PHYS 621 Lecture Notes 16

Ehrenfest's Theorem — Expectation values vs classical mechanics

N 11.1 Define $\langle \hat{A} \rangle_\psi = \langle \psi | \hat{A} | \psi \rangle$

$$\frac{d}{dt}\langle \hat{A}\rangle_\psi = \left(\frac{d\langle\psi|}{dt}\right)\hat{A}|\psi\rangle + \langle\psi|\hat{A}\left(\frac{d}{dt}|\psi\rangle\right) + \langle\psi|\frac{\partial\hat{A}}{\partial t}|\psi\rangle.$$

$|\psi\rangle$ satisfies the Schrödinger Eq:

$$\frac{d}{dt}|\psi\rangle = \frac{1}{i\hbar}\hat{H}|\psi\rangle, \qquad \frac{d}{dt}\langle\psi| = -\frac{1}{i\hbar}\langle\psi|\hat{H}$$

because $i^* = -i$

$$\boxed{\frac{d}{dt}\langle\hat{A}\rangle_\psi = \frac{1}{i\hbar}\langle\psi|[\hat{A},\hat{H}]|\psi\rangle + \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle}$$ ← Ehrenfest's Thm.

(c.f. Heisenberg eqs. of motion)

Recall that in the Heisenberg picture, for $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$,

$$\frac{d\hat{x}_H}{dt} = \frac{1}{i\hbar}[\hat{x},\hat{H}]_H = \frac{\hat{p}_H}{m}$$

$$\frac{d\hat{p}_H}{dt} = \frac{1}{i\hbar}[\hat{p},\hat{H}]_H = -\left(\frac{\partial V}{\partial\hat{x}}\right)_H$$

Expectation values are the same in any picture (Heisenberg/Schrödinger etc.)

Ehrenfest's Thm ⇒
$$\left\langle\frac{d\hat{x}}{dt}\right\rangle_\psi = \frac{1}{m}\langle\hat{p}\rangle_\psi$$
$$\left\langle\frac{d\hat{p}}{dt}\right\rangle_\psi = -\left\langle\frac{\partial V}{\partial\hat{x}}\right\rangle_\psi$$

Expectation values satisfy this form of the classical eqs of motion.

Note! $\left\langle\frac{\partial V}{\partial\hat{x}}\right\rangle_\psi \neq \frac{\partial V}{\partial\langle\hat{x}\rangle_\psi}$, e.g. $\langle\hat{x}^2\rangle \neq \langle\hat{x}\rangle^2$, so expectation values do not precisely satisfy classical eqs. except in special cases.

Connection with the classical Hamilton-Jacobi Eq. (3D)

$\rho = |\psi(\vec{x}, t)|^2$

continuity Eq: $\dfrac{\partial \rho}{\partial t} = -\nabla \cdot \vec{J}$,

$$\vec{J} = \frac{\hbar}{2mi}\left(\psi^* \nabla \psi - \psi \nabla \psi^*\right)$$

polar representation of the wavefunction:

$$\psi = \sqrt{\rho}\, e^{iS/\hbar}, \quad \rho, S \in \mathbb{R}$$

Then the probability current can be written:

$$\boxed{\vec{J}} = \frac{\hbar}{2mi}\left\{\cancel{\sqrt{\rho}\nabla\sqrt{\rho}} - \cancel{\sqrt{\rho}\nabla\sqrt{\rho}} + \frac{i}{\hbar}\rho \nabla S - \left(-\frac{i}{\hbar}\rho\nabla S\right)\right\}$$

$$\boxed{= \frac{\rho}{m}\nabla S}$$

For a fluid with density ρ and current $\vec{J}$, the continuity equation is

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\underbrace{\rho \vec{v}}_{\vec{J} \equiv \rho \vec{v}}) = 0$$

fluid velocity.

→ The probability density evolves like a fluid with local velocity

$$\boxed{\vec{v} \equiv \frac{1}{m}\nabla S}$$

The Schrödinger Eq. becomes:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right]\left(\sqrt{\rho}\, e^{iS/\hbar}\right) = i\hbar \frac{\partial}{\partial t}\left(\sqrt{\rho}\, e^{iS/\hbar}\right)$$

$$= -\frac{\hbar^2}{2m} e^{iS/\hbar}\left[\nabla^2\sqrt{\rho} + \underbrace{\frac{2i}{\hbar}\nabla\sqrt{\rho}\cdot\nabla S} + \underbrace{\frac{i\sqrt{\rho}}{\hbar}\nabla^2 S} + \left(\frac{i}{\hbar}\right)^2\sqrt{\rho}(\nabla S)^2\right]$$

$$+ V(\vec{x})\sqrt{\rho}\, e^{iS/\hbar}$$

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

Continuity eq. $\Rightarrow \dfrac{\partial\sqrt{\rho}}{\partial t} = \dfrac{1}{2\sqrt{\rho}}\dfrac{\partial\rho}{\partial t} = \dfrac{1}{2\sqrt{\rho}}\nabla\cdot\left[\dfrac{\rho}{m}\nabla S\right]$

$$= \frac{1}{2\sqrt{\rho}}\frac{1}{m}\left[\nabla\rho\cdot\nabla S + \rho\nabla^2 S\right]$$

$$= \frac{1}{m}\left[\nabla\sqrt{\rho}\cdot\nabla S + \frac{\sqrt{\rho}}{2}\nabla^2 S\right]$$

$\rightarrow$ The underlined terms cancel

$$\Rightarrow \boxed{\frac{1}{2m}(\nabla S)^2 + V(\vec{x}) + \frac{\partial S}{\partial t} - \frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}} = 0}$$

– Quantum Hamilton-Jacobi Eq.

$\hbar \to 0$: This becomes the classical Hamilton-Jacobi eq. if $S = S_{cl}(\vec{x}, t; \vec{x}_0, t_0)$ $\Leftarrow$ Hamilton's principle function

action along classical path

cf. path integral: $\psi(\vec{x}, t) \approx e^{i S_{cl}(\vec{x},t;\vec{x}_0,t_0)/\hbar}(\ldots)$

WKB semiclassical approximation

write $S(\vec{x},t) = W(\vec{x}) - Et$ for stationary state!

Quantum Hamilton-Jacobi Eq:

$$\frac{1}{2m}(\nabla W)^2 + V(\vec{x}) - E \underbrace{- \frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}}_{V_Q = \text{quantum potential}} = 0$$

1D, semiclassical approx — drop V_Q term

$$\frac{1}{2m}\left(W'(x)\right)^2 + V(x) - E = 0$$

$$\Rightarrow W(x) = \pm \int dx' \underbrace{\sqrt{2m(E - V(x'))}}_{= p(x')}$$

$$\psi(x,t) \simeq \sqrt{\rho}\, \exp\left[\pm i \int_{x_0}^{x} dx'\, p(x') - iEt/\hbar\right]$$

Continuity Eq. again: $\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\left(\frac{\rho}{m}\frac{\partial S}{\partial x}\right) = 0$

$$= \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}\left(\frac{\rho}{m}\frac{\partial W}{\partial x}\right)$$

Stationary state: $\frac{\partial \rho}{\partial t} = 0$

$\Rightarrow \rho W'(x) = \rho \sqrt{2m(E-V(x))} = \text{constant}$

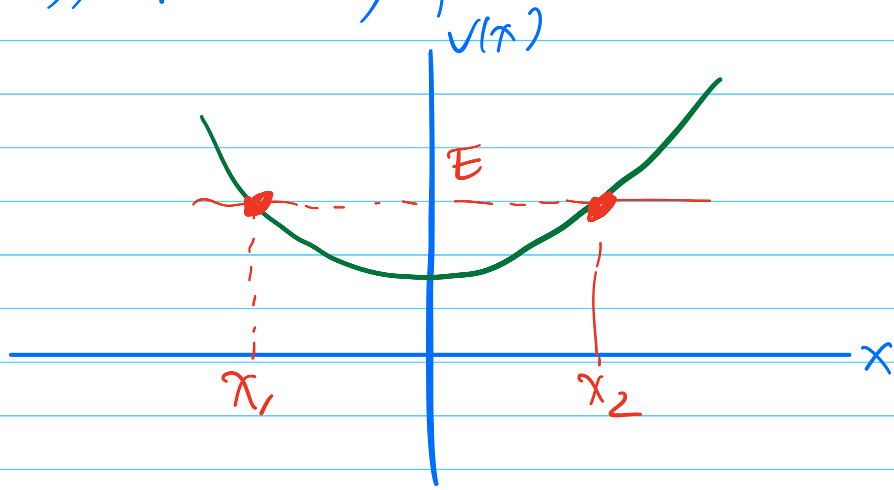
$\Rightarrow \rho = \frac{\text{const.}}{\sqrt{E-V(x)}}$

$\Rightarrow$ WKB solution for semiclassical approx. in 1D:

$$\boxed{\begin{aligned} \psi(x,t) &= \sqrt{\rho}\, e^{iS/\hbar} \\ &\approx \frac{\text{constant}}{(E-V(x))^{1/4}} \exp\left[\pm \frac{i}{\hbar} \int_{x_0}^{x} dx' \sqrt{2m(E-V(x'))} \right. \\ &\qquad \left. - iEt/\hbar \right] \end{aligned}}$$

Turning points:

The WKB approx. breaks down near the classical turning points where $E = V(x)$.



x_1, x_2 — classical turning pts

Near the turning pts, approximate

$$\frac{2m}{\hbar^2}\left(V(x)-E\right) \approx \underbrace{v_1}_{\text{const.}} (x-x_1)$$

Schrödinger Eq:

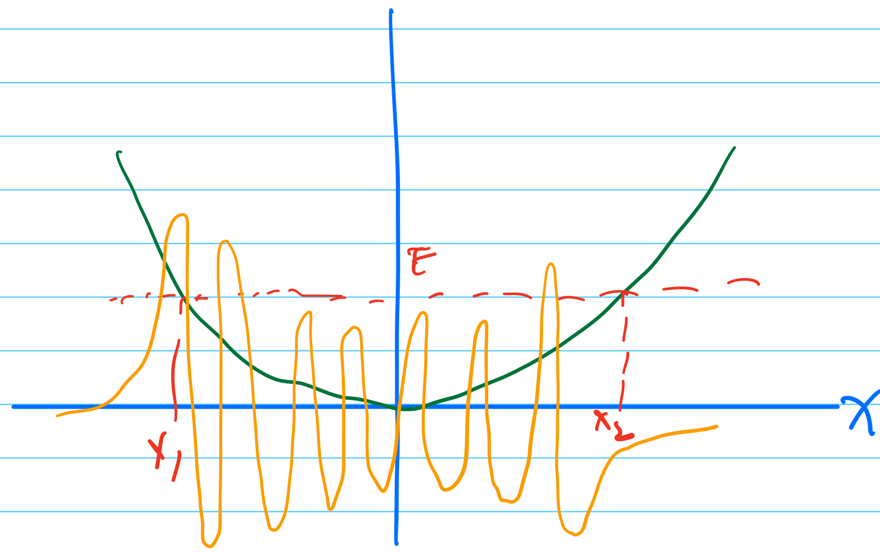
$$\psi''(x) \approx v_1 (x-x_1)\, \psi(x)$$

solutions are Airy functions:

$$\psi(x) = C_A \, Ai\left(\sqrt[3]{v_1}\,(x-x_1)\right) + C_B \, Bi\left(\overbrace{\sqrt[3]{v_1}\,(x-x_1)}^{\equiv u}\right)$$

$$\equiv C_A \, Ai(u) + C_B \, Bi(u)$$

We can use this to match solutions on either side of the turning pt.



$\psi_{WKB}(x)$

Result of matching at turning pts:

$$\psi_{WKB}(x) = \begin{cases} \dfrac{N}{\sqrt{|p(x)|}} \exp\left(-\dfrac{1}{\hbar}\displaystyle\int_x^{x_1} |p(x)|\,dx\right) & x < x_1 \\ \dfrac{N}{\sqrt{|p(x)|}} \sin\left(\dfrac{1}{\hbar}\displaystyle\int_x^{x_1} |p(x)|\,dx - \pi/4\right) & x_1 < x < x_2 \end{cases}$$

and $$\psi_{WKB}(x) = \begin{cases} \dfrac{N'}{\sqrt{|p(x)|}} \cos\left(\dfrac{1}{\hbar}\displaystyle\int_x^{x_2} |p(x)|\,dx - \pi/4\right) & x_1 < x < x_2 \\ \dfrac{N'}{2\sqrt{|p(x)|}} \exp\left(-\dfrac{1}{\hbar}\displaystyle\int_{x_2}^{x} |p(x)|\,dx\right) & x > x_2 \end{cases}$$

Matching solutions in region $x_1 < x < x_2$ requires

$$\int_{x_1}^{x_2} |p(x)|\,dx = \left(n+\tfrac{1}{2}\right)\pi\hbar \quad \text{, or}$$

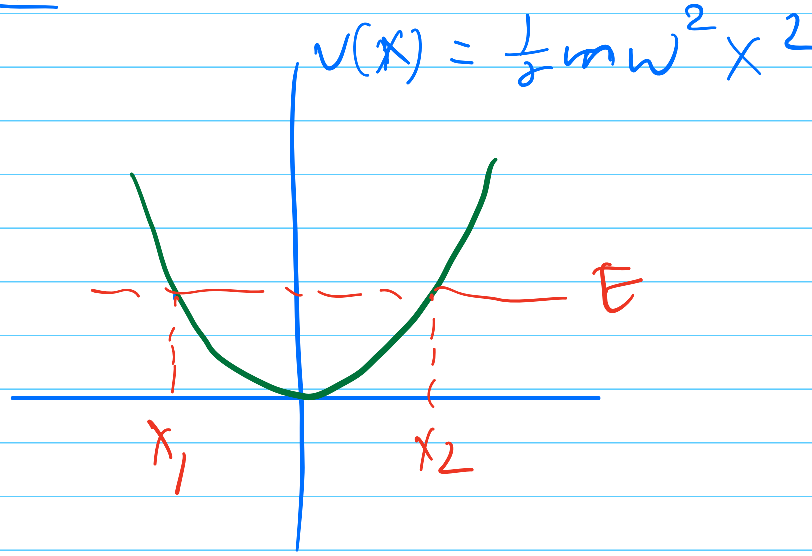
$$\boxed{\int_{x_1}^{x_2} \sqrt{2m\left(E-V(x)\right)}\,dx = \left(n+\tfrac{1}{2}\right)\pi\hbar}\ , \ n\in\mathbb{Z}$$

Bohr-Sommerfeld quantization condition

Maslov correction

— WKB approx gives condition on allowed energies

Example: $V(x) = \frac{1}{2} m\omega^2 x^2$



$$x_1 = -\sqrt{\frac{2E}{m\omega^2}}, \quad x_2 = \sqrt{\frac{2E}{m\omega^2}}$$

$$\int_{x_1}^{x_2} dx \sqrt{2m\left(E - \frac{1}{2} m\omega^2 x^2\right)}$$

From WKB approx.

$$= \frac{E\pi}{\omega} = (n + 1/2)\pi\hbar$$

$$\Rightarrow \boxed{E = (n + 1/2)\hbar\omega}$$

Maslov-corrected Bohr-Sommerfeld quantization of the simple harmonic oscillator.