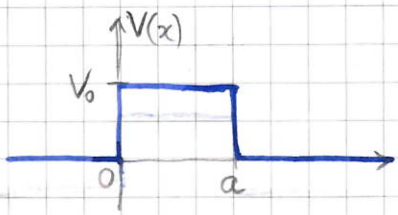
PROBLEMS CLASS 5 – 2/2/2024

Ex 53

TISE $$\left(-\frac{d^2}{dx^2} + V(x)\right)\psi(x) = k^2\psi(x)$$

SQUARE BARRIER/WELL POTENTIAL $$V(x) = \begin{cases} 0, & x<0 \\ V_0, & 0<x<a \\ 0, & x>a \end{cases}$$



1. Show that the matching conditions at $x = 0, a$, where $V(x)$ is discontinuous (but finite) are that $\psi(x)$, $\psi'(x)$ are continuous.

This can be proven in generality for a potential that is finite in a neighbourhood of x_0. Consider the infinitesimal neighbourhood $(x_0-\varepsilon, x_0+\varepsilon)$, with $\varepsilon>0$. Integrate the TISE once and twice:

ONCE: $$-\left[\psi'(x)\right]_{x_0-\varepsilon}^{x_0+\varepsilon} + \int_{x_0-\varepsilon}^{x_0+\varepsilon} dx\, V(x)\psi(x) = k^2\int_{x_0-\varepsilon}^{x_0+\varepsilon} dx\,\psi(x)$$

ψ, V bounded near $x_0 \Rightarrow$ integrals $\xrightarrow[\varepsilon\to 0^+]{} 0$.

$\Rightarrow \psi'(x)$ continuous at x_0.

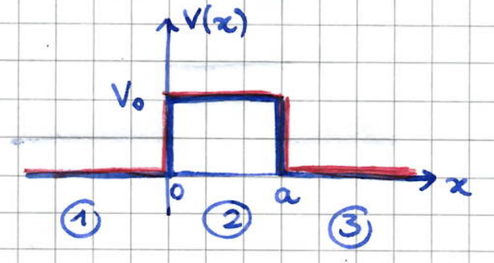
TWICE: $\int_{x_0-\varepsilon}^{x_0+\varepsilon} dx \int_{x_0-\varepsilon}^{x} dx'$

$$-\left[\psi(x)\right]_{x_0-\varepsilon}^{x_0+\varepsilon} + \underset{\substack{\downarrow\, \varepsilon\to 0\\ 0}}{2\varepsilon\,\psi'(x_0-\varepsilon)} + \underset{\substack{\downarrow\, \varepsilon\to 0\\ 0}}{\int_{x_0-\varepsilon}^{x_0+\varepsilon} dx \int_{x_0-\varepsilon}^{x} dx' \left(V(x')-k^2\right)\psi(x')} = 0.$$

$\Rightarrow \psi(x)$ continuous at x_0.

(YOU CAN QUOTE THIS RESULT IN THE EXAM IF USEFUL.)

2. Solve the SE in the three regions and impose the matching conditions to find the scattering solutions associated to $k^2>0$ (continuous spectrum), and determine $R(k), T(k)$ in terms of a & $\ell=\sqrt{k^2-V_0}$.



①, ③ : $-\frac{d^2}{dx^2}\psi = k^2\psi \quad \Rightarrow$ solutions $e^{\pm ikx}$

② : $-\frac{d^2}{dx^2}\psi = (k^2-V_0)\psi = \ell^2\psi \quad \Rightarrow$ " $e^{\pm i\ell x}$ $\quad (\ell^2 = k^2-V_0)$

Scattering solution:

$$\psi(x) = \begin{cases} e^{ikx} + R(k)e^{-ikx}, & x<0 \quad ① \\ A^{(k)}e^{i\ell x} + B^{(k)}e^{-i\ell x}, & 0<x<a \quad ② \\ T(k)e^{ikx}, & x>a \quad ③ \end{cases}$$

4 unknowns. Impose 2+2 matching conditions at $x=0, a$ to find unique scattering solution with unit flux of incident waves of wavenumber $k>0$.

ψ continuous at $x=0$: $\quad 1+R = A+B \quad$ ⓐ

" $\quad x=a$: $\quad Ae^{i\ell a}+Be^{-i\ell a} = Te^{ika} \quad$ ⓑ

ψ' continuous at $x=0$: $\quad ik(1-R) = i\ell(A-B) \quad$ ⓒ

" $\quad x=a$: $\quad i\ell(Ae^{i\ell a}-Be^{-i\ell a}) = ikTe^{ika} \quad$ ⓓ

First eliminate A & B. Since the RHS's of ⓑ & ⓓ are simpler, I'll use them to eliminate A & B.

$$ⓑ + \frac{ⓓ}{il} : \quad 2A e^{ila} = \left(1+\frac{k}{l}\right) T e^{ika}$$

$$ⓑ - \frac{ⓓ}{il} : \quad 2B e^{-ila} = \left(1-\frac{k}{l}\right) T e^{ika}$$

$$\Rightarrow \quad A = \frac{1}{2}\left(1+\frac{k}{l}\right) e^{i(k-l)a} T \,, \qquad B = \frac{1}{2}\left(1-\frac{k}{l}\right) e^{i(k+l)a} T \,.$$

Sub in ⓐ & ⓒ :

$$ⓐ : \quad 1 + R = \frac{1}{2}\left[\left(1+\frac{k}{l}\right) e^{-ila} + \left(1-\frac{k}{l}\right) e^{ila}\right] e^{ika} T$$

$$\frac{ⓒ}{ik} : \quad 1 - R = \frac{1}{2}\frac{l}{k}\left[\left(1+\frac{k}{l}\right) e^{-ila} - \left(1-\frac{k}{l}\right) e^{ila}\right] e^{ika} T$$

$$\Rightarrow ⓐ + \frac{ⓒ}{ik} : \quad 2 = \frac{1}{2} e^{ika} T \left[\left(1+\frac{l}{k}\right)\left(1+\frac{k}{l}\right) e^{-ila} + \left(1-\frac{k}{l}\right)\left(1-\frac{l}{k}\right) e^{ila}\right]$$

$$= \frac{1}{2} e^{ika} T \left[\frac{(k+l)^2}{kl} e^{-ila} - \frac{(k-l)^2}{kl} e^{ila}\right]$$

$$\Rightarrow \boxed{T(k) = \frac{4kl\, e^{-ika}}{(k+l)^2 e^{-ila} - (k-l)^2 e^{ila}} = \frac{4kl\, e^{-ika}}{-2i(k^2+l^2)\sin(la) + 4kl\cos(la)}} \qquad \left(l = \sqrt{k^2 - V_0}\right)$$

$$ⓐ - \frac{ⓒ}{ik} : \quad 2R = \frac{1}{2} e^{ika} T \left[\left(1-\frac{l}{k}\right)\left(1+\frac{k}{l}\right) e^{-ila} + \left(1-\frac{k}{l}\right)\left(1+\frac{l}{k}\right) e^{ila}\right]$$

$$= \frac{e^{ika} T}{2lk}\left[(k^2-l^2) e^{-ila} - (k^2-l^2) e^{ila}\right]$$

$$= \frac{e^{ika} T}{2lk}\, 2i \sin(la)\, (l^2-k^2) = -\sin(la)\cdot i\, \frac{k^2-l^2}{lk} e^{ika} T$$

$$\Rightarrow \boxed{R(k) = -i \sin(la)\, \frac{k^2-l^2}{2lk} e^{ika} T(k) = \frac{-2i(k^2-l^2)\sin(la)}{-2i(k^2+l^2)\sin(la) + 4kl\cos(la)}}$$

3. For which values of k is the square potential "transparent", i.e. $R(k) = 0$?

$R(k)=0$:

$$k^2 - \ell^2 = V_0 = 0 \quad \text{(no potential - trivial)}$$

or

$$\sin(\ell a) = 0 \iff \ell a = n\pi, \qquad n \in \mathbb{Z}$$

$$\iff k^2 - V_0 = \ell^2 = \left(\frac{n\pi}{a}\right)^2$$

$$\iff k^2 = V_0 + \left(\frac{n\pi}{a}\right)^2 .$$

For these values of k the incident wave is transmitted but not reflected:

$$R(k) = 0, \qquad T(k) = \frac{e^{-ika}}{\cos(n\pi)} = (-1)^n e^{-ika} .$$

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4. Write down the bound state solutions corresponding to the discrete spectrum $k^2 = -\mu^2 < 0$. Find the equations that determine implicitly the allowed values of μ in terms of ℓ (or V_0).

TO WRITE DOWN THE BOUND STATE SOLUTIONS (I won't do it explicitly):

1) Sub $k = i\mu$ in scattering solution, $\mu > 0$.
2) Divide through by $T(i\mu)$.
3) Choose $k = i\mu$ s.t. $\frac{1}{T(i\mu)} = 0$ to get rid of the unbounded $e^{-\mu x}$ term for $x \to -\infty$.

So look for poles of $T(k)$ on the positive imaginary axis.

- Poles of $T(k)$: $(k+\ell)^2 e^{-i\ell a} = (k-\ell)^2 e^{i\ell a}$

$$\Rightarrow \frac{k+\ell}{k-\ell} = \varepsilon e^{i\ell a}, \qquad \varepsilon = \pm 1$$

$$\Rightarrow k\left(1 - \varepsilon e^{i\ell a}\right) = -\ell\left(1 + \varepsilon e^{i\ell a}\right)$$

$$\Rightarrow k = -\ell \frac{1+\varepsilon e^{i\ell a}}{1-\varepsilon e^{i\ell a}} = \ell \frac{e^{i\ell a} + \varepsilon}{e^{i\ell a} - \varepsilon} = \ell \frac{e^{i\ell a/2} + \varepsilon e^{-i\ell a/2}}{e^{i\ell a/2} - \varepsilon e^{-i\ell a/2}}$$

$$\varepsilon = -1 \ : \quad k = i\,\ell \tan\left(\frac{\ell a}{2}\right) \quad\Updownarrow\quad \mu = \ell \tan\left(\frac{\ell a}{2}\right) \qquad , \qquad \varepsilon = +1 : \quad k = -i\ell \cot\left(\frac{\ell a}{2}\right) \quad\Updownarrow\quad \mu = -\ell \cot\left(\frac{\ell a}{2}\right) .$$

But we also have

$$\ell^2 = k^2 - V_0 \qquad \Leftrightarrow \qquad \ell^2 + \mu^2 = -V_0 \quad .$$

So we <u>need</u>

$$\begin{cases} \mu = \ell \tan\left(\frac{\ell a}{2}\right) \quad \vee \quad \mu = -\ell \cot\left(\frac{\ell a}{2}\right) \\ \ell^2 + \mu^2 = -V_0 \quad . \end{cases} \qquad (*)$$

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5. Do bound state solutions exist for $V_0 > 0$? And for $V_0 < 0$? In the latter case, use a graphical argument to show that a new bound state solution appears every time $\sqrt{-V_0}$ crosses a non-negative multiple of $\frac{\pi}{4a}$.

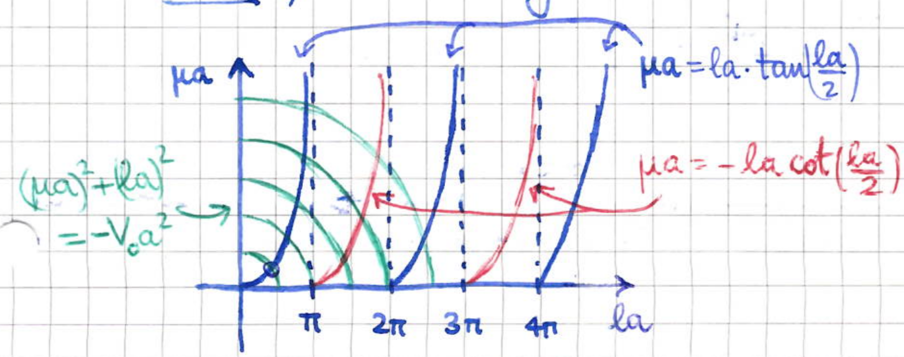
We seek solutions with <u>$\mu > 0$</u>.

- If <u>$V_0 > 0$</u>, need $\ell^2 < 0$. Set $\ell = iL$, ($L > 0$ wlog) and get

$$\mu = -L \tanh\left(\frac{aL}{2}\right) \leq 0 \quad \text{or} \quad \mu = -L \coth\left(\frac{aL}{2}\right) < 0 \ .$$

$\Rightarrow$ No bound state solutions, as expected since .

- If <u>$V_0 < 0$</u>, we can again exclude $\ell^2 < 0$ as above. For $\ell, \mu > 0$



Bound state solutions exist in correspondence of the intersections of the green $\frac{1}{4}$-circles with the blue or red curves.

- Since $\quad la\cdot\tan\left(\frac{la}{2}\right) \approx \frac{(la)^2}{2} \quad$ for $\quad la \ll 1$,

there is always at least a bound state solution if $V_0 < 0$.

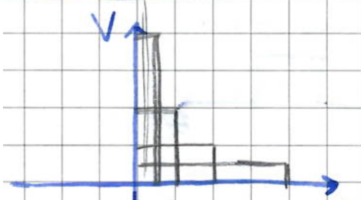
- A new bound state solution appears every time

$$\underbrace{\sqrt{-V_0}\cdot a}_{\text{Radius of the circle}} = n\pi \,, \qquad n = 0, 1, 2, \dots$$

$$\Leftrightarrow \underline{\sqrt{-V_0} = \frac{n\pi}{a}} \,, \qquad \underline{n = 0, 1, 2, \dots}$$

The eigenvalues k^2 in the discrete spectrum move down as $-V_0$ increases, and whenever $\sqrt{-V_0}$ crosses an integer multiple of $\frac{\pi}{a}$ a new bound state solution appears with $k^2 = 0$.

6. Show that when $a \to 0$, $V_0 \to \infty$ with $aV_0 = b$ fixed, the reflection and transmission coeff's reduce to those for $V(x) = b\,\delta(x)$.



$V(x) \to b\delta(x)$.

$$V_0 = \frac{b}{a} \to \infty \,, \quad \Rightarrow \quad l = \sqrt{k^2 - V_0} \approx \frac{\sqrt{-b}}{\sqrt{a}} \to \infty \Rightarrow la \to 0 .$$

$$T(k) = \frac{4kl\, e^{-ika}}{-2i(k^2+l^2)\sin(la) + 4kl\cos(la)} \approx \frac{4kl}{-2il^3 a + 4kl} \xrightarrow{l^2 a \to -b} \frac{2k}{2k + ib} = \frac{2ik}{2ik - b}$$

$$R(k) = -i\sin(la)\,\frac{k^2 - l^2}{2lk}\, e^{ika}\, T(k) \approx \frac{-l^2 a}{2ik}\,\frac{2ik}{2ik-b} \to \frac{b}{2ik-b} .$$