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Simple 1D problems

Digression: Gaussian integrals

$$I(\alpha) = \int_{-\infty}^{\infty} e^{-\alpha x^2} dx$$

$$I^2(\alpha) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\alpha r^2} dx\,dy$$

$$= \int_0^\infty \int_0^{2\pi} r\,dr\,d\theta \; e^{-\alpha r^2}$$

$$= \pi/\alpha$$

$$\therefore I = \sqrt{\frac{\pi}{\alpha}}$$

$$I(\alpha,\beta) = \int_{-\infty}^{\infty} e^{-\alpha x^2+\beta x} dx$$

$$= e^{\beta^2/4\alpha} \left(\frac{\pi}{\alpha}\right)^{\frac{1}{2}}$$

$$I_{2n}(\alpha) = \int_{-\infty}^{\infty} x^{2n} e^{-\alpha x^2} dx$$

$$= \left(-\frac{d}{d\alpha}\right)^n \int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \left(-\frac{d}{d\alpha}\right)^n \sqrt{\frac{\pi}{\alpha}}$$

$$I_2(\alpha) = \frac{1}{2}\frac{\sqrt{\pi}}{\alpha^{3/2}}$$

1. Free particle

$$H = \frac{p^2}{2m}$$

$$i\hbar \frac{d}{dt}|\psi\rangle = \frac{p^2}{2m}|\psi\rangle$$

step (1) find ~~I~~ $H|\omega\rangle = E|\omega\rangle$

Obviously, $|\omega\rangle = |p\rangle$, $E = \frac{p^2}{2m}$

$p = \pm(2mE)^{\frac{1}{2}}$ for any given E (continuous,

$\therefore$ For each E, there are two eigenkets

$|p=\sqrt{2mE}\rangle$ & $|p=-\sqrt{2mE}\rangle$ (degeneracy!)

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in general, eigenket of E $= \alpha|\sqrt{2mE}\rangle + \beta|-\sqrt{2mE}\rangle$

∴ it describes moving left or right at the same time !

In this case, $\hat{H}$ has degeneracy which can be lifted by $\hat{P}$.

∴ $\hat{p}, \hat{H}$ are complete $\underbrace{\text{commuting}}_{\text{set of}}$ observables in this case

(disregarding spins ...)

∴ We can label ~~them~~ eigenstates by

$|p, E\rangle$ or simply $|p\rangle$

$$U(t) = \int_{-\infty}^{\infty} dp \; |p\rangle\langle p| \; e^{-\frac{iE_pt}{\hbar}}$$

↑ see over

$$= \int_{-\infty}^{\infty} dp \; |p\rangle\langle p| \; e^{-\frac{ip^2t}{2m\hbar}}$$

same as Green's function for the diffusion eq.

$$U(x,t;x') \equiv \langle x|U(t)|x'\rangle$$

Satisfying $i\hbar\frac{d}{dt}U(x t, x') = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}U$

(Sometimes, denoted as G as the Green's function)

$$= \int_{-\infty}^{\infty} dp \; \langle x|p\rangle\langle p|x'\rangle \; e^{-\frac{ip^2t}{2m\hbar}}$$

if we impose $\underline{t>0}$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp \; e^{\frac{ip(x-x')}{\hbar}} \; e^{-\frac{ip^2t}{2m\hbar}}$$

i.e, $U = (\cdots)\,\theta(t)$

$$= \left(\frac{m}{2\pi\hbar i t}\right)^{\frac{1}{2}} \; e^{\frac{im(x-x')^2}{2\hbar t}}$$

$i\hbar\frac{d}{dt}U + \frac{\hbar^2}{2m}\frac{d^2}{dx^2}U = i\hbar\,\delta(t-t')\,\delta(x-x')$

~~$\frac{\partial T}{\partial t} = D\nabla^2 T$~~

∵ $|\psi(t)\rangle = \hat{U}(t)\,|\psi(0)\rangle$

$$\langle x|\psi(t)\rangle = \psi(x,t) = \int dx' \; U(x,t;x') \; \psi(x',0)$$

~~diffusion~~

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The above is for the origin of $t = 0$.

If the origin is at t', we have

$$\psi(xt) = \int dx \; U(xt; x't') \; \psi(x't') \quad \text{——} ①$$

$$U(xt; x't') = \langle x | \underbrace{\hat{U}(t-t')}_{\Downarrow} | x' \rangle$$

in general, $\hat{U}(t, t')$

If at t', the particle is localized at x_0,

, i.e., $\psi(x't') = \delta(x' - x_0)$

random walk

$\psi(x,t) = U(xt, x_0 t')$. In other words, $U(xt, x't')$

is the amplitude that a particles at x, t when

initially, it was at (x', t').

① is some kind of "Huygen's" principle :

✗ the total amplitude at (x, t) = sum of contributes

~~from~~ progating from (x', t') with a weight

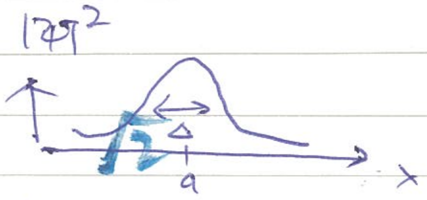
$\psi(x', t')$ U has the meaning of Green's function

$t > t'$

$\psi(x,t)\big|_{t=t'} = \psi(x,$

2. Gaussian Packet

$$\psi(x) = A \, e^{-\frac{(x-a)^2}{2\Delta^2}}$$



Eigenstates of $\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\psi + \frac{1}{2}K(x-a)^2\psi = E\psi$
(Simple harmonic oscillator)

Landauer
tunning

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Direct substitution, we get

$$+\frac{\hbar^2}{2m}\frac{1}{\Delta^4}=\frac{1}{2}K$$

$$\therefore K=\frac{\hbar^2}{m\Delta^4}$$

$$E=\frac{\hbar^2}{2m}\frac{1}{\Delta^2}$$

normalization:

$$\langle\psi|\psi\rangle=|A|^2\int_{-\infty}^{\infty}e^{-\frac{(x-a)^2}{\Delta^2}}dx$$

$$=A^2(\pi\Delta^2)^{\frac{1}{2}}\equiv 1$$

$$\therefore A=\frac{1}{(\pi\Delta^2)^{\frac{1}{4}}}$$

$$\langle x\rangle=\langle\psi|\hat{x}|\psi\rangle$$

$$=A^2\int_{-\infty}^{\infty}x\,e^{-\frac{(x-a)^2}{\Delta^2}}dx$$

$$=a$$

$$\langle x^2\rangle=A^2\int_{-\infty}^{\infty}x^2e^{-\frac{(x-a)^2}{\Delta^2}}dx$$

$$=A^2\int_{-\infty}^{\infty}(y+a)^2e^{-\frac{y^2}{\Delta^2}}dy$$

$$\int_{-\infty}^{\infty}y^2e^{-y^2/\Delta^2}dy=\frac{1}{2}\sqrt{\pi}\Delta^3$$

$$=\frac{\Delta^2}{2}+a^2$$

$$\therefore\Delta x\equiv\langle(\hat{x}-\langle x\rangle)^2\rangle^{\frac{1}{2}}=[\langle x^2\rangle-\langle x\rangle^2]^{\frac{1}{2}}$$

$$=\left[\frac{\Delta^2}{2}+a^2-a^2\right]^{\frac{1}{2}}=\frac{\Delta}{\sqrt{2}}$$

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$$\langle p \rangle = A^2 \int_{-\infty}^{\infty} e^{-\frac{(x-a)^2}{2\Delta^2}} \frac{\hbar}{i}\frac{d}{dx}\, e^{-\frac{(x-a)^2}{2\Delta^2}}\, dx = 0$$

$\because \psi(x)$ is real!

$$\langle p^2 \rangle = A^2 \int_{-\infty}^{\infty} e^{-\frac{(x-a)^2}{2\Delta^2}} \, -\hbar \frac{d^2}{dx^2}\, e^{-\frac{(x-a)^2}{2\Delta^2}}\, dx$$

$$= \ldots$$

or do Fourier transformation

$$\Phi(p) = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}}\, e^{-ipx/\hbar}\, A e^{-\frac{(x-a)^2}{2\Delta^2}}$$

$$= \left(\frac{\Delta^2}{\pi\hbar^2}\right)^{\frac{1}{4}} e^{-ipa/\hbar}\, e^{-p^2\Delta^2/2\hbar^2}$$

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} dp\, p^2\, |\Phi(p)|^2$$

$$= \frac{\Delta}{\sqrt{\pi\hbar^2}} \int_{-\infty}^{\infty} dp\, p^2\, e^{-\frac{\Delta^2}{\hbar^2}p^2}$$

$$= \frac{\Delta}{\sqrt{\pi\hbar^2}} \left(-\frac{d}{ds}\right) \underbrace{\int_{-\infty}^{\infty} dp\, e^{-sp^2}}_{\sqrt{\frac{\pi}{s}}} \Bigg|_{s = \Delta^2/\hbar^2}$$

$$= \frac{\Delta}{\sqrt{\pi\hbar^2}} \frac{\sqrt{\pi}}{2} \frac{1}{\left(\frac{\Delta}{\hbar}\right)^3} = \frac{\hbar^2}{2\Delta^2}$$

$$\therefore \Delta p = \left(\frac{\hbar^2}{2\Delta^2}\right)^{\frac{1}{2}} = \frac{1}{\sqrt{2}}\frac{\hbar}{\Delta}$$

$\Delta x \cdot \Delta p = \frac{\hbar}{2}$, in general $\Delta x\, \Delta p \geq \frac{\hbar}{2}$

— Heisenberg uncertainty Relation (will be proved later!)

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General features of energy eigenfunctions in 1D

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

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

Given intial conditions $\psi(x_0)$ $\left.\frac{d\psi}{dx}\right|_{x=x_0}$

$\Rightarrow$ $\psi(x)$ can be solved.

bound state : $\psi(x)\to 0$ as $x\to\pm\infty$

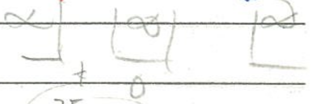
Theorem 1. No degeneracy in 1D bound states (up to a scale factor)

pf: Assume ψ_1, ψ_2 have the same E

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2}+V\psi_1=E\psi_1 \quad — ①$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2}+V\psi_2=E\psi_2 \quad — ②$$

$\boxed{V \text{ smooth}}$

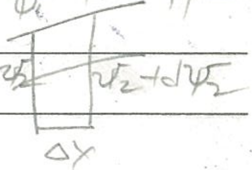


$\psi_2 = 0$
$d\psi_2$

① × ψ_2 − ② × ψ_1

$$\psi_1\frac{d^2\psi_2}{dx^2}-\psi_2\frac{d^2\psi_1}{dx^2}=0$$

i.e. $$\frac{d}{dx}\left(\psi_1\frac{d\psi_2}{dx}-\psi_2\frac{d\psi_1}{dx}\right)=0$$



$$\psi_1\frac{d\psi_2}{dx}-\psi_2\frac{d\psi_1}{dx}=\text{const}$$

$\because$ $|x|\to\infty$. $\psi_1,\psi_2\to 0$ (bound states) ($\psi_2\neq 0$)

$$\frac{\psi_1}{\psi_2}=\frac{d\psi_1}{d\psi_2}=\frac{\psi_1+d\psi_1}{\psi_2+d\psi_2}$$

$\therefore$ const $=0$ $\quad\therefore$ $\frac{1}{\psi_1}\frac{d\psi_1}{dx}=\frac{1}{\psi_2}\frac{d\psi_2}{dx}\Rightarrow\frac{1}{|\psi_1|}\frac{d|\psi_1|}{dx}=\frac{1}{|\psi_2|}\frac{d|\psi_2|}{dx}$

i.e. $$\frac{d\ln|\psi_1|}{dx}=\frac{d\ln|\psi_2|}{dx}$$

$$\ln|\psi_1|=\ln|\psi_2|+\text{const}\Rightarrow|\psi_1|=C|\psi_2|$$

Q.E.D.

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↙H Hermitian

Theorem 2. If U(x) is real, the eigenfunctions are real up to scale factors in 1D.

Pf: If $\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n + U(x)\,\psi_n(x) = E\psi_n$

then $\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n^* + U(x)\,\psi_n^*(x) = E\psi_n^*$

Theorem 1. $\psi_n^* = C\psi_n$ (non-degenerate)

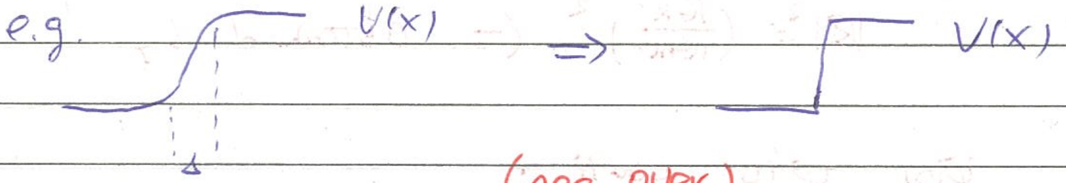
⇒ ψ_R, ψ_I are solutions
real imaginary parts

∴ $\psi_I = C\psi_R$ (non-degenerate)

∴ $\psi = \psi_R + i\psi_I = (1+Ci)\,\psi_R$ QED.

3. A real potential U(x) is always smooth, but some times for mathematical convenience, we idealized and approximate it to some "unphysical" potential.

e.g.



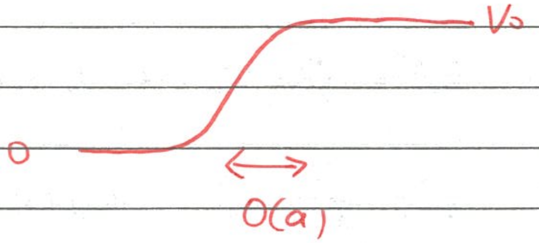
(see over)

Solutions thus obtained are good only above the lengthscale Δ, i.e., using V(x) to get ψ(x), ψ(x)'s resolution can't be better than Δ.

No matter what idealization we made for U(x), ψ(x) must obey the following requirements.

A real example is to consider

$$U(x) = \frac{V_0}{2}\left(1+\tanh\frac{x}{2a}\right)$$



rigorous solution $y = \frac{1}{1+e^{x/a}}$ $\psi \to u(y) \Rightarrow$

$x \to -\infty$. $\psi = e^{ikx} + e^{-ikx}R$ $k = \sqrt{\frac{2mE}{\hbar^2}}$

$x \to \infty$ $\psi = Te^{ik'x}$ $k' = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$

$$|R|^2 = \left\{\frac{\sinh\pi(k-k')a}{\sinh\pi(k+k')a}\right\}^2$$

$a \to 0$ $|R|^2 = \left(\frac{k-k'}{k+k'}\right)^2$ (= obtained by

$\psi(0)$, $\psi'(0)$ conti :

$$1+R=T$$
$$ik(1-R)=ik'T$$
$>$ $R=\frac{k-k'}{k+k'}$ $T=\frac{2k}{k+k'}$

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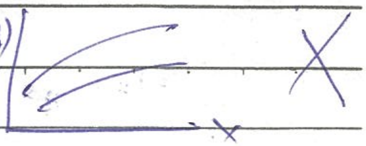
打 X is ambiguous for example θ, $\theta+2\pi$

$\Psi(x)$: single valued $\overset{\nLeftarrow}{\Rightarrow}$ ($|\Psi|^2$ single valued)



$\Psi(x)$: finite ($|\Psi|^2$ finite)

$\therefore e^{\alpha x}$ for $x>0$ is not allowed

($\because e^{\alpha x} \to \infty$ as $x \to \infty$)

$\Psi(x)$: Continuous so that $\frac{d\Psi}{dx}$ is well defined.

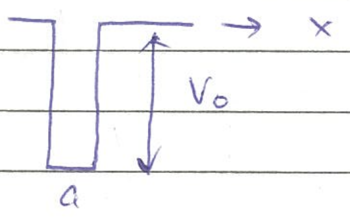
$\frac{d\Psi(x)}{dx}$: single valued

in some more "violent" case, $\frac{d\Psi}{dx}$ needs not to be continuous. However, if $V(x)$ is not bad, $\Psi(x)$, $\frac{d\Psi}{dx}$ should be continuous.

~~e.g. $V(x) = \delta(x)$~~

e.g. $U(x) = -a V_0 \delta(x)$

o



$U(x) = 0 \qquad |x| > \frac{a}{2}$

$U(x) = -V_0 \qquad |x| < \frac{a}{2}$

$= -V_0\, a \cdot \frac{1}{a} \qquad |x| < \frac{a}{2}$

$a \to 0 \quad \frac{1}{a} \to \delta(x)$, aV_0 fixed

$\therefore V(x) = -aV_0\, \delta(x)$

$$\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\Psi = (E - U(x))\,\Psi(x) = (E + aV_0\delta(x))\,\Psi(x) \quad ①$$

$$\varepsilon \to 0^+, \int_{-\varepsilon}^{\varepsilon} ① \Rightarrow \frac{-\hbar}{2m}\left(\frac{d\Psi}{dx}\Big|_{0^+} - \frac{d\Psi}{dx}(0^-)\right) = \int_{-\varepsilon}^{\varepsilon} (E + aV_0\delta(x))\Psi(x$$

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$\psi(x)$ finite

$$\therefore \int_{-\varepsilon}^{\varepsilon} E\,\psi(x)\,dx \to 0 \quad \text{as } \varepsilon \to 0$$

but $\int_{-\varepsilon}^{\varepsilon} aV_0\,\delta(x)\,\psi(x)\,dx = aV_0\,\psi(0)$

$$\therefore \frac{-\hbar^2}{2m}\left(\frac{d\varphi(0^+)}{dx} - \frac{d\varphi(0^-)}{dx}\right) = aV_0\,\psi(0) \quad -- ②$$

$x>0$ $\quad \frac{-\hbar^2}{2m}\frac{d^2\varphi}{dx^2} = E\psi$

$$\therefore \psi = A\,e^{-Kx}, \quad K = \sqrt{-2mE}/\hbar$$

Similarly

$x<0$ $\quad \psi = B\,e^{Kx}$ $\quad \psi(0)$ cont! $\Rightarrow A=B$

$$② \Rightarrow \frac{-\hbar^2}{2m}\left[-KA - BK\right] = aV_0 A$$

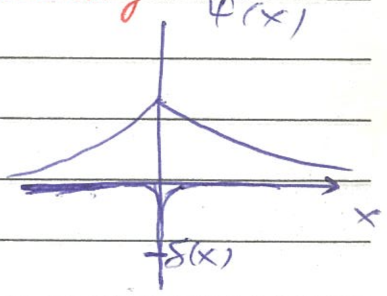
$$\therefore \frac{\hbar^2}{2m}\cdot 2K = aV_0$$

$$K = \frac{aV_0 m}{\hbar^2} = \sqrt{-2mE}/\hbar$$

attractive potential in

(mention superconductivity at $d \le 2$)

$$\therefore E = -\frac{ma^2V_0^2}{2\hbar^2}$$



$\therefore$ There is only one bound state.

Which means when we shrink the width of a potential well, while keeping aV_0 fixed, there will be only one bound state survived!

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Another derivation :

$$\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) - V_0\delta(x)\psi(x) = E\psi(x)$$

$$\psi(x) = \int\frac{dk}{2\pi}\psi(k)e^{ikx} \quad \Rightarrow \quad \psi(k) = \frac{V_0}{\frac{\hbar^2 k^2}{2m}+|E|}\int\frac{dk'}{2\pi}\psi(k')$$

$$\Rightarrow \frac{1}{V_0} = \int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{1}{\frac{\hbar^2}{2m}k^2+|E|} \qquad k = \sqrt{\frac{2m|E|}{\hbar^2}}\,x$$

$$= \frac{1}{2\pi}\frac{1}{|E|}\sqrt{|E|}\underbrace{\int_{-\infty}^{\infty}\frac{dx}{x^2+1}}_{\substack{\shortparallel\\ \pi}} \times \sqrt{\frac{2m}{\hbar^2}}$$

$$= \frac{1}{2}\frac{1}{\sqrt{|E|}}\sqrt{\frac{2m}{\hbar^2}}$$

$$\therefore \frac{4}{V_0^2} = \frac{2m}{\hbar^2}\frac{1}{|E|}, \qquad |E| = \frac{m}{2\hbar^2}V_0^2$$

$$\therefore E = -\frac{mV_0^2}{2\hbar^2}$$

Let $\int\frac{dk'}{2\pi}\psi(k') = \alpha$

$$\psi(k) = \frac{\alpha V_0}{\frac{\hbar^2}{2m}\left(k^2+\left(\frac{m}{\hbar^2}V_0\right)^2\right)} \equiv \frac{2m\alpha V_0}{\hbar^2}\frac{1}{k^2+\beta^2}$$

$$\therefore \psi(x) = \int\frac{dk}{2\pi}\frac{1}{k^2+\beta^2}e^{ikx}\cdot\frac{2m\alpha V_0}{\hbar^2}$$

$$= \frac{1}{2\beta}e^{-\beta|x|}\frac{2m\alpha V_0}{\hbar^2}, \qquad \beta = \frac{mV_0}{\hbar^2}$$

$$= k$$

Attractive potential for $d=1,2,3$

$$V(\vec{r}) = -U_0\delta(\vec{r})$$

$$-\nabla^2\psi - V_0\delta(\vec{r})\,\psi = E\psi$$

$$\psi(r) = \sum_k \psi_k e^{i\vec{k}\cdot\vec{r}}$$

$$\delta(\vec{r})\psi(\vec{r}) = \psi(0)\delta(\vec{r})$$

$$\Rightarrow \sum_k (k^2-E)\,\psi_k\, e^{i\vec{k}\cdot\vec{r}} \overset{\swarrow}{=} \sum_k V_0\,\psi(0)\, e^{ik\cdot r}$$

$$\therefore\ \psi_k = \frac{v_0}{k^2-E}\psi(0) = \frac{v_0}{k^2-E}\sum_{k'}\psi_{k'}$$

$$\sum_k \quad \therefore \Rightarrow \frac{1}{v_0} = \sum_{k^2>0}\frac{1}{k^2-E}$$

weak attraction. $v_0 \to 0^+$ if $E<0$. $\sum_{k^2>0}\frac{1}{k^2+|E|}$ has $\to\infty$

$$\because \sum_{k^2}\frac{1}{k^2+|E|} \propto \int_0^{\frac{2\pi}{a}} d\vec{k}\,\frac{1}{k^2+|E|} \underset{\uparrow}{\sim} \int_0^{\frac{2\pi}{a}} d\vec{k}\,\frac{1}{k^2}$$

$\because v_0\to 0.\ E\to 0$

diverges only for $d=1,$ & 2

$\therefore$ a bound state allows !

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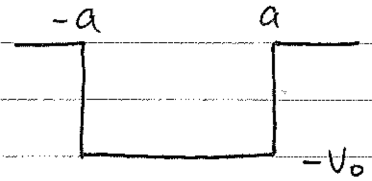
Two types of states

example



$V = 0 \qquad |x| > a$

$\;\; = -V_0 \qquad |x| < a$

$|x| > a, \qquad \psi'' + \frac{2m}{\hbar^2} E \psi = 0$

$|x| < a, \qquad \psi'' + \frac{2m}{\hbar^2} (E + V_0) \psi = 0$

bound state $\quad E < 0 \quad , \quad \alpha \equiv \sqrt{\frac{2m}{\hbar^2} |E|} \quad , \quad \beta = \sqrt{\frac{2m}{\hbar^2} (V_0 - |E|)}$

$$\psi(x) = \begin{cases} \cancel{A e^{\alpha x}} + B e^{-\alpha x} & x > a \\ C \sin\beta x + D \cos\beta x & |x| < a \\ F e^{\alpha x} + \cancel{G e^{-\alpha x}} & x < -a \end{cases}$$

quantum tunneling : $\quad |\psi|^2 \neq 0 \quad$ for $\quad |x| > a$

$\psi(a^+) = \psi(a^-) \Rightarrow B e^{-\alpha a} = C \sin\beta a + D \cos\beta a$

$\psi(-a^+) = \psi(-a^-) \Rightarrow F e^{-\alpha a} = -C \sin\beta a + D \cos\beta a$

$$\Rightarrow \begin{array}{l} 2C \sin\beta a = (B - F) e^{-\alpha a} \quad \text{---} ① \\ 2D \cos\beta a = (B + F) e^{-\alpha a} \quad \text{---} ② \end{array}$$

$\frac{d\psi}{dx}\Big|_{a^+} = \frac{d\psi}{dx}\Big|_{a^-} \Rightarrow -\alpha B e^{-\alpha a} = C\beta \cos\beta a - D\beta \sin\beta a$

$\frac{d\psi}{dx}\Big|_{-a^+} = \frac{d\psi}{dx}\Big|_{-a^-} \Rightarrow \alpha F e^{-\alpha a} = C\beta \cos\beta a + D\beta \sin\beta a$

$$\Rightarrow \begin{array}{l} 2\beta C \cos\beta a = \alpha (F - B) e^{-\alpha a} \quad \text{---} ③ \\ 2\beta D \sin\beta a = \alpha (F + B) e^{-\alpha a} \quad \text{---} ④ \end{array}$$

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$C \neq 0$, $B \neq F$ ③/① ⇒ $\beta \cot \beta a = -\alpha$

$D \neq 0$, $B \neq -F$ ④/② ⇒ $\beta \tan \beta a = \alpha$ >

Can't be satisfied at the same time $[\,|\tan\theta + \cot\theta| \geq 2\,]$

∴ Two classes of solutions

(i) $C \neq 0$, $B \neq F$, $D = 0$, $B = -F$

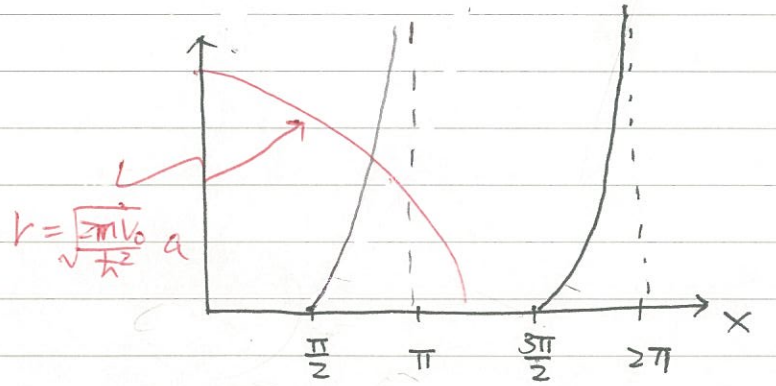
$$\psi(x) = \begin{cases} B e^{-\alpha x} & x > a \\ C \sin \beta x & |x| < a \\ -B e^{\alpha x} & x < -a \end{cases}$$

odd

$\beta \cot \beta a = -\alpha$

$\beta a \equiv X$, $\alpha a \equiv Y$, $X \cot X = -Y$

$$X^2 + Y^2 = a^2(\alpha^2 + \beta^2) = \frac{2mV_0}{\hbar^2} a^2$$



⇒ only $Y > \frac{\pi}{2}$

i.e. $V_0 a > \frac{\pi^2 \hbar^2}{8ma}$

has solutions !!

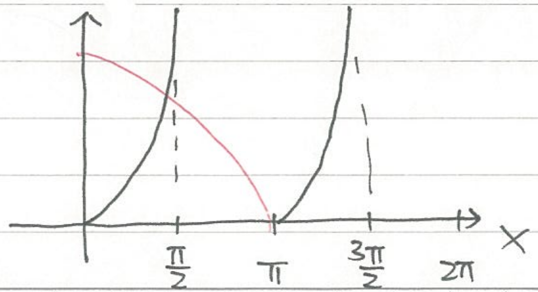
(ii) $D \neq 0$, $B \neq -F$, $C = 0$, $B = F$

$$\psi(x) = \begin{cases} B e^{-\alpha x} & x > a \\ D \cos \beta x & |x| < a \\ B e^{\alpha x} & x < a \end{cases}$$

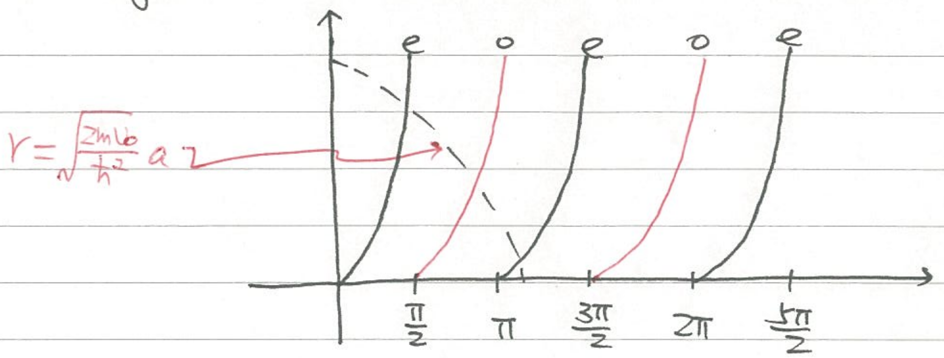
even ⇒ always has solutions !

$$X^2 + Y^2 = \frac{2mV_0}{\hbar^2} a^2$$

$Y = X \tan X$



Altogether we have



several important features

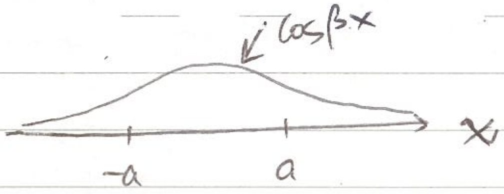
(i) ground state has no node (even), $\underline{\bar{X} < \frac{\pi}{2}}$

π

βa

true for other dimension

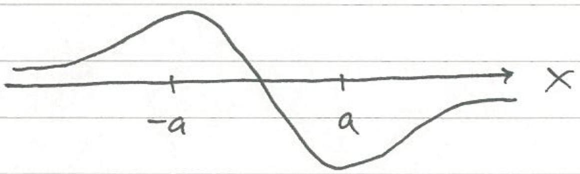
$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\right.$ is small if no node!$\left.\right)$



1st excited state $\frac{\pi}{2} < \bar{X} < \pi$

↓

λ. smaller



one node

K.E. ↑

2st .. 2 nodes

⋮

Oscillation theorem

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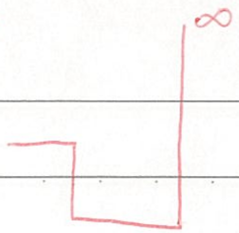
4.

therefore ↳



~~not~~ necessarily have bound state!

(ii) $\boxed{A=\underset{\sim}{2}V_0a}$ fixed. $a \to 0$

$$r=\sqrt{\frac{2mV_0a}{\hbar^2}}\sqrt{a} \to 0$$

only one solution survives

$$Y = X\tan X \simeq X^2$$

$$(\beta a)^2 \simeq \alpha a \quad \therefore \quad \alpha \simeq \beta^2 a = \frac{2m}{\hbar^2}(V_0a - |E|a)$$

with $\nearrow 0$ over $|E|a$

$$\rightarrow \frac{2m}{\hbar^2}V_0a = \frac{m}{\hbar^2}A$$

$$\therefore |E| = \frac{m}{2\hbar^2}A^2, \quad \text{i.e.} \quad E = -\frac{m}{2\hbar^2}A^2.$$

$$\Leftrightarrow \quad V=-A\delta(x), \quad E=-\frac{m}{2\hbar^2}A^2,$$

Valid when $r<\pi/2$

$$V_0a^2 \le \frac{\pi^2\hbar^2}{8m}$$

$\therefore$ for a given V_0, $a^2 \le \frac{\pi^2\hbar^2}{8mV}$

(iii) $V_0 \to \infty$

$E+V_0 \Rightarrow E$

First shift $0 \to V_0$, $-V_0 \to 0$

$$\Rightarrow \underline{E>0} \qquad \alpha=\sqrt{\frac{2m(V_0-E)}{\hbar^2}}, \quad \beta=\sqrt{\frac{2mE}{\hbar^2}}$$

$\alpha \to \infty \quad \therefore \quad \psi(x) \to 0 \quad$ for $|x|>a$

$$X^2+Y^2=\frac{2mV_0a^2}{\hbar^2} \to \infty$$

intersections happen at $X=\frac{\pi}{2}, \pi, \frac{3\pi}{2}, 2\pi, \ldots$

$Y = X\tan x$, $X\cot x$, ...

$$\therefore X=\frac{n\pi}{2}, =\beta a, \quad E_n=\frac{n^2\pi^2\hbar^2}{8ma^2}$$

n=odd, $Y=X\tan X$, $\psi = D\cos\beta x \quad |x|<a$

n=even, $Y=-X\cot X$, $\psi = C\sin\beta x$, $|x|<a$

$n=1$, $\psi = D\cos\frac{\pi}{2a}x$ ground state

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Scattering state : $(E>0)$

$\xrightarrow{F}$ $\quad$ $\xrightarrow{A}$

$\xleftarrow[G]{}$

$$\psi(x) = Ae^{ikx} \qquad x>a. \qquad k=\sqrt{\frac{2m}{\hbar^2}E}$$

$$= C\sin\beta x + D\cos\beta x \qquad |x|<a \qquad \beta=\sqrt{\frac{2m}{\hbar^2}(E+V_0)}$$

$$= Fe^{ikx} + Ge^{-ikx} \qquad x<-a$$

$k=i\alpha$

$F=0$

$$G = i\frac{\sin 2\beta a}{2k\beta}(\beta^2-k^2)A$$

$$A = \frac{e^{-2ika}}{\cos 2\beta a - i\frac{\sin 2\beta a}{2k\beta}(k^2+\beta^2)}F$$

$\frac{A}{F}=\infty$

transmission coefficient $T \equiv \left|\frac{A}{F}\right|^2 \Rightarrow$

$$T^{-1} = 1+\frac{V_0^2}{4E(E+V_0)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)$$

$x>-a$, $J=\frac{\hbar^2}{2mi}(\psi^*\partial\psi-\psi\partial\psi^*) = \underbrace{\frac{\hbar k}{m}|F|^2}_{J_{incident}} - \underbrace{\frac{\hbar k}{m}|G|^2}_{J_{reflection}}$

x a, $\underbrace{J=\frac{\hbar k}{m}|A|^2}_{J_{transimission}}$

7

$\therefore$ $T=\left|\frac{J_{transimission}}{J_{incident}}\right|$

$$R=\left|\frac{J_{ref}}{J_{inc}}\right| = \left|\frac{G}{F}\right|^2$$

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Complete set must include both scattering states and bound states :

$$|\psi\rangle = \sum_{E<0} a_E |E\rangle + \overset{\swarrow \int dE}{\sum_{E>0}} b(E)\,|E\rangle$$

if $a_E = 0$ for all E

$$\langle\psi|\hat{H}|\psi\rangle = \int dE\, |b(E)|^2 \text{ always} > 0$$

this implies for $E<0$ $|E\rangle$ can not be expressed in terms $\sum_{E>0} b(E)\,|E\rangle$!

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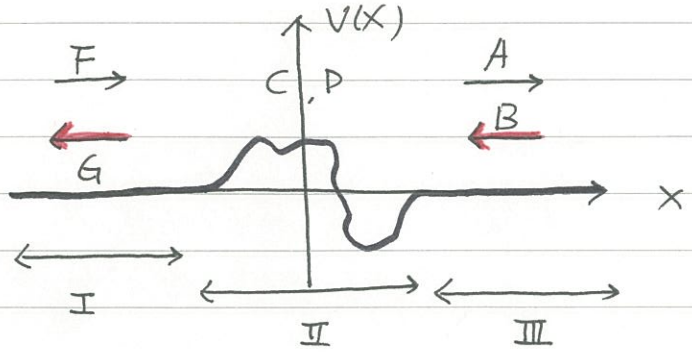
The Scattering matrix

* The most general situation that one considers is as follows :



A, G out going
B. F in coming

III : $\psi(x) = Ae^{ikx} + Be^{-ikx}$

II : $\psi(x) = Cf(x) + Dg(x)$ ⇒ $f(x), g(x)$ two linearly independent particular solutions. ↓ can be choosen to be real !

I : $\psi(x) = Fe^{ikx} + Ge^{-ikx}$

boundary conditions : I/II ψ, ψ' continuous
II/III ψ, ψ'

⇒ 4 equations eliminate 4 variables leave two independent unknowns.

We may choose them to be B & F !

∵ All equations are linear in A, B, C, D, F & G.

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∴ We can write :

$$G = S_{11}F + S_{12}B$$

$$A = S_{21}F + S_{22}B$$

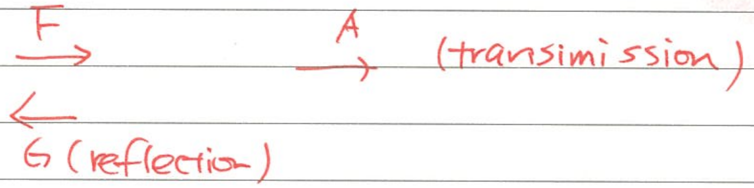
independent of A, B, G, F

or equivalently

$$\underset{\underset{\text{outgoing}}{\leftarrow\ \rightarrow}}{\begin{pmatrix}G\\A\end{pmatrix}} = \underbrace{\begin{pmatrix}S_{11} & S_{12}\\ S_{21} & S_{22}\end{pmatrix}}_{S}\underset{\underset{\text{incomming}}{\rightarrow\ \leftarrow}}{\begin{pmatrix}F\\B\end{pmatrix}} \qquad — ①$$

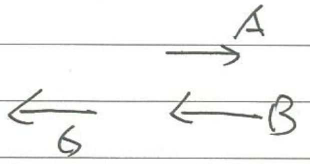
S ≡ Scattering matrix or simply S-matrix

$B=0$:



$$\therefore R_L = \left|\frac{G}{F}\right|^2_{B=0} = |S_{11}|^2 , \quad T_L = \left|\frac{A}{F}\right|^2_{B=0} = |S_{21}|^2$$

$F=0$



$$R_R = \left|\frac{A}{B}\right|^2_{F=0} = |S_{22}|^2 , \quad T_R = \left|\frac{G}{B}\right|^2_{F=0} = |S_{21}|^2$$

Obviously, if II is symmetric, one has

$R_L = R_R$, $T_L = T_R$

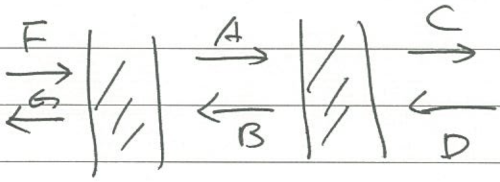
In 1D,

it is more convenient to use another representation, called the transfer matrix:

independent of A, B, G, F.

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} F \\ G \end{pmatrix} \equiv T \begin{pmatrix} F \\ G \end{pmatrix} \quad — ②$$

This has the advantage for combining sequent scattering centers:



$$\begin{pmatrix} C \\ D \end{pmatrix} = T^{(2)} \begin{pmatrix} A \\ B \end{pmatrix} \qquad \begin{pmatrix} A \\ B \end{pmatrix} = T^{(1)} \begin{pmatrix} F \\ G \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} C \\ D \end{pmatrix} = T^{(2)} T^{(1)} \begin{pmatrix} F \\ G \end{pmatrix} \qquad \therefore T \equiv T^{(2)} T^{(1)}$$

The relation of T to S is:

$$\because B = T_{21} F + T_{22} G \quad \therefore G = -\frac{T_{21}}{T_{22}} F + \frac{1}{T_{22}} B$$

$$\therefore A = T_{11} F + T_{12} G$$

$$= \frac{T_{11} T_{22} - T_{12} T_{21}}{T_{22}} F + \frac{T_{12}}{T_{22}} B$$

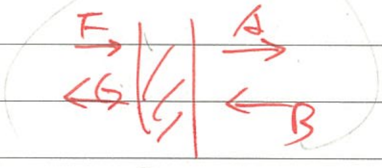
$$\therefore S_{21} = \frac{T_{11} T_{22} - T_{12} T_{21}}{T_{22}}, \quad S_{22} = \frac{T_{12}}{T_{22}}$$

$$S_{11} = -\frac{T_{21}}{T_{22}}, \quad S_{12} = \frac{1}{T_{22}}$$

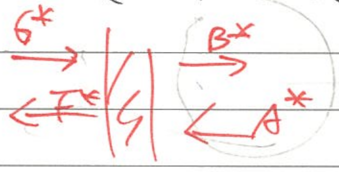
The symmetry properties of T is easier to be explored.

Time - reversal invariant

if
$$\begin{cases} Ae^{ikx}+Be^{-ikx} \\ \cancel{Cf(x)+Dg(x)} \\ Fe^{ikx}+Ge^{-ikx} \end{cases}$$
is a solution



$$\Rightarrow \begin{cases} A^{*}e^{-ikx}+B^{*}e^{ikx} \\ \cancel{C^{*}f(x)+D^{*}g(x)}, \\ F^{*}e^{-ikx}+G^{*}e^{ikx} \end{cases}$$
must be a solution too!



but (B^{*}, G^{*}) play the role of (A, F)

(A^{*}, F^{*}) " " (B, G)

Since T is independent of A, B, G, F, we have

$$\begin{pmatrix} B^{*} \\ A^{*} \end{pmatrix} = T \begin{pmatrix} G^{*} \\ F^{*} \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} G^{*} \\ F^{*} \end{pmatrix}$$

rearranging it

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} T_{22}^{*} & T_{21}^{*} \\ T_{12}^{*} & T_{11}^{*} \end{pmatrix} \begin{pmatrix} F \\ G \end{pmatrix}$$

Comparing with ② $\Rightarrow$ $T_{11} = T_{22}^{*}$. $T_{12} = T_{21}^{*}$

$$\therefore \quad T = \begin{pmatrix} T_{11} & T_{12} \\ T_{12}^{*} & T_{11}^{*} \end{pmatrix} \quad (\text{not Hermitian})$$

Unitarity

One can imagine that at $t=-\infty$, a wavepacket $\begin{pmatrix} F \\ B \end{pmatrix}$ comes in and at $t=\infty$, it comes out as $\begin{pmatrix} G \\ A \end{pmatrix}$

probability is conserved

$$\therefore \quad |A|^2 + |G|^2 = |B|^2 + |F|^2$$

$$\text{i.e.} \quad |A|^2 - |B|^2 = |T_{11} \overset{\updownarrow A}{F} + T_{12} G|^2 - |T_{12}^{*} F + T_{11}^{*} G|^2$$

$$= |F|^2 - |G|^2$$

$\therefore \; |T_{11}|^2 - |T_{12}|^2 = 1$ (coefficients of $|F|^2$ & $|G|^2$)

i.e. $\det T = I$.

Now, if $\begin{pmatrix} F \\ G \end{pmatrix} = \begin{pmatrix} 1 \\ r \end{pmatrix}$, $\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} t \\ 0 \end{pmatrix}$ (Substitute to ①
$\Rightarrow S_{11} = r$
$S_{21} = t$)

we have $\quad 0 = T_{12}^{*}\,{}^{\times} 1 + T_{11}^{*}\,{}^{\times} r$

$$\therefore r = -\frac{T_{12}^{*}}{T_{11}^{*}} \qquad t = T_{11} + T_{12} r$$

(reflection amplitude)

$$= \frac{|T_{11}|^2 - |T_{12}|^2}{T_{11}^{*}} = \frac{1}{T_{11}^{*}}$$

(transition amplitude)

$$\therefore T = \begin{pmatrix} \frac{1}{t^*} & -r^*/t^* \\ -r/t & \frac{1}{t} \end{pmatrix} \qquad T_{12} = -r^* T_{11} = -r^*/t^*$$

$$\det T = 1 \Rightarrow \frac{1}{|t|^2} - \frac{|r|^2}{|t|^2} = 1$$

$$\text{ie. } 1 = |r|^2 + |t|^2$$

Using these relations, we have

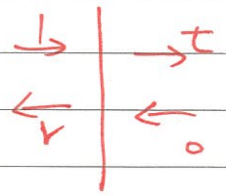
$$S_{12} = \frac{1}{T_{22}} = t$$

$$S_{21} = \frac{T_{11}T_{22} - T_{12}T_{21}}{T_{22}} = \frac{|T_{11}|^2 - |T_{12}|^2}{T_{22}} = \frac{1}{T_{22}} = t.$$

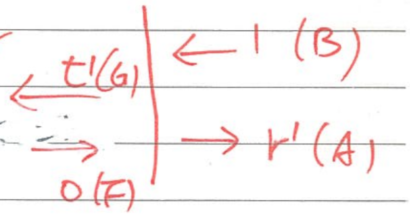
$$S_{11} = -\frac{T_{21}}{T_{22}} = -(-r/t) \times t = r$$

$$S_{22} = \frac{T_{12}}{T_{22}} = t \cdot \left(-\frac{r^*}{t^*}\right) = -r^*(t/t^*)$$

$$\therefore S = \begin{pmatrix} r & t \\ t & -r^*(t/t^*) \end{pmatrix}$$



or



$$\begin{pmatrix} t' \\ r' \end{pmatrix} = S \begin{pmatrix} 0 \\ 1 \end{pmatrix} \leftarrow$$

(for delta potential $-r^* t/t^* = r$!)

$\therefore t' = t, \; r' = -r^*(t/t^*)$

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* bound - state energies as poles of S

For bound states $E<0$, $\psi(x)$ must take the following form

$$\psi(x) = \begin{cases} Ae^{-\kappa x} & \text{III} \\ C f(x) + D g(x) & \text{II} \\ G e^{\kappa x} & \text{I} \end{cases}$$

$$\kappa = \sqrt{\frac{-2mE}{\hbar^2}}$$

This is the same as the scattering state by the substitution : $k = i\kappa$, $B=0$, $F=0$

But since $R_L = \left|\frac{G}{F}\right|^2_{B=0,\,F=0} = |S_{11}|^2$

$$T_L = \left|\frac{A}{F}\right|^2_{B=0,\,F=0} = |S_{21}|^2$$

$\therefore$ R_L, T_L must go to ∞ , Similarly
(i.e. $S_{11}, S_{21} \to \infty$)

S_{22}, S_{12} must $\to \infty$ too !

Indeed, from the calculation of scattering state, we have $S_{21} = \dfrac{A}{F} = \dfrac{\bar{e}^{i2ka}}{\cos 2\beta a - i\frac{\sin 2\beta a}{2k\beta}(k^2+\beta^2)}$

Substitute $k \to i\kappa$. $S_{21} = \dfrac{e^{2\kappa a}}{\cos 2\beta a - \frac{\sin 2\beta a}{2\kappa\beta}(\beta^2-\kappa^2)}$

which blows up at $\cot 2\beta a = \frac{\beta^2-K^2}{2K\beta}$

where $\beta=\sqrt{\frac{2m}{\hbar^2}(V_0-|E|)}$ $\quad K=\sqrt{\frac{2m|E|}{\hbar^2}}$ = previous α

$$\because \tan\frac{\phi}{2} = \pm\sqrt{1+\cot^2\phi} - \cot\phi$$

$$\therefore \tan\beta a = \pm\sqrt{1+\left(\frac{\beta^2-K^2}{2K\beta}\right)^2} - \frac{\beta^2-K^2}{2K\beta}$$

$$= \pm\frac{\beta^2+K^2}{2K\beta} - \frac{\beta^2-K^2}{2K\beta} = \begin{cases} \frac{K}{\beta} & + \\ -\beta/K & - \end{cases}$$

$\therefore \tan\beta a = K/\beta$ or $\cot\beta a = -K/\beta$

i.e. $\beta\tan\beta a = \alpha$ or $\beta\cot\beta a = -\alpha$

which are exactly the equations that bound-state energies must satisfy!