Lecture 30. Semiclassical Approximation (WKB - appr)

Energy spectrum.

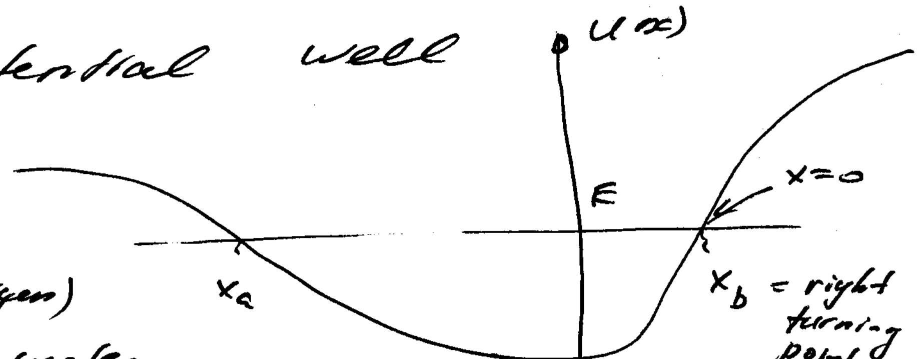
$$\psi(x) = \frac{C}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int_{x_i}^{x} p(x')\,dx'}$$

where $p(x') = \sqrt{2m(E-U(x'))}$

Applicability $\frac{m\hbar|F|}{p^3} \ll 1$, or $|F|\lambda_{dB} \ll E_{kin}$

The above solution is not applicable near the "classical turning points", where $p(x)=0$ or $E=U(x)$.

Consider a potential well



We will evaluate the stationary (= eigen) states of the system.

$$(*)\ \psi(x) = C\begin{cases} \frac{1}{\sqrt{p(x)}}\left(Be^{\frac{i}{\hbar}\int_x^0 p(x')dx'} + Ce^{-\frac{i}{\hbar}\int_x^0 p(x')dx'}\right) \\ \frac{1}{\sqrt{|p(x)|}} De^{-\frac{1}{\hbar}\int_0^x |p(x')|dx'} \end{cases}$$

← only decreasing exp. is allowed.

30.2| At $x=0$ $p(x)=0$ and the approximation is not applicable.

$$V(x) = E + \overset{=F}{V'(x)} \cdot x$$

And the Schrödinger equation is

$$-\frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2}|F| \cdot x\psi(x)$$

Make this equation dimensionless

$$\frac{d^2\psi(\xi)}{d\xi^2} = \xi\psi, \quad \alpha = \sqrt[3]{\frac{2mF}{\hbar^2}} \quad ; \quad \xi = \alpha x$$

This equation has two solutions

$$\psi = a \cdot Ai(\alpha x) + b\, \underset{\substack{\uparrow \\ \text{growing solution,}}}{Bi(\alpha x)} \qquad b \equiv 0.$$

Asymptotes for $Ai(\alpha x)$ are

$$\begin{cases} Ai(z) \propto \dfrac{1}{2\sqrt{\pi}\, z^{1/4}} e^{\mp\frac{2}{3} z^{3/2}} \quad (+ \text{ for } Bi(z)) & z \to +\infty \\ Ai(z) \propto \dfrac{1}{\sqrt{\pi}\,(-z)^{1/4}} \sin\left(\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right), & z \to -\infty \end{cases}$$

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$$\frac{d^2}{dz^2}\left(e^{-\frac{2}{3}z^{3/2}}\right) = \frac{d}{dz}\left[\left(-\frac{2}{3}\cdot z^{1/2}\cdot\frac{3}{2}\right)e^{-\frac{2}{3}z^{3/2}}\right] = \frac{d}{dz}\left(\sqrt{z}\, e^{-\frac{2}{3}z^{3/2}}\right)$$

$$= z\, e^{-\frac{2}{3}z^{3/2}}$$

Now we can ~~solve~~ write down $\psi(x)$ from $(*)$: $\quad p(x) = \hbar\alpha^{3/2}\sqrt{-x}$

$$\int_0^x \frac{p(x')dx'}{\hbar} = \int_0^x \sqrt{\frac{2m x'|F|}{\hbar^2}}\, dx' = +\frac{2}{3}\alpha^{3/2} x^{3/2} = +\frac{2}{3}(\alpha x)^{3/2}$$

$\sqrt{p(x)} \propto \sqrt[4]{x}$ and for $x>0$

$$\psi(x) = \frac{D}{\sqrt[4]{x}}\frac{1}{\sqrt{\hbar}\,\alpha^{3/4}} e^{-\frac{2}{3}(\alpha x)^{3/2}}$$

Compare to $\psi_{en}(x) = \dfrac{a}{2\sqrt{\pi}(\alpha x)^{1/4}} e^{-\frac{2}{3}x^{3/2}}$ we obtain $a = \sqrt{\dfrac{4\pi}{\alpha\hbar}}\, D$

For $x<0$ we obtain from $(*)$

$$\psi(x) = \frac{1}{\sqrt{\hbar}\,\alpha^{3/4}(-x)^{1/4}}\left[B e^{i\frac{2}{3}(-\alpha x)^{3/2}} + C e^{-\frac{2i}{3}(-\alpha x)^{3/2}}\right]$$

$$\frac{a}{2i\sqrt{\pi}} e^{i\pi/4} = \frac{B}{\sqrt{\hbar\alpha}} \qquad \frac{C}{\sqrt{\alpha\hbar}} = \frac{-a}{2i\sqrt{\pi}} e^{-i\pi/4}$$

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$$p(x) = \sqrt{2m\left[-V'(x_2)\cdot(x-x_2)\right]} = \sqrt{2m|F|(x-x_2)}$$

And we had the applicability condition

$$\frac{m\hbar\cdot|F|}{p^3} \ll 1 \qquad \frac{m\hbar\cdot|F|}{(2m)^{3/2}|F|^{3/2}|x-x_2|^{3/2}} \ll 1$$

$$|x-x_2|^{3/2} \gg \frac{\hbar}{2^{3/2}\sqrt{mF}}$$

$$|x-x_2| \gg \sqrt[3]{\frac{\hbar^2}{mF}}$$ is exactly the

large distance asymptote for the "Airy" solution in the linearized potential

$$\psi_{lin}(x) = a_1 Ai(\xi) = a\,Ai(\alpha(x-x_2)),$$

$$\alpha = \sqrt[3]{\frac{2m|F|}{\hbar^2}}$$

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$$\psi(x) = \begin{cases} \frac{2D}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int_x^{x_2} p(x')dx' + \frac{\pi}{4}\right) \\ \frac{D}{\sqrt{|p(x)|}} \exp\left(-\frac{1}{\hbar}\int_{x_2}^{x} |p(x')|dx'\right) \end{cases}$$

Similar analysis for $\psi(x)$ near left classical point

$$\frac{2D}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int_x^{x_2} p(x')dx' + \frac{\pi}{4}\right) = \psi_{right}(x)$$

$$\frac{2D'}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int_{x_1}^{x} p(x')dx' + \frac{\pi}{4}\right) = \psi_{left}(x)$$

these two functions coincide if ....

$$\int_{x_1}^{x_2} p(x')dx' = \hbar\pi(n - 1/2) \quad \text{for } n = 1, 2; \ldots$$

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

$$p = \sqrt{2m(E - U(x))} \qquad E = \frac{m\omega^2 x_{1;2}^2}{2}$$

$$\sqrt{2m}\int_{-\sqrt{\frac{2E}{m\omega^2}}}^{+\sqrt{\frac{2E}{m\omega^2}}} \sqrt{E - \frac{m\omega^2 x^2}{2}}\, dx = \hbar\pi(n - \tfrac{1}{2}) \qquad \pm\sqrt{\frac{2E}{m\omega^2}} = x_{1;2}$$

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$$\frac{\sqrt{2E}}{\omega\sqrt{m}} \sqrt{E}\cdot\sqrt{2m}\int_{-\sqrt{\frac{2E}{m\omega^2}}}^{+\sqrt{\frac{2E}{m\omega^2}}} \sqrt{1-\frac{m\omega^2x^2}{2E}}\, \frac{dx\,\omega\sqrt{m}}{\sqrt{2E}} \quad \hbar\pi(n+1/2) \quad n=0,1,\ldots$$

$$I\,E = \hbar\omega\,\frac{\pi}{2}(n+1/2); \qquad I = \int_{-1}^{1}\sqrt{1-\xi^2}\,d\xi = \frac{\pi}{2}$$

half of a circle

$$E = \hbar\omega(n+1/2)$$

Consider an infinite rectangular well.

$$p = \sqrt{2mE}$$

$$p\int_{x_1}^{x_2} dx' = Lp = \pi\hbar(n-\cancel{1/2})$$

$$E = \frac{\pi^2\hbar^2 n^2}{2mL^2}$$

31.4

Number of states in a given phase-volume.

$$\int_{x_1}^{x_2} p(x)\,dx = \frac{1}{2}\oint p(x)\,dx = \pi\hbar(n+1/2), \quad n=0,1,\ldots$$

$$\Gamma = 2\pi\hbar(n+1/2) \qquad \Delta\Gamma = 2\pi\hbar\,\Delta n,$$

Number of states $\Delta n = \dfrac{\Delta\Gamma}{2\pi\hbar}$ for ~~a~~ volume in the phase space $\Delta\Gamma$.
Is a reliable way to build statistical mechanics.

One more interesting observation

$$\Delta E \oint \frac{\partial p}{\partial E}\,dx = 2\pi\hbar, \quad \text{but} \quad \frac{\partial E}{\partial p} = v,$$

and $\Delta E \oint \dfrac{dx}{v} = 2\pi\hbar$, or $\Delta E = \dfrac{2\pi\hbar}{T} = \hbar\omega(E)$

The energy between two levels in semiclassical approximation is equal to the cyclotron frequency of oscillations, multiplied by $\hbar$.