Chapter 7: Variational Principle

If E_{gs} ground state energy

then $\langle H \rangle \geq E_{gs}$

$\rightarrow \langle \psi | H | \psi \rangle \geq E_{gs}$ for any normalized ψ

this forms an upper bound of ground-state energy.

e.g. $$H = \underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}}_{T} \underbrace{- \alpha \delta(x)}_{V}$$ delta well

Suppose $\psi = A e^{-bx^2}$ $\quad A = \left(\frac{2b}{\pi}\right)^{1/4}$

$$\langle T \rangle = -\frac{\hbar^2}{2m}\sqrt{\frac{2b}{\pi}}\int_{-\infty}^{\infty} e^{-bx^2}\frac{d^2}{dx^2}e^{-bx^2}\,dx = \frac{\hbar^2 b}{2m}$$

$$\langle V \rangle = -\alpha\sqrt{\frac{2b}{\pi}}\int_{-\infty}^{\infty} e^{-bx^2}\delta(x)e^{-bx^2}\,dx$$

$$= -\alpha\sqrt{\frac{2b}{\pi}}$$

$$\langle H \rangle = \frac{\hbar^2 b}{2m} - \alpha\sqrt{\frac{2}{\pi}}\, b^{1/2}$$ $\quad E_{gs} \leq$ for all b.

to find best bound,

$$0 = \frac{d\langle H \rangle}{db} = \frac{\hbar^2}{2m} - \frac{1}{2}\alpha\sqrt{\frac{2}{\pi}}\, b^{-1/2} \rightarrow b = \frac{2m^2}{\pi\hbar^4}\alpha^2$$

$$\langle H \rangle = \frac{\hbar^2}{2m}\left(\frac{2m^2}{\pi\hbar^4}\alpha^2\right) - \alpha\sqrt{\frac{2}{\pi}}\sqrt{\frac{2}{\pi}}\frac{m}{\hbar^2}\alpha$$

$$= \frac{m\alpha^2}{\pi\hbar^2} - \frac{2m\alpha^2}{\pi\hbar^2}$$

$$= -\frac{m\alpha^2}{\pi\hbar^2}$$ compare $E_{gs} = -\frac{m\alpha^2}{2\hbar^2}$

more negative

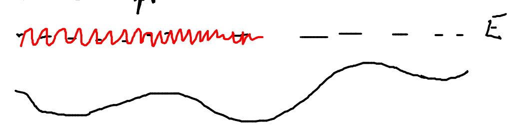
Delta barrier $+\alpha\delta(x)$

$$\langle H \rangle_{best} = \frac{m\alpha^2}{\pi\hbar^2} + \frac{2m\alpha^2}{\pi\hbar^2} = \frac{3m\alpha^2}{\pi\hbar^2}$$

$E_{gs} = 0$
scattering state

variational principle not so helpful for scattering states

Chapter 8: WKB Approximation

$V(x) =$ 

Suppose that $\psi(x)$ is a scattering state solution

$$\psi(x) = Ae^{\pm ikx} \qquad k = \sqrt{2m(E-V)}/\hbar$$

but A & k both vary with x, slowly

or for bound state,

$$\psi(x) = A e^{\kappa x} \qquad \kappa = \sqrt{2m(E-V)}/\hbar$$

This is fine so long as $\frac{1}{k}$ or $\frac{1}{\kappa}$ are small compared to fluctuations in $V(x)$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

$$\rightarrow \frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2}\psi$$

$$p(x) = \sqrt{2m(E-V(x))} \qquad \text{"momentum"}$$

Let $E > V(x)$ so $p(x)$ is real "classical region"

Let $\psi(x) = A(x)\, e^{i\phi(x)}$ $\qquad A, \phi$ are real

$$\psi'(x) = (A' + iA\phi')e^{i\phi}$$

$$\psi'' = \left(A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2\right)e^{i\phi}$$

$$A'' + \underline{2iA'\phi'} + \underline{iA\phi''} - A(\phi')^2 = -\frac{p^2}{\hbar^2}A$$

real part: $A'' - A(\phi')^2 = -\frac{p^2}{\hbar^2}A \rightarrow A'' = A\left[(\phi')^2 - \frac{p^2}{\hbar^2}\right]$

imaginary part: $2A'\phi' + A\phi'' = 0 \rightarrow (A^2\phi')' = 0$

$\hookrightarrow A^2\phi' = C^2 \rightarrow A = \frac{C}{\sqrt{\phi'}}$

Assum $A(x)$ changes slowly $\rightarrow A'' \approx 0$.

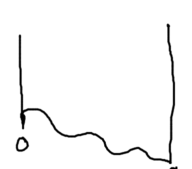
$$(\phi')^2 \approx \frac{p^2}{\hbar^2} \rightarrow \frac{d\phi}{dx} = \pm\frac{p}{\hbar}$$

$$\rightarrow \phi(x) = \pm\frac{1}{\hbar}\int^x p(x')\,dx'$$

$$A(x) = \frac{C}{\sqrt{\phi'}} = \frac{C}{\sqrt{p(x)}}$$

$$\psi(x) = \frac{C}{\sqrt{p(x)}}\, e^{\pm\frac{i}{\hbar}\int p(x)\,dx}$$

$\pm$: whether wave travels to right (+) or left (−)

e.g.  ∞ square well with bumpy bottom

$$\psi(x) = \frac{1}{\sqrt{p(x)}}\left[C_+ e^{i\phi(x)} + C_- e^{-i\phi(x)}\right] \qquad \phi(x) = \frac{1}{\hbar}\int_0^x p(x)\,dx$$

$$= \frac{1}{\sqrt{p(x)}}\left[C_1 \sin\phi(x) + C_2\cos\phi(x)\right]$$

$\psi(0) = 0$ & $\phi(0) = 0$ $\quad \frac{1}{\hbar}\int_0^0 p(x)\,dx$

$$\psi(0) = \frac{1}{\sqrt{p(x)}}C_2 \rightarrow C_2 = 0$$

$$0 = \psi(a) = \frac{1}{\sqrt{p(a)}}C_1 \sin\phi(a)$$

$$\rightarrow \phi(a) = n\pi \qquad n = 1, 2, 3, \ldots$$

$$\longrightarrow \int_0^a p(x)\,dx = n\pi\hbar \qquad n = 1, 2, 3, \ldots$$

$$p(x) = \sqrt{2m(E - V(x))}$$

e.g. $V(x) = 0 \qquad p(x) = \sqrt{2mE}$

$$\int_0^a \sqrt{2mE}\,dx = n\pi\hbar$$

$$a\sqrt{2mE} = n\pi\hbar$$

$$2mE = \frac{n^2\pi^2\hbar^2}{a^2}$$

$$E = \frac{n^2\pi^2\hbar^2}{2ma^2} \qquad \boxtimes$$