Physics 491
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Lecture #5: Schrödinger 1D Bound State

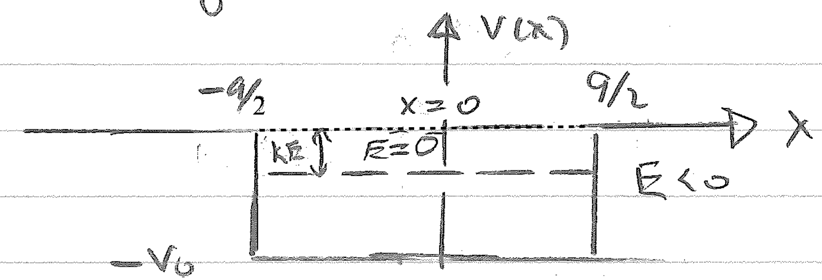
① Boundary Conditions

(i) normalizable $\lim_{|x|\to\infty} \Psi(x) = 0$

(ii) continuity of $\Psi(x)$ PDF defined for all x

(iii) continuity of $\Psi'(x)$ everywhere $V(x)$ finite.
ensures $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$ continuous and $\frac{\hat{p}^2}{2m}$ finite

② Finite square well



usually take $V=0$ at ∞ (free particle)

$$|a| < \frac{a}{2} \qquad \Psi_I'' = -k^2 \Psi_I \qquad k = \sqrt{2m(V_0 - |E|)}/\hbar \ \text{ real}$$

$$|a| > \frac{a}{2} \qquad \Psi_{II}'' = q^2 \Psi_{II} \qquad q = \sqrt{2m(-E)}/\hbar$$

$$= \sqrt{2m|E|}/\hbar$$

QM particle penetrates (tunnels) into classically forbidden region

$$k^2 + q^2 = \frac{2m}{\hbar^2}\left[V_0 + E - E\right] = \frac{2mV_0}{\hbar^2} \ \text{ constant}$$

(i) implies exponential decay $|x| > \frac{a}{2}$

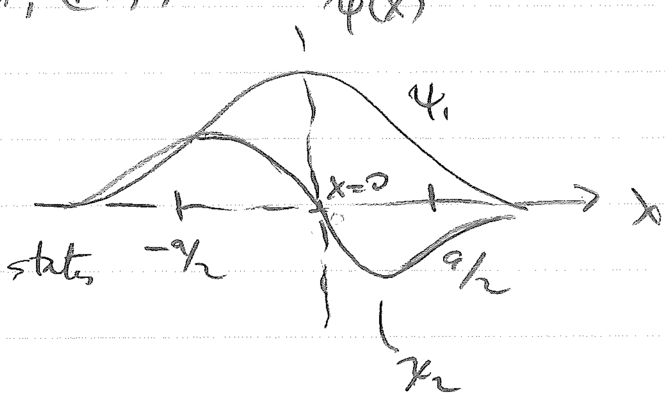
$x < -\frac{a}{2}$ $\quad \psi_{II} = C e^{\beta x}$

$x > a/2$ $\quad \psi_{II} = D e^{-\beta x}$

$-a/2 < x < \frac{a}{2}$ $\quad \psi_I = A \sin kx + B \cos kx$

because $V(x) = V(-x)$ solutions will be even or odd. Three constants determined by (ii), (iii).

sketch of ground and first excited states



<u>even</u> $\quad \psi_I = B \cos kx$

$$B \cos \frac{ka}{2} = D e^{-\beta a/2} \qquad \text{at } x = \frac{a}{2}$$

$$-kB \sin ka/2 = -\beta D e^{-\beta a/2}$$

$$\tan\left(\frac{ka}{2}\right) = \frac{\beta}{k}$$

transcendental equations

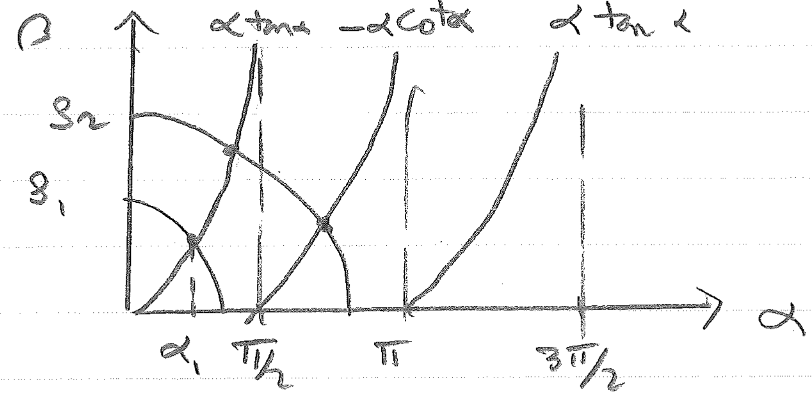
<u>odd</u> $$\cot\left(\frac{ka}{2}\right) = -\frac{\beta}{k}$$

define $\alpha \equiv \frac{ka}{2}$, $\beta \equiv \frac{\beta a}{2}$, $\gamma \equiv \frac{a}{2\hbar}\sqrt{2mV_0}$

all dimensionless, γ = constant characterizing strength of well.

$$\alpha^2 + \beta^2 = \gamma^2$$

Graphical Solution



Always at least 1 solution in 1D. δ_2 is example with 2 solutions.

$$E_n = -V_0 + \frac{\hbar^2}{2m}k^2 = -V_0 + \frac{\hbar^2}{2ma^2}(2\alpha_n)^2$$

Recover ∞ well in limit $V_0 \to \infty$ (redefine as zero of potential) $\delta \to \infty$, $\alpha \to \frac{n\pi}{2}$

$$E_n \to \frac{\hbar^2}{2ma^2}(n\pi)^2.$$

Free particle wave packet

expand in terms of plane waves.

$$E = \frac{(\hbar k)^2}{2m} \quad \text{non-relativistic energy}$$

dispersion relation $\omega(k) = \frac{1}{\hbar}\left(\frac{\hbar^2 k^2}{2m}\right)$

plane wave states, choose normalization

$$\phi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

Fourier transform of $\Psi(x) \to \tilde{\Psi}(k)$

$$\Psi(x,0) = \int_{-\infty}^{\infty} \tilde{\Psi}(k) \frac{1}{\sqrt{2\pi}} e^{ikx} dk$$

$$\Psi(x,t) = \int_{-\infty}^{\infty} \tilde{\Psi}(k) \frac{1}{\sqrt{2\pi}} e^{i(kx-\omega(k)t)} dk$$

Because there is no confining potential, over time Δx will increase.

If we take $\Psi(x,0)$ to be Gaussian

$$\Psi(x,0) = \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2}$$

you will find on HW

$$\Psi(x,t) = \left(\frac{2a}{\pi}\right)^{1/4} \frac{1}{\sqrt{\alpha}} e^{-ax^2/\alpha}$$

where $\alpha = 1 + \frac{2i\hbar a t}{m}$ (complex) and

Δx increases with time. Wave packet has multiple momentum components that propagate with different speeds.

<u>Plane wave normalization</u>

$$\int_{-\infty}^{\infty} \phi_{k'}^* \phi_k \, dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k-k')x} \, dx$$

$$\equiv \delta(k-k')$$

Dirac "delta function". Technically not a function.

Analogous to Kronecker δ_{ij} in limit of continuous domain.

<u>Coefficients $\tilde{\Psi}(k)$</u>:

$$\Psi(x,0) = \int_{-\infty}^{\infty} \tilde{\Psi}(k')\, \phi_{k'}(x)\, dk'$$

where $\phi_{k'}(x) = \frac{1}{\sqrt{2\pi}} e^{ik'x}$

multiply by orthogonal $\phi_k^*(x)$ and integrate over x:

$$\int_{-\infty}^{\infty} \phi_k^*(x)\, \Psi(x,0)\, dx =$$

$$\int_{-\infty}^{\infty} dx\, \phi_k^*(x) \int_{-\infty}^{\infty} \tilde{\Psi}(k')\, \phi_{k'}(x)\, dk'$$

$$= \int_{-\infty}^{\infty} dk'\, \tilde{\Psi}(k') \underbrace{\int_{-\infty}^{\infty} dx\, \phi_k^*(x)\, \phi_{k'}(x)}_{\delta(k-k')}$$

$$= \int_{-\infty}^{\infty} dk'\, \tilde{\Psi}(k')\, \delta(k-k') = \tilde{\Psi}(k)$$

$$\boxed{\tilde{\Psi}(k) = \int \phi_k^*(x)\, \Psi(x,0)\, dx}$$

Suppose $\Psi(x,0)$ is just plane wave

$$\phi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

then

$$\tilde{\Psi}(k) = \int \phi_k^*(x)\, \phi_{k'}(x)\, dx$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k'-k)x}\, dx = \delta(k-k')$$

giving:

$$\Psi(x,0) = \int \delta(k-k')\, \phi_{k'}(x)\, dk'$$

$$= \phi_k(x)$$

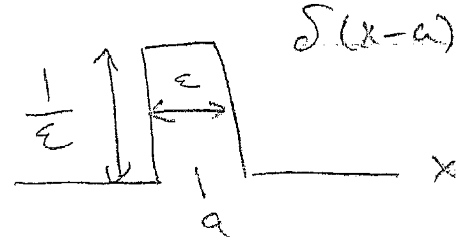
of course!

⑥ Delta function

Dirac delta function defined by

$$\int_{x_1}^{x_2} f(x)\,\delta(x-a)\,dx = \begin{cases} f(a) & x_1 < a < x_2 \\ 0 & \text{otherwise} \end{cases}$$

picture unit-area spike at $x=a$



Mathematically, "δ function" is distribution with many representations.

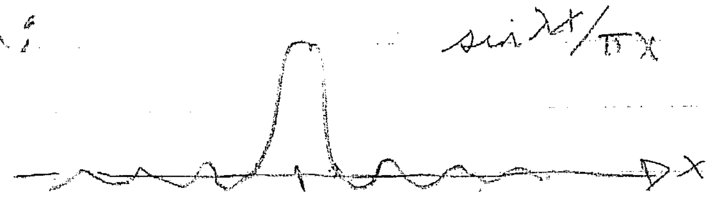
$\delta(x)$ has dimension $\dfrac{1}{\dim x}$

Important representation

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ikx} = \lim_{\lambda\to\infty} \frac{1}{2\pi}\int_{-\lambda}^{\lambda} dk\, e^{ikx}$$

$$= \lim_{\lambda\to\infty} \frac{\sin(\lambda x)}{\pi x}$$

sketch:



note ① $\lim_{x\to 0}\left[\lim_{\lambda\to\infty}\frac{\sin(\lambda x)}{\pi x}\right]$

$= \lim_{\lambda\to\infty}\left[\lim_{x\to 0}\frac{\sin\lambda x}{\pi x}\right] = \lim_{\lambda\to\infty}\frac{\lambda}{\pi}\to\infty$

② $\int_{-\infty}^{\infty}dx\left[\lim_{\lambda\to\infty}\frac{\sin\lambda x}{\pi x}\right] = \lim_{\lambda\to\infty}\frac{2}{\pi}\int_0^{\infty}\frac{\sin u}{u}\,du$

$u \equiv \lambda x$

$= \lim_{\lambda\to\infty}\left(\frac{2}{\pi}\right)\left(\frac{\pi}{2}\right) = 1$

(6) δ-function potential

$$V(x) = -\frac{\hbar^2}{2m}\frac{\lambda}{b}\delta(x)$$

λ dimensionless strength
b a length

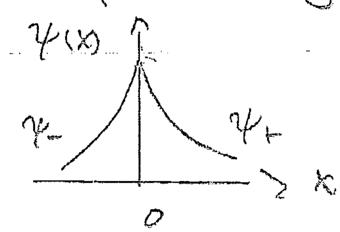
$$-\frac{\hbar^2}{2m}\psi'' + V\psi = E\psi$$

$$\psi'' = -\frac{\lambda}{b}\delta(x)\psi - \frac{2mE}{\hbar^2}\psi$$

when you see δ, integrate! for λ > 0, we look for bound state (E < 0)

$$\psi_\pm(x) = A e^{\mp kx}, \quad k = \sqrt{2m|E|}/\hbar$$

must decay exponentially



kink at x = 0 determined by strength λ

Integrate over infinitessimal neighborhood of x = 0

$$\int_{-\varepsilon}^{\varepsilon}\psi''\,dx = -\frac{\lambda}{b}\int_{-\varepsilon}^{\varepsilon}\delta(x)\psi(x)\,dx + k^2\int_{-\varepsilon}^{+\varepsilon}\psi\,dx$$

$$\left.\frac{d\psi}{dx}\right|_{-\varepsilon}^{\varepsilon} = -\frac{\lambda}{b}\psi(0) + k^2(2\varepsilon)\psi(0)$$

lim ε → 0 $\quad \left.\frac{d\psi_+}{dx}\right|_{0^+} - \left.\frac{d\psi_-}{dx}\right|_{0^-} = -\frac{\lambda}{b}\psi(0)$

$$= -\frac{\lambda}{b}A$$

$$-2kA = -\frac{\lambda}{b}A$$

$$k = \frac{\lambda}{2b}$$

$$E = -\frac{1}{2m}\left(\frac{\hbar\lambda}{2b}\right)^2 \quad \text{1 bound state}$$

normalization: $2|A|^2\int_0^\infty e^{-2kx}\,dx = \frac{|A|^2}{k}\int_0^\infty e^{-y}\,dy$

$$= \frac{|A|^2}{k} = 1 \;;\; A = \sqrt{\lambda/2b} \quad \text{choosing real}$$

$$\boxed{\psi_\pm(x) = \left(\frac{\lambda}{2b}\right)^{1/2} e^{\mp\frac{\lambda}{2b}x}}$$