Phys 503

Lectures 24-25

Hamilton-Jacobi theory

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Geometric optics approximation to quantum mechanics

Particle in 3-d: $\psi(\vec{x},t)$ satisfying $-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}$

If $V=0$, there are plane-wave solutions

$$\psi_{\vec{p}}(\vec{x},t) \propto \exp\left(\frac{i}{\hbar}(\vec{p}\cdot\vec{x} - Et)\right), \quad E = \frac{p^2}{2m}$$

$$\frac{S}{\hbar} = \frac{1}{\hbar}(\vec{p}\cdot\vec{x} - Et) = \vec{k}\cdot\vec{x} - \omega t = \begin{pmatrix}\text{phase of}\\ \text{wave function}\end{pmatrix}$$

Picture ←

$$k = \frac{p}{\hbar} = (\text{wave number})$$

$$\omega = \frac{E}{\hbar} = (\text{angular frequency}) = \frac{\hbar k^2}{2m}$$

$$\lambda\!\!\!^{-} = \frac{1}{k} = \frac{\hbar}{k} = (\text{reduced wavelength}) = \frac{\lambda}{2\pi}$$

$$\nabla S = \vec{p} \quad \text{and} \quad \frac{\partial S}{\partial t} = -E$$

$$S = \underbrace{\int (\vec{p}\cdot d\vec{x} - E\,dt)}_{\substack{\text{line integral of}\\ \text{4-d gradient}}} = \begin{pmatrix}\text{indefinite}\\ \text{action}\end{pmatrix}$$

$V \neq 0$: $\psi(\vec{x},t) = R(\vec{x},t)\exp\left(\frac{i}{\hbar}S(\vec{x},t)\right)$

$$P(\vec{x},t)\,d^3x = |\psi(\vec{x},t)|^2\,d^3x = R^2(\vec{x},t)\,d^3x = \begin{pmatrix}\text{probability to}\\ \text{find particle}\\ \text{in } d^3x\end{pmatrix}$$

$$\frac{S(\vec{x},t)}{\hbar} = (\text{phase of wave function})$$

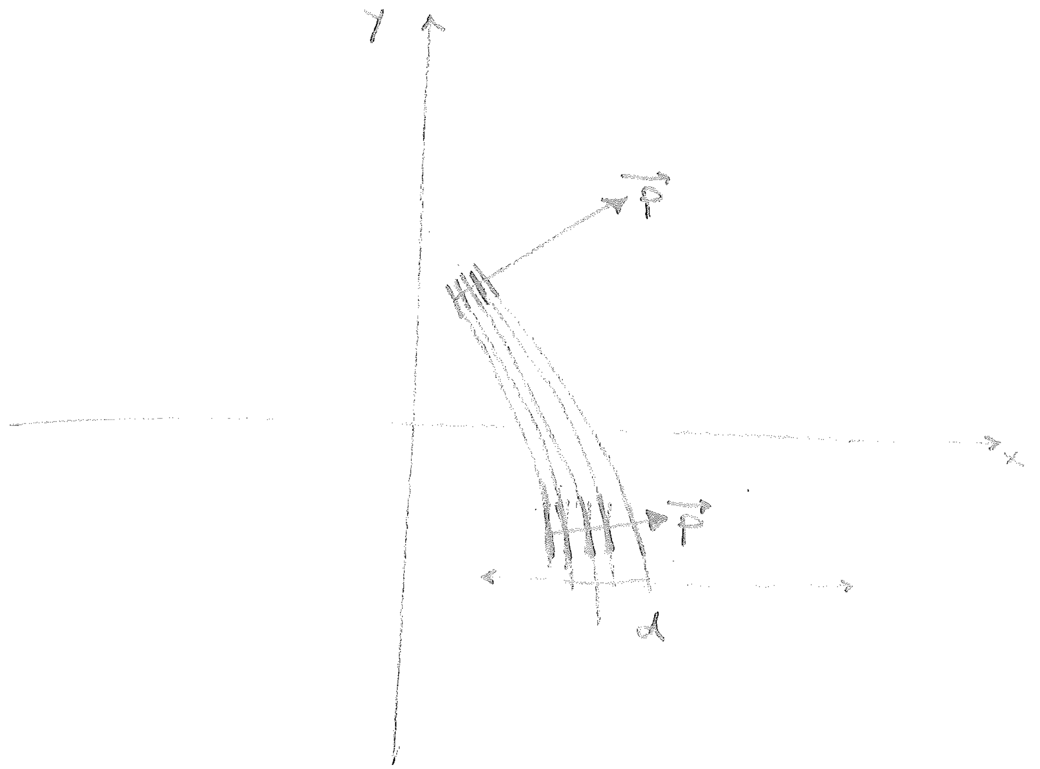
$$\vec{p}(\vec{x},t) = \nabla S = \begin{pmatrix}\text{local momentum}\end{pmatrix}$$

$$E(\vec{x},t) \equiv -\frac{\partial S}{\partial t} = \begin{pmatrix}\text{local energy}\end{pmatrix}$$

Geometric (ray) optics: short wavelengths (no diffraction)

$$\bar{\lambda} = \frac{\hbar}{p} \ll d = \begin{pmatrix}\text{typical scale of variation} \\ \text{of } V, R, \vec{p}, \text{ and } E\end{pmatrix}$$

On scales small compared to d, we have plane waves



$$\hbar \ll pd = \begin{pmatrix}\text{typical action over} \\ \text{length } d\end{pmatrix}$$

↑

quantum of action (uncertainty principle)

By choosing units such that d and p are $O(1)$, we make $\hbar \ll 1$ the small parameter

$$mE = p^2/2 \sim O(1)$$

$$\partial/\partial x \sim O(1)$$

$$m\,\partial/\partial t \sim p\frac{\partial}{\partial x} \sim O(1)$$

$$\nabla\psi = \left(\nabla R + \frac{i}{\hbar}R\nabla S\right)e^{iS/\hbar}$$

$$\nabla^2\psi = \Big(\nabla^2 R + \frac{i}{\hbar}\nabla R\cdot\nabla S + \frac{i}{\hbar}R\nabla^2 S$$
$$+ \frac{i}{\hbar}\nabla S\cdot\left(\nabla R + \frac{i}{\hbar}R\nabla S\right)\Big)e^{iS/\hbar}$$

$$= \Big[\left(\nabla^2 R - \frac{1}{\hbar^2}R\nabla S\cdot\nabla S\right) +$$
$$+ \frac{i}{\hbar}\left(2\nabla S\cdot\nabla R + R\nabla^2 S\right)\Big]e^{iS/\hbar}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi = \Big[\left(-\frac{\hbar^2}{2m}\nabla^2 R + R\frac{|\nabla S|^2}{2m}\right)$$
$$-\frac{i\hbar}{2m}\left(2\nabla S\cdot\nabla R + R\nabla^2 S\right)\Big]e^{iS/\hbar}$$

$$\frac{\partial\psi}{\partial t} = \left(\frac{\partial R}{\partial t} + \frac{i}{\hbar}R\frac{\partial S}{\partial t}\right)e^{iS/\hbar}$$

$$i\hbar\frac{\partial\psi}{\partial t} = \left(i\hbar\frac{\partial R}{\partial t} - R\frac{\partial S}{\partial t}\right)e^{iS/\hbar}$$

Gather it together

$$R\frac{|\nabla S|^2}{2m} + VR + R\frac{\partial S}{\partial t} - i\hbar\left[\frac{2\nabla S\cdot\nabla R + R\nabla^2 S}{2m} + \frac{\partial R}{\partial t}\right]$$
$$-\frac{\hbar^2}{2m}\nabla^2 R = 0$$

Schrödinger equation $\Leftrightarrow$

(1)

$$-\frac{\hbar^2}{2m}\nabla^2 R + R\frac{|\nabla S|^2}{2m} + VR + R\frac{\partial S}{\partial t} = 0$$

$$\boxed{\frac{|\nabla S|^2}{2m} + V - \frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} + \frac{\partial S}{\partial t} = 0}$$

"quantum potential"

(2)

$$+\frac{1}{2m}\left(2\nabla S \cdot \nabla R + R\nabla^2 S\right) + \frac{\partial R}{\partial t} = 0$$

$$\nabla P = 2R\nabla R\,; \quad \frac{\partial P}{\partial t} = 2R\frac{\partial R}{\partial t}$$

$$\frac{\partial P}{\partial t} + \frac{1}{m}\nabla S \cdot \nabla P = -\frac{1}{m}P\nabla^2 S$$

$$\frac{dP}{dt} = \frac{\partial P}{\partial t} + \frac{\vec{p}}{m}\cdot\nabla P = -\frac{1}{m}P\nabla\cdot\vec{p}$$

Conservation law if $\vec{p}/m = d\vec{x}/dt$

Geometric optics limit: $\hbar \to 0$ (Subtle because R can develop fine structures due to chaotic dynamics)

$$\boxed{\underbrace{\frac{|\nabla S|^2}{2m} + V}_{H(\vec{x}, \nabla S)} + \frac{\partial S}{\partial t} = 0}$$

Hamiltonian-Jacobi equation

Is this classical mechanics? Can we make classical trajectories out of rays defined by $\vec{p}$?

$$p_j(\vec{x},t) = \frac{\partial S}{\partial x_j}$$

$$\dot{p}_j = \frac{\partial^2 S}{\partial x_j \partial x_k}\dot{x}_k + \frac{\partial^2 S}{\partial x_j \partial t}$$

$$= \frac{\partial}{\partial x_j}\left(-\frac{1}{2m}\frac{\partial S}{\partial x_k}\frac{\partial S}{\partial x_k} - V\right)$$

$$= -\frac{1}{m}\frac{\partial^2 S}{\partial x_j \partial x_k}\frac{\partial S}{\partial x_k} - \frac{\partial V}{\partial x_j}$$

$$= -\frac{\partial^2 S}{\partial x_j \partial x_k}\frac{p_k}{m} - \frac{\partial V}{\partial x_j}$$

$$\Rightarrow \boxed{\dot{p}_j = -\frac{\partial V}{\partial x_j} + \frac{\partial^2 S}{\partial x_j \partial x_k}\underbrace{\left(\dot{x}_k - \frac{p_k}{m}\right)}_{\text{Get classical trajectories if choose } \dot{x}_k = p_k/m}}$$

Take a broader view that gets us into phase space. Integration of H-J equation gives

$$S = S(\vec{x}, \vec{p}_0, t)$$

3 integration constants chosen to be initial momenta of the classical trajectories; 4th integration constant is an irrelevant additive constant

Notice $p_j = \dfrac{\partial S}{\partial x_j}$

$x_{0j} = \dfrac{\partial S}{\partial p_{0j}}$

S is a generating function of F_2 type for a time-dependent canonical transformation from $\vec{x}, \vec{p}$ to initial coordinates $\vec{x}_0, \vec{p}_0$.

$$\dot{x}_{0j} = \frac{\partial^2 S}{\partial p_{0j}\,\partial x_k}\,\dot{x}_k + \underbrace{\frac{\partial^2 S}{\partial p_{0j}\,\partial t}}$$

$$= \frac{\partial}{\partial p_{0j}}\left(-\frac{1}{2m}\frac{\partial S}{\partial x_k}\frac{\partial S}{\partial x_k} - V\right)$$

$$= -\frac{1}{m}\frac{\partial^2 S}{\partial x_k\,\partial p_{0j}}\frac{\partial S}{\partial x_k}$$

$$= -\frac{\partial^2 S}{\partial x_k\,\partial p_{0j}}\frac{p_k}{m}$$

$$= \frac{\partial^2 S}{\partial p_{0j}\,\partial x_k}\left(\dot{x}_k - \frac{p_k}{m}\right)$$

$$= 0$$

Now do this in classical theory. Time-dependent canonical transformation from q_i, p_i to constant coördinates β_j, α_j (these can be any canonical transformation of the initial values)

Generating function $F_2(q, \alpha, t) = S(q_1, \ldots, q_n, \alpha_1, \ldots, \alpha_n, t)$. (Hamilton's principal function)

$$p_j = \frac{\partial S}{\partial q_j}$$

$$\beta_j = \frac{\partial S}{\partial \alpha_j}$$

$$\boxed{0 = K = H + \frac{\partial S}{\partial t} = H\left(q_1, \dots, q_n; \frac{\partial S}{\partial q_1}, \dots, \frac{\partial S}{\partial q_n}; t\right) + \frac{\partial S}{\partial t}}$$

H-J equation

α_j's are integration constants for this equation

Special case: $\partial H / \partial t = 0$

$$\Rightarrow \quad S = -\alpha_1 t + W(q_1, \dots, q_n; \alpha_1, \dots, \alpha_n)$$

Hamilton's characteristic function

$$\boxed{H\left(q_1, \dots, q_n; \frac{\partial W}{\partial q_1}, \dots, \frac{\partial W}{\partial q_n}\right) = \alpha_1}$$

Hamilton's characteristic equation

Can use W to generate a <u>time-independent</u> canonical transformation from q_j, p_j to $Q_j, P_j = \alpha_j$.

$$p_j = \frac{\partial W}{\partial q_j}$$

$$Q_j = \frac{\partial W}{\partial P_j} = \frac{\partial W}{\partial \alpha_j} = \frac{\partial S}{\partial \alpha_j} + \frac{\partial(\alpha_1 t)}{\partial \alpha_j} = \beta_j + \delta_{j1} t$$

$$K = H + \frac{\partial W'}{\partial t} = H = \alpha_1$$

$$\Longrightarrow \quad \dot{P}_j = -\frac{\partial H}{\partial Q_j} = 0 \quad \Rightarrow \quad P_j = \alpha_j$$

$$\dot{Q}_j = +\frac{\partial H}{\partial P_j} = \frac{\partial H}{\partial \alpha_j} = \delta_j \quad \Rightarrow \quad Q_j = \delta_j t + \beta_j$$