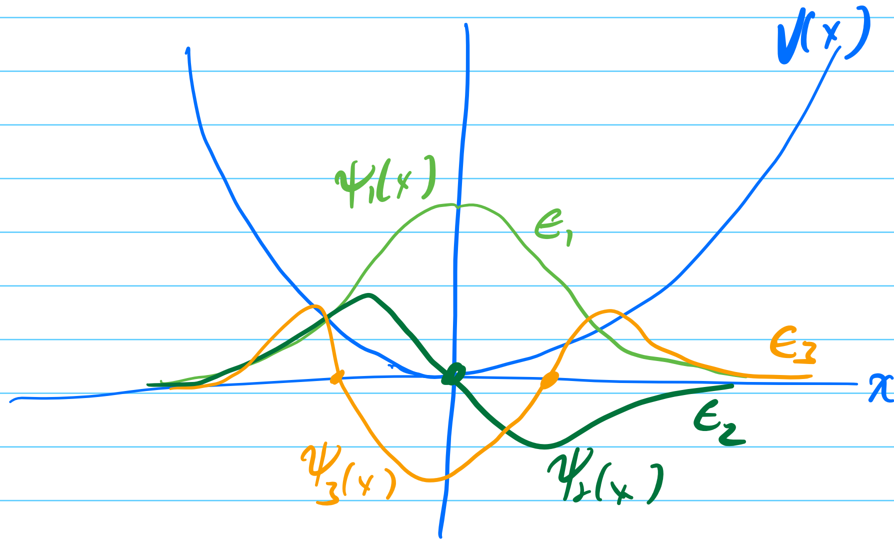
PHYS 621 Lecture Notes 11

N7.1

Nodes of the wavefunction

We will show that in 1D, ordering bound states by energy, the n^{th} bound state has $(n-1)$ nodes.

Node = zero of the wavefunction.



The proof relies on the Wronskian Theorem:

Suppose $y_1'' + f_1(x) y_1 = 0$

$y_2'' + f_2(x) y_2 = 0$

$f_1(x)$ and $f_2(x)$ piecewise continuous in $x \in (a,b)$.

Define Wronskian $W(y_1, y_2) \equiv y_1 y_2' - y_2 y_1'$

$$\frac{d}{dx}\left(y_1 y_2' - y_2 y_1'\right) = \left(f_1(x) - f_2(x)\right) y_1 y_2$$

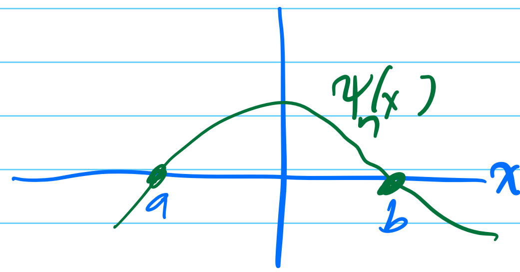
$$\int_a^b dx \frac{d}{dx}\left(y_1 y_2' - y_2 y_1'\right) = \int_a^b dx \left(f_1(x) - f_2(x)\right) y_1 y_2$$

$$\boxed{\left(y_1 y_2' - y_2 y_1'\right)\Big|_a^b = \int_a^b dx\, \left(f_1(x) - f_2(x)\right) y_1 y_2}$$

Wronskian Theorem

Suppose $x=a$, $x=b$ are locations of two consecutive nodes.

Suppose $\psi_n(x)$ is the wavefunction of the n^{th} bound state, with energy ϵ_n, and $\psi_{n+1}(x)$ is the wavefunction of the $(n+1)^{st}$ bound state, with energy ϵ_{n+1}.



$$\psi_n'' + \left(\epsilon_n - U(x)\right)\psi_n(x) = 0$$

$$\psi_{n+1}'' + \left(\epsilon_{n+1} - U(x)\right)\psi_{n+1}(x) = 0$$

By the Wronskian theorem,

$$\star \quad \left(\psi_{n+1}\psi_n' - \psi_n \psi_{n+1}'\right)\Big|_a^b = \int_a^b dx\, \left(\epsilon_{n+1} - \epsilon_n\right)\psi_n \psi_{n+1}$$

Suppose $\psi_n(x) > 0$ between nodes $a < x < b$.
Then $\psi_n'(a) > 0$, $\psi_n'(b) < 0$.

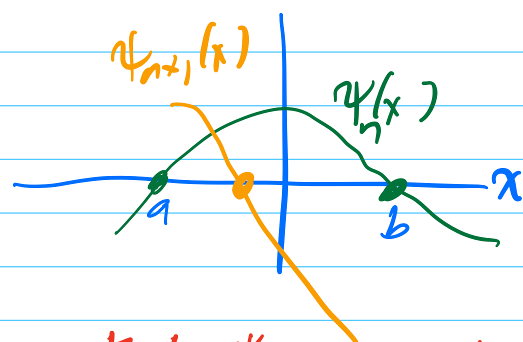
Suppose ψ_{n+1} has no node between $a < x < b$, e.g. $\psi_{n+1} > 0$.
The right-hand side of $\star$ is > 0.

The first term on the left-hand side of ☆ is the opposite sign of ψ_{n+1} because $\psi_n'(b)<0$, $\psi_n'(a)>0$.

The second term vanishes because $\psi_n(b)=\psi_n(a)=0$.

Hence, the LHS has the opposite sign as the RHS.

$\Rightarrow$ The assumption that ψ_{n+1} has no node in $a<x<b$ must be false.



We have shown that ψ_{n+1} has at least one node between any pair of nodes of ψ_n. Hence ψ_{n+1} has at least one more node than ψ_n. In general, ψ_{n+1} has precisely n nodes. This follows by considering the infinite square well, which has that property, and tracking the wavefunction as the potential is deformed to the actual potential. To introduce a new node would require a pt. where $\psi(c)=\psi'(c)=0$, which is not possible for nonvanishing $\psi(x)$.

Orthogonality: If $\epsilon_i \neq \epsilon_j$ for two bound states, taking $a\to-\infty$, $b\to+\infty$ in the wronskian theorem, using $\psi(x)\to 0$ as $x\to\pm\infty$,

$$\boxed{\int_{-\infty}^{\infty} dx\, \psi_i(x)\,\psi_j(x) = 0.}$$

(Note $\psi_i(x)$ can be taken to be real because the time-independent Schrödinger eq. is real.)

7.3 Infinitely deep square well

$$U(x) = \begin{cases} 0 & 0 < x < L \\ \infty & x < 0 \,,\; x > L \end{cases} \rightarrow \psi(x) = 0 \text{ for } x<0, x>L$$

$0<x<L$: $\psi''(x) = -\epsilon\psi(x)$, $\epsilon = \frac{2mE}{\hbar^2}$

Solution: $\psi(x) = A\sin(\sqrt{\epsilon}\,x) + B\cos(\sqrt{\epsilon}\,x)$

Boundary conditions: $\psi(0) = 0 \rightarrow B = 0$

$\psi(L) = 0 \rightarrow \sin(\sqrt{\epsilon}L) = 0$

$\rightarrow \sqrt{\epsilon_n}L = n\pi$ for $n \in \mathbb{Z}$.

$\rightarrow \boxed{E_n = \frac{\hbar^2 n^2\pi^2}{2mL^2}}$ Bound state energies

$\boxed{\psi_n(x) = A\sin\frac{n\pi x}{L}}$

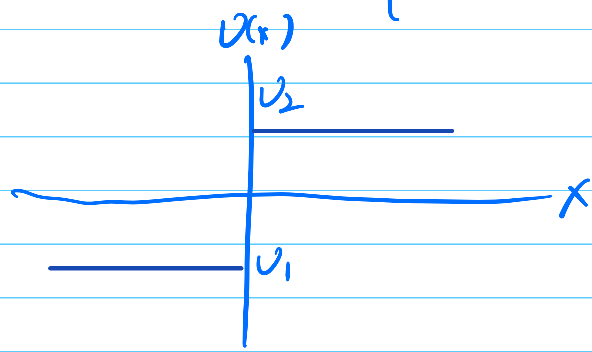
Normalization: $\int dx\, |\psi_n(x)|^2 = 1$

$\rightarrow \int_0^L |A|^2 \sin^2\frac{n\pi x}{L}\,dx = |A|^2\frac{L}{2} = 1$

$\rightarrow \boxed{|A| = \sqrt{\frac{2}{L}}}$ (independent of n)

7.4 Potential Step: Reflection and Transmission

Suppose $U_2 > U_1$, $U(x) = \begin{cases} U_1 & x<0 \\ U_2 & x>0 \end{cases}$



If $\epsilon < U_1$ — no solution (exponential solution not normalizable)

If $U_1 < \epsilon < U_2$: $\boxed{\psi(x) = \begin{cases} A\sin(k_1 x + \phi) & x<0 \\ B\, e^{-\kappa_2 x} & x>0 \end{cases}}$ continuum nondegenerate solutions

$$k_1 = \sqrt{\epsilon - U_1}\,, \quad \kappa_2 = \sqrt{U_2 - \epsilon}$$

$\psi(x)$ continuous at $x=0$:

$$\boxed{A\sin\phi = B}$$

$\psi'(x)$ continuous at $x=0$: $Ak_1\cos\phi = -B\kappa_2$

Divide by $\psi(0) = A\sin\phi = B$:

$$k_1\cot\phi = -\kappa_2$$

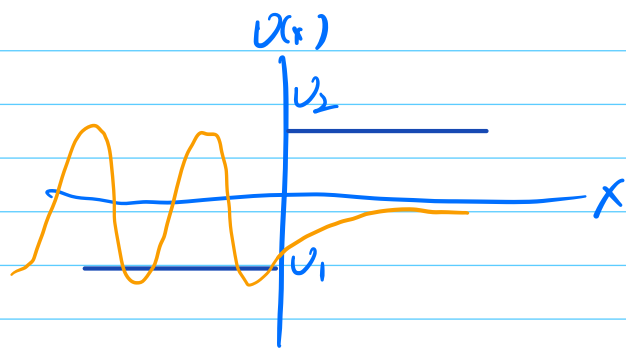
$$\Rightarrow \boxed{\phi = \arctan\left(-\frac{k_1}{\kappa_2}\right)}$$

$$\frac{\sin\phi}{\cos\phi} = \frac{\sin\phi}{\sqrt{1-\sin^2\phi}} = -\frac{\kappa_1}{\kappa_2}$$

$$\sin^2\phi = \left(\frac{\kappa_1}{\kappa_2}\right)^2(1-\sin^2\phi) \rightarrow \sin\phi = \frac{-\kappa_1}{\sqrt{\kappa_1^2+\kappa_2^2}}$$

$$B = A\sin\phi = \frac{-A\kappa_1}{\sqrt{\kappa_1^2+\kappa_2^2}}$$

$$\Rightarrow \boxed{\psi_E(x) = \begin{cases} A\sin\left(\kappa_1 x + \arctan\left(-\kappa_1/\kappa_2\right)\right) & x<0 \\ \frac{-A\kappa_1}{\sqrt{\kappa_1^2+\kappa_2^2}}\, e^{-\kappa_2 x} & x>0 \end{cases}}$$



$$x<0:\ \Psi_E(x,t) = \psi_E(x)\, e^{-iEt/\hbar}$$

$$= \frac{A}{2i}\left[e^{i(\kappa_1 x - Et/\hbar)+\phi} - e^{-i(\kappa_1 x + Et/\hbar)+\phi}\right]$$

$\phi(E)$ $\phi(E)$

Right-moving "incident" plane wave

Left-moving "reflected" plane wave.

If $\epsilon > V_2$:

Suppose $\psi(x) = \begin{cases} e^{ik_1 x} + R e^{-ik_1 x} & , x<0 \\ S e^{ik_2 x} & x>0 \end{cases}$

$$k_1 = \sqrt{\epsilon - V_1}\,, \quad k_2 = \sqrt{\epsilon - V_2}$$

Continuity of $\psi(x)$ at $x=0$: $\boxed{1+R=S}$

Continuity of $\dfrac{\psi'(x)}{\psi(x)}$ at $x=0$:

$$ik_1 \frac{(1-R)}{1+R} = ik_2 \Rightarrow \boxed{R = \frac{k_1-k_2}{k_1+k_2}}$$

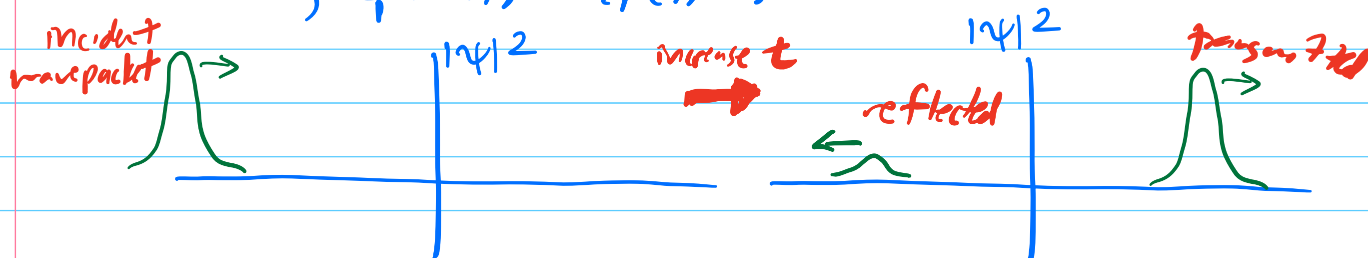
$$\boxed{S = \frac{2k_1}{k_1+k_2}}$$

Including time dependence:

$$\Psi_\epsilon(x,t) = \begin{cases} e^{ik_1 x - i\epsilon t/\hbar} + \dfrac{k_1-k_2}{k_1+k_2}\, e^{-ik_1 x - i\epsilon t/\hbar} & x<0 \\ \dfrac{2k_1}{k_1+k_2}\, e^{ik_2 x - i\epsilon t/\hbar} & x>0 \end{cases}$$

Suppose $f(k_1)$ is a Gaussian centered around $\bar{k}_1 \gg \sqrt{V_2}$.

$$\Psi(x,t) = \int dk_1\, f(k_1)\, \Psi_{k_1}(x,t)$$



Probability of reflection $\sim |R|^2 = \dfrac{(k_1-k_2)^2}{(k_1+k_2)^2}$

probability of transmission $\sim 1-|R|^2 = \dfrac{k_2}{k_1}|S|^2 = \dfrac{4k_1k_2}{(k_1+k_2)^2}$

$\equiv T$

transmission coefficient