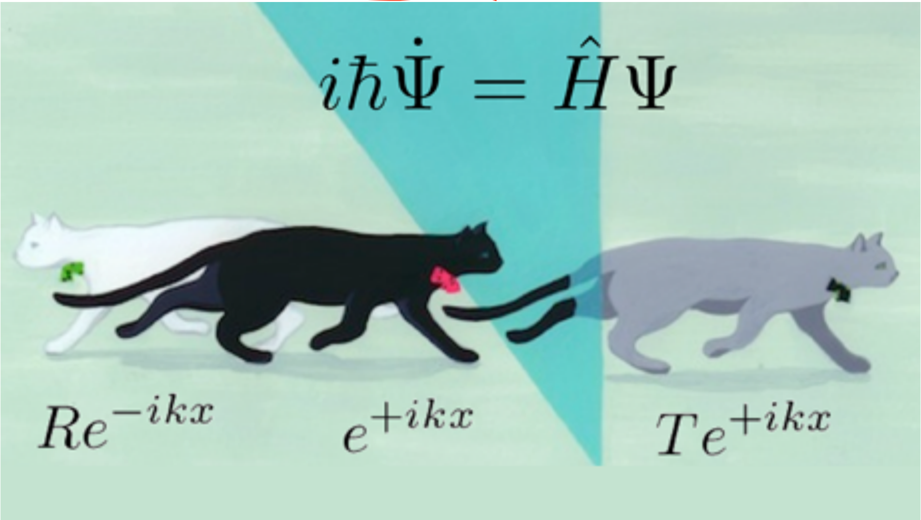
Exploring Quantum Physics

Coursera, Spring 2013 Instructors: Charles W. Clark and Victor Galitski

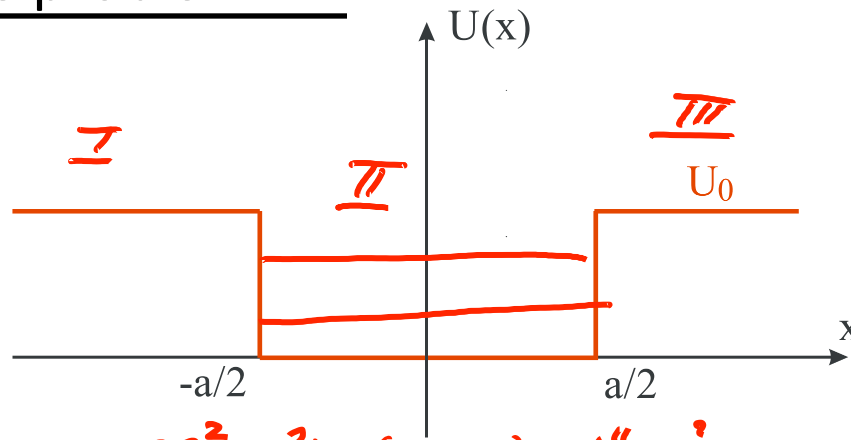
Bound states in quantum potential wells

Part II: *Finite potential well*



Formulation of the problem

$$U(x) = \begin{cases} U_0, & \text{if } |x| > a/2 \\ 0, & \text{if } |x| < a/2, \end{cases}$$



- For $|x| > a/2$: $-\frac{\hbar^2}{2m}\psi''(x) + U_0\psi(x) = E\psi(x)$
- For $|x| < a/2$: $-\frac{\hbar^2}{2m}\psi''(x) = E\psi(x)$

$\gamma^2 = \frac{2m}{\hbar^2}(U_0 - E)$ $\quad \psi'' - \gamma^2\psi = 0$

$k^2 = \frac{2mE}{\hbar^2}$ $\quad \psi'' + k^2\psi = 0$

- We're interested in finding bound state(s) (with $0 < E < U_0$) satisfying the following continuity constraints:

$$\psi(\pm a/2 + 0) = \psi(\pm a/2 - 0) \text{ and } \psi'(\pm a/2 + 0) = \psi'(\pm a/2 - 0)$$

along with the conditions $\psi(x \to \pm\infty) \to 0$.

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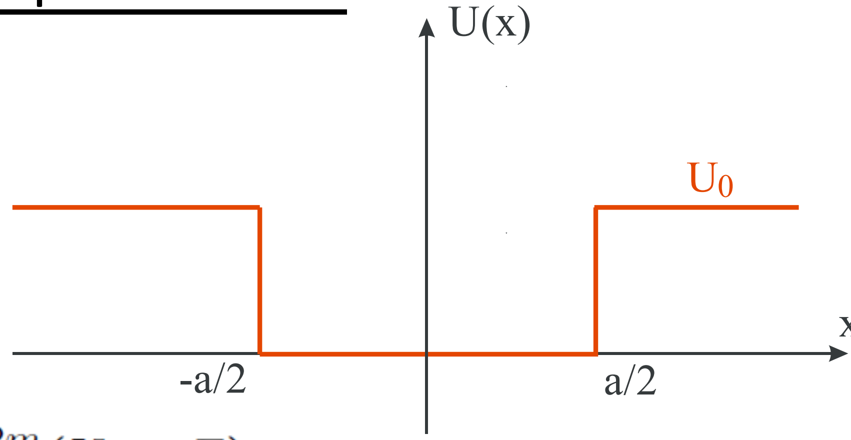

$e^{\pm\gamma x}$

- For $|x| > a/2$: $\underline{\psi''(x) - \gamma^2\psi(x) = 0,\ \gamma^2 = \frac{2m}{\hbar^2}(U_0 - E)}$
- For $|x| < a/2$: $\underline{\psi''(x) + k^2\psi(x) = 0,\ k^2 = \frac{2m}{\hbar^2}E}$ $e^{\pm ikx}$
- We're interested in finding bound state(s) (with $0 < E < U_0$) satisfying the following continuity constraints:

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Using the symmetry

- In general, if the Hamiltonian commutes with an operator, $\hat{A}$,

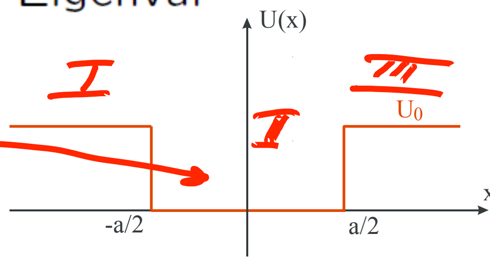
$$\left[\hat{H},\, \hat{A}\right] = \hat{H}\hat{A} - \hat{A}\hat{H} = 0,$$

solutions to the S. Eqn. can be chosen to have definite a and E, $\psi_{aE}(x)$.

$\hat{H}\psi = E\psi$

$\hat{A}\psi = a\psi$

- Our potential is inversion symmetric $\hat{I}U(x) = U(-x) \equiv U(x)$. Eigenvalues of $\hat{I}$ are $p = \pm 1$.



- General solution of $\left(\frac{d^2}{dx^2} + k^2\right)\psi(x) = 0$:

$$\psi(x) = C_1 e^{ikx} + C_2 e^{-ikx}$$

- We can choose solutions with a definite parity, or in other words:

$$\psi_+(x) = C\cos(kx) \text{ and } \psi_-(x) = \tilde{C}\sin(kx)$$

Using the constraints at infinities

- General solution of $\left(\frac{d^2}{dx^2} - \gamma^2\right)\psi(x) = 0$:

$$\psi(x) = Ae^{-\gamma x} + \cancel{Be^{+\gamma x}}$$

- *E.g.*, for $x > a/2$ we must request that the wave-function ~~remains finite~~ $\to 0$ at $x \to +\infty$. Otherwise, the probabilty for particle to "leak" to infinity would explode exponentially (does not make sense).

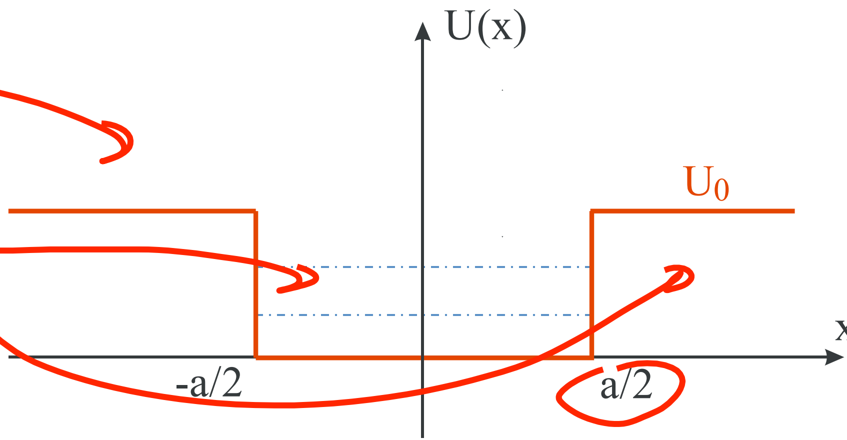
- So, we drop the B-term and the solution is

$$\psi(x) = Ae^{-\gamma x}, \quad \text{for } x > a/2$$

Using the matching conditions at x=a/2

- So, we found

$$\psi_+(x) = \begin{cases} Ae^{\gamma x}, & \text{if } x < -a/2 \\ C\cos(kx), & \text{if } |x| < a/2 \\ \underline{Ae^{-\gamma x}}, & \text{if } x > a/2 \end{cases}$$



- Lets match solutions at $x = a/2$

$$C\cos\left(\frac{ka}{2}\right) = A\,e^{-\frac{\gamma a}{2}} \qquad (1)$$

$$-Ck\sin\left(\frac{ka}{2}\right) = -A\gamma\,e^{-\frac{\gamma a}{2}} \qquad (2)$$

$$\frac{Eq(2)}{Eq(1)} : \quad \underbrace{k\tan\left(\frac{ka}{2}\right) = \gamma}$$

Making the self-consistency equation dimensionless

- The non-linear self-consistency equation is not solvable analytically:

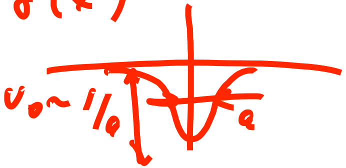
$$\tan\left(\frac{ka}{2}\right) = \frac{\gamma}{k} \equiv \sqrt{\frac{U_0}{E} - 1}, \quad \text{with } k = \sqrt{2mE/\hbar^2}$$

- The starting point of analysis is to introduce dimensionless parameters. In our case, $x = ka/2$ and $\xi^2 = \frac{mU_0a^2}{2\hbar^2}$

$$\tan x = \sqrt{(\xi/x)^2 - 1}$$

- Two limiting cases: a deep, $\frac{mU_0a^2}{\hbar^2} \gg 1$, and shallow, $\frac{mU_0a^2}{\hbar^2} \ll 1$, well.

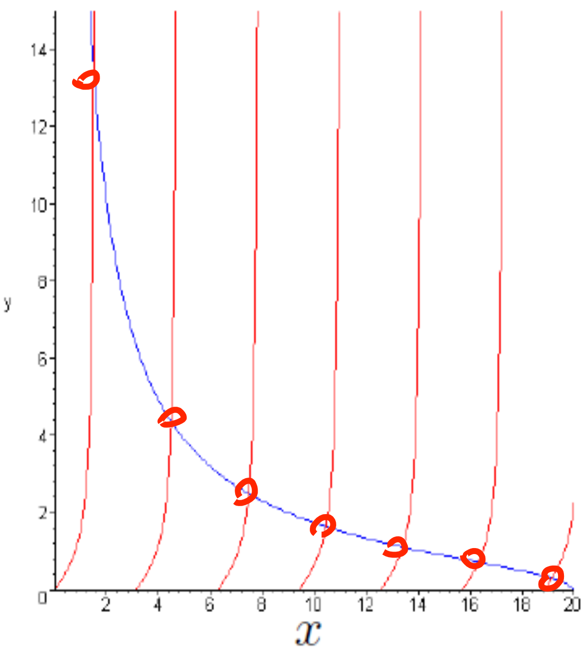
$U(x) = -\alpha\,\delta(x)$



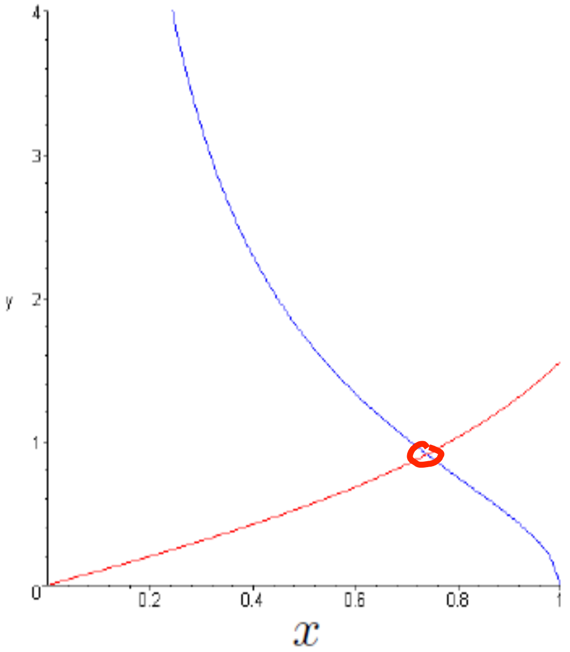
Solving the self-consistency equation

$$\tan x = \sqrt{(\xi/x)^2 - 1}$$

Deep potential, $\xi = 20$



Relatively shallow potential, $\xi = 1$



See, Michael Fowler's lectures at UVa for a more details analysis
http://galileo.phys.virginia.edu/~mf1i/home.html