Physics III **Series 10**

1) Well, play!

2a) $x = y \cdot L \rightarrow \frac{dy}{dx} = \frac{1}{L} \rightarrow \frac{d}{dx} = \frac{1}{L} \cdot \frac{d}{dy}$

$V(x) = V_0 \cdot v(y)$

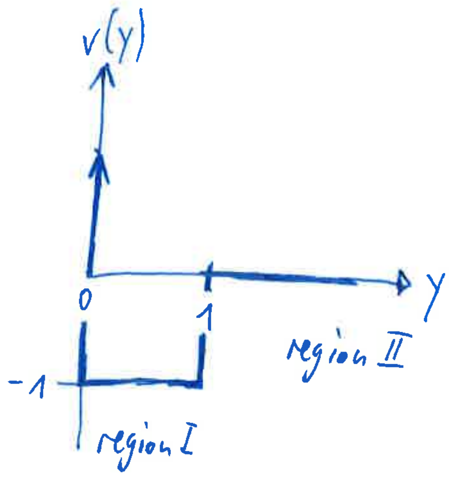
$E = V_0 \cdot \varepsilon$

Schrödinger equation:

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

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{1}{L^2}\frac{\partial^2 \psi}{\partial y^2} + V_0 v(y) = V_0 \cdot \varepsilon \cdot \psi(y) \quad \Big| : V_0$$

$$\underbrace{-\frac{\hbar^2}{2mV_0L^2}}_{=:\lambda} \cdot \frac{\partial^2 \psi}{\partial y^2} + v(y) = \varepsilon \psi(y)$$



b) generally: bound states $\rightarrow \varepsilon < 0$

i) Region I: $\psi(y<0) \equiv 0$; Schrödinger equation: $-\lambda \frac{\partial^2 \psi_I}{\partial y^2} + \underbrace{v_I(y)}_{=-1} = \varepsilon \psi_I(y)$

$$\Rightarrow \frac{\partial^2 \psi_I}{\partial y^2} = -\frac{\varepsilon + 1}{\lambda}\psi_I$$

ii) Region II: Schrödinger eq.: $v = 0$

$$\Rightarrow \frac{\partial^2 \psi_{II}}{\partial y^2} = -\varepsilon/\lambda \, \psi_{II}$$

Boundary conditions: $\psi_I(y=0) \overset{!}{=} 0$

$\psi_{II}(y \rightarrow \infty) \overset{!}{=} 0$ (normalization)

$\left.\begin{array}{l}\psi_I(y=1) = \psi_{II}(y=1) \\ \psi_I'(y=1) = \psi_{II}'(y=1)\end{array}\right\}$ wave function is continuous

Solution in region I: Ansatz (flat potential $\rightarrow$ plane waves!):

$$\psi_I = A_1 e^{-iky} + A_2 \cdot e^{iky}$$

$$\Rightarrow \frac{\partial^2 \psi}{\partial y^2} = -k^2 A_1 e^{-iky} - k^2 A_2 e^{+iky} = -k^2 \psi_I \overset{!}{=} -\frac{\varepsilon+1}{\lambda}\psi_I$$

$$\Rightarrow k^2 = \frac{\varepsilon + 1}{\lambda}$$

boundary condition: $\psi_I(y=0) \stackrel{!}{=} 0 = A_1 e^0 + A_2 e^0 = A_1 + A_2 \Rightarrow A_2 = -A_1$ (2)

$$\Rightarrow \underline{\underline{\psi_I}} = A\cdot(e^{-iky} - e^{+iky}) = \underline{\underline{2A\cdot\sin(ky)}}$$

ii) Ansatz for region 2: $\underline{\psi_{II} = B\cdot e^{-\kappa y}}$ (not $e^{+\kappa y} \to \infty$ for $y\to\infty$), $\underline{\underline{\kappa \in \mathbb{R}^+}}$

$$\Rightarrow \frac{\partial^2\psi_{II}}{\partial y^2} = \kappa^2 B e^{-\kappa y} \stackrel{!}{=} -\varepsilon/\lambda\, e^{-\kappa y} \Rightarrow \underline{\underline{\kappa^2 = -\varepsilon/\lambda}} \quad (>0 \text{ for } \varepsilon<0)$$

Boundary conditions: $\psi_I(1) = 2A\cdot\sin(k) \stackrel{!}{=} \psi_{II}(1) = B\cdot e^{-\kappa} \Rightarrow B = 2A\sin(k)\cdot e^{\kappa}$

$$\psi_I'(1) = \cancel{2}k\cancel{A}\cdot\cos(k) \stackrel{!}{=} \psi_{II}'(1) = -\kappa B e^{-\kappa} = -\kappa\cdot\cancel{2A}\sin(k)\cdot\underbrace{e^{\kappa}\cdot e^{-\kappa}}_{=1}$$

$$\Rightarrow \frac{\sin(k)}{\cos(k)} \equiv \tan(k) = -\frac{k}{\kappa}$$

or $\underline{\underline{\tan\left(\sqrt{\frac{\varepsilon+1}{\lambda}}\right)}} = -\frac{\sqrt{\frac{\varepsilon+1}{\lambda}}}{\sqrt{-\varepsilon/\lambda}} = \underline{\underline{-\sqrt{\frac{\varepsilon+1}{-\varepsilon}}}}$

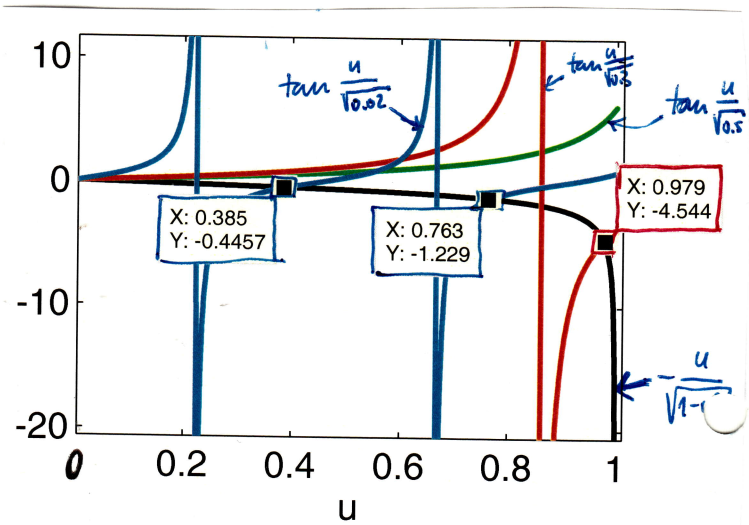
Finding the solutions graphically:

set $u = \sqrt{\varepsilon+1} \Rightarrow \varepsilon = u^2-1$

$$\Rightarrow \tan(u/\sqrt{\lambda}) = -\frac{u}{\sqrt{1-u^2}}$$

Since $\varepsilon\in[-1,0] \Rightarrow u\in[0,1]$

To the right, both sides are plotted for different λ. (right side is independent of λ!)



The values for u can be read off graphically or found numerically [Matlab: find 0 in $y = \tan(\frac{u}{\sqrt{\lambda}}) + \frac{u}{\sqrt{1-u^2}}$]

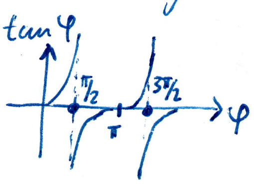
From the values of u we obtain ε and thus the energy of the bound state, E.

For a given λ, how many bound states are there?.

We obtain a bound state for every divergence of the tan in the interval $[0,1]$ of u.

$\Rightarrow$ Divergences of $\tan(\varphi)$ are at $\varphi = (2n+1)\frac{\pi}{2}$, $n\in\mathbb{N}_0$ (rest not relevant)

$$\stackrel{!}{=} \frac{u}{\sqrt{\lambda}} \quad \text{(argument of tan)}$$



$\Rightarrow$ with decreasing λ more divergences move into $[0,1]$ at $u=1$

At $u=1$ we have thus $(2n+1)\frac{\pi}{2} = \frac{1}{\sqrt{\lambda}}$ or $\lambda_n = \frac{4}{(2n+1)^2 \cdot \pi^2}$, which is the smallest λ that has n bound states (divergences), not more.

③

For example: $n=0 \Rightarrow \lambda_0 = \frac{4}{\pi^2} \Rightarrow$ For $\lambda > \lambda_0$ there are no bound states

$n=1 \Rightarrow \lambda_1 = \frac{4}{9\pi^2} \Rightarrow$ For $\lambda_1 < \lambda < \lambda_0$ there ~~are~~ is exactly one bound state.

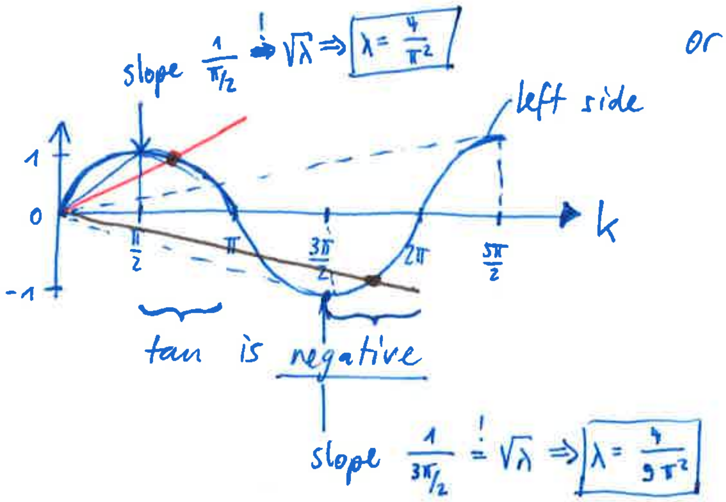
$n=2 \Rightarrow \ldots$

Alternative graphical solution:

We can write the matching condition $\frac{\sin(k)}{\cos(k)} = -\frac{k}{\kappa}$ (<0 !) a bit different:

$$\frac{\cos^2 k}{\sin^2 k} = \frac{\kappa^2}{k^2} \overset{!}{=} \frac{1-\sin^2 k}{\sin^2 k} = \frac{1}{\sin^2 k} - 1 \Rightarrow \sin^2(k) = \frac{k^2}{k^2+\kappa^2} = \frac{\frac{\varepsilon+1}{\lambda}}{\frac{\varepsilon+1}{\lambda} - \frac{\varepsilon}{\lambda}} = \varepsilon + 1 \underset{\substack{\uparrow \\ \lambda = \frac{\varepsilon+1}{k^2}}}{=} \lambda \cdot k^2$$

or $\sin(k) = \pm\sqrt{\lambda} \cdot k \propto k$ with slope $\sqrt{\lambda}$



$\Rightarrow$ same result as above

(note that the other crossing points lead to $\tan(k) > 0$ and are thus no solutions)

2c) For $E>0$ all energies are larger than the potential energy step and we expect that the particle can move freely in $y>0$ and that all energies are allowed (i.e. no discrete state due to confinement).

We show the continuous (all $E>0$!) spectrum by explicit construction.

Our intuition (to be) remembers that for free states the following Ansatz for the wave function is often a solution (we will briefly show another below):

region 1: $\Psi_I = A \cdot \sin(k_I y)$ as above, e.g. $\Psi_I(y=0) = 0$.

$\Psi_{II} = B \cdot \sin(k_{II} y + \delta)$, i.e. a phase shifted harmonic oscillation (plane wave)

Boundary conditions at $y=1$ (as above): $\Psi_I(1) = A \cdot \sin(k_I) \overset{!}{=} \Psi_{II}(1) = B \cdot \sin(k_{II} + \delta)$

and $\Psi_I'(1) = k_I A \cdot \cos(k_I) \overset{!}{=} \Psi_{II}'(1) = k_{II} B \cdot \cos(k_{II} + \delta)$

Dividing the two equations gives us

$$\tan(k_I) = \frac{k_I}{k_{II}}\cdot\tan(k_{II}+\delta) \underset{\uparrow}{=} \frac{k_I}{k_{II}}\cdot\frac{\tan(k_{II})+\tan(\delta)}{1-\tan(k_{II})\cdot\tan(\delta)}$$

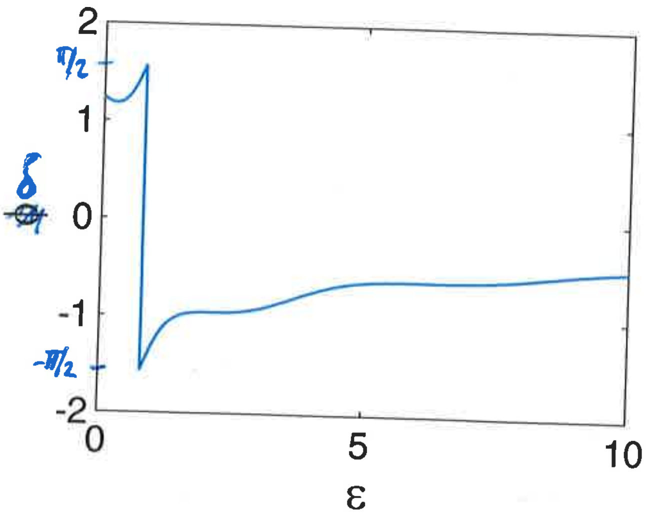
Bronstein, p80
eq. 2.86

$\Rightarrow$ solving for $\tan(\delta)$: $\frac{k_{II}}{k_I}\left[\tan(k_I) - \tan(k_I)\tan(k_{II})\tan(\delta)\right] = \tan(k_{II})+\tan(\delta)$

$$\frac{k_{II}}{k_I}\tan(k_I) - \tan(k_{II}) = \tan(\delta)\left[1+\frac{k_{II}}{k_I}\tan(k_I)\tan(k_{II})\right]$$

or $$\tan(\delta) = \frac{k_{II}/k_I\cdot\tan(k_I) - \tan(k_{II})}{1+\frac{k_{II}}{k_I}\tan(k_I)\cdot\tan(k_{II})}$$

Since the Schrödinger equation is identical to 2b, one obtains directly $k_I = \sqrt{\frac{\varepsilon+1}{\lambda}}$ and $k_{II} = \sqrt{\varepsilon/\lambda}$. A and B one would obtain from normalization. The resulting phase δ is plotted to the right.



Alternative Ansatz (only one is required!)

also plane waves!

One can also use the Ansatz $\varphi_{II} = B\sin(k_{II}y)+C\cdot\cos(k_{II}y)$, which leads to the boundary conditions: i) $A\cdot\sin(k_I) \overset{!}{=} B\cdot\sin(k_{II}) + C\cdot\cos(k_{II})$

ii) $k_I A\cos(k_I) \overset{!}{=} k_{II}B\cos(k_{II}) - k_{II}C\sin(k_{II})$

Solving for B: $$C \overset{i)}{=} \frac{A\sin(k_I) - B\sin(k_{II})}{\cos(k_{II})} \overset{ii)}{=} \frac{Bk_{II}\cos(k_{II}) - Ak_I\cos(k_I)}{k_{II}\cdot\sin(k_{II})}$$

$$\frac{B\sin(k_{II})}{\cos(k_{II})} + \frac{B\cos(k_{II})}{\sin(k_{II})} = \frac{A\sin(k_I)}{\cos(k_{II})} + \frac{k_I}{k_{II}}\frac{A\cos(k_I)}{\sin(k_{II})}$$

$$B\cdot\frac{\overbrace{\sin^2(k_{II})+\cos^2(k_{II})}^{\equiv 1}}{\cancel{\sin(k_{II})\cdot\cos(k_{II})}} = A\cdot\frac{k_{II}\sin(k_I)\sin(k_{II}) + k_I\cos(k_I)\cos(k_{II})}{k_{II}\cancel{\sin(k_{II})\cdot\cos(k_{II})}}$$

$$\Rightarrow B = A\left(\sin(k_I)\sin(k_{II}) + \frac{k_I}{k_{II}}\cos(k_I)\cos(k_{II})\right)$$

and $$C = \frac{A}{\cos(k_{II})}\left(\underbrace{\sin(k_I) - \sin^2(k_{II})\sin(k_I)}_{\sin(k_I)[\underbrace{1-\sin^2(k_{II})}_{\cos^2(k_{II})}]} - \frac{k_I}{k_{II}}\sin(k_{II})\cos(k_I)\cos(k_{II})\right)$$

$$= A\left[\sin(k_I)\cos(k_{II}) \underset{\uparrow}{-} \frac{k_I}{k_{II}}\cos(k_I)\sin(k_{II})\right]$$, i.e. a solution for all E!

(we can obtain the phase δ by $\tan(\delta) = \frac{C}{B}$ to connect to the above solution)

$$V(x) := -\alpha\,\delta(x)$$

$$P(k > k_0) = ? \qquad k_0 = m\alpha/\hbar^2$$

From lecture: $\psi(x) = B\,e^{-\kappa|x|}$

normalize:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx := 1 = 2|B|^2 \int_0^{\infty} e^{-2\kappa|x|} dx = \frac{|B|^2}{\kappa}$$

$$B = \sqrt{\kappa} = \frac{\sqrt{m\alpha}}{\hbar} \Rightarrow k_0 = \kappa\,!$$

$$\psi(x) = \sqrt{\frac{m\alpha}{\hbar^2}}\, e^{-m\alpha|x|/\hbar^2} \qquad E = -\frac{m\alpha^2}{2\hbar^2} < 0 \quad \text{Bound-state}$$

$\downarrow$

$$\psi(x,t) = \sqrt{\frac{m\alpha}{\hbar^2}}\, e^{-m\alpha|x|/\hbar^2}\, \underbrace{e^{-iEt/\hbar}}_{k \text{ and } x \text{ independent}}$$

momentum distribution

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx}\,\psi(x)\,dx = \frac{1}{\sqrt{2\pi}}\sqrt{\kappa}\, \underbrace{\int_{-\infty}^{\infty} e^{-ikx} e^{-\kappa|x|} dx}$$

$$\int_{-\infty}^{\infty} e^{ikx} e^{-\kappa|x|} dx = \int_{-\infty}^{0} e^{-i(k+i\kappa)x} dx + \int_0^{\infty} e^{-i(k-i\kappa)x} dx$$

$$= \left.\frac{e^{-i(k+i\kappa)x}}{-i(k+i\kappa)}\right|_{-\infty}^{0} + \left.\frac{e^{-i(k-i\kappa)x}}{-i(k-i\kappa)}\,(*)\right|_0^{\infty} = \frac{1}{-i(k+i\kappa)} - \frac{1}{-i(k-i\kappa)} =$$

$$= \frac{+ik+\kappa-ik+\kappa}{k^2+\kappa^2} = \frac{2\kappa}{k^2+\kappa^2} \qquad \tilde{F}(\exp\ \cancel{\text{decay}}\ \text{decay}) \to \text{Lorentzian}$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \sqrt{\kappa} \cdot \frac{2\kappa}{k^2+\kappa^2} = \sqrt{\frac{2}{\pi}} \frac{\kappa^{3/2}}{k^2+\kappa^2}$$

$$\phi(k,t) = \sqrt{\frac{2}{\pi}} \frac{\kappa^{3/2} \cdot e^{-iEt/\hbar}}{k^2+\kappa^2}$$

$$P(k>\kappa) = \int_\kappa^\infty |\phi(k,t)|^2 \, dk = \frac{2}{\pi} \int_\kappa^\infty \frac{\kappa^3}{(k^2+\kappa^2)^2} \, dk$$

$$= \frac{1}{\pi} \left[\frac{k \cdot \kappa}{k^2+\kappa^2} + \operatorname{arctg}\left(\frac{k}{\kappa}\right) \right]_\kappa^\infty = \frac{1}{\pi} \cdot 0 - \frac{1}{\pi} \cdot \frac{1}{2} + \frac{1}{\pi} \frac{1}{2} \pi - \frac{1}{\pi} \cdot \pi/4$$

$$= \underline{\underline{\frac{1}{4} - \frac{1}{2\pi}}} \sim 0.091$$