{2\,m} + V(x) = E \quad \Rightarrow \quad p(x) = \sqrt{2\,m\,(E - V(x))}$$

$$S = \int_{x_{\mathrm{init}}}^{x_{\mathrm{final}}} \mathrm{d}x'\,\sqrt{2\,m\,(E - V(x))}$$

The classical trajectories are given by $\delta S = 0$. $\delta R = 0$ gives the path a particle takes in a given time. $\delta S = 0$ gives the path a particle takes at a given energy. This is closely related to Fermat's principle in Optics:

$$\delta \int_{\text{path}} \mathrm{d}s\, n(x) = 0$$

What you should know about classical mechanics (look it up, if you have to)

• Lagrangian mechanics is determined from the Lagrange function $L = T - V$. You calculate an action R from it

$$R = \int_0^t \mathrm{d}t'\, L(x, \dot{x}, t) = R(x_{\text{init}}, x_{\text{final}}, t)$$

and the path is determined by $\delta R = 0$.

$$\frac{\partial R}{\partial x} = p, \quad \frac{\partial R}{\partial x_0} = -\, p_0, \quad \frac{\partial R}{\partial t} = -\, E$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} = 0$$

• Hamiltonian mechanics (where L does not depend explicitly on t)

$$H(x, p) = -\, L(x, \dot{x}) + \dot{x} p, \quad p = \frac{\partial L}{\partial \dot{x}}$$

$$\mathrm{d}H = \frac{\partial H}{\partial x}\,\mathrm{d}x + \frac{\partial H}{\partial p}\,\mathrm{d}p = \dot{x}\;\mathrm{d}p + p\,\mathrm{d}\dot{x} - \frac{\partial L}{\partial x}\,\mathrm{d}x - \frac{\partial L}{\partial \dot{x}}\,\mathrm{d}\dot{x}$$

$$\frac{\partial H}{\partial p} = \dot{x}, \quad \frac{\partial H}{\partial x} = -\, \dot{p}$$

These are Hamilton's equations. $H = T + V = \frac{p^2}{2\,m} + V(x)$.

$$\frac{p}{m} = \dot{x}, \quad \dot{p} = -\, \frac{\partial V}{\partial x}$$

• Hamilton-Jacobi $E = H(x, p)$. A partial differential equation for R:

$$H\left(x, \frac{\partial R}{\partial x}\right) + \frac{\partial R}{\partial t} = 0$$