ECE 162A
Mat 162A

Lecture #6: Stationary Solutions
Read Chapter 5,6 of Eisberg,Resnick

Eigenvalue Equation

- Using operators, Schroedinger's equation can be expressed as an eigenvalue equation

$$E_{op}\psi = E\psi$$

where

$$E_{op} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V$$

- The solution of the equation involves finding the particular solutions ψ_n, called eigenfunctions and E_n called eigenvalues.

Solutions to SE

- Free particle
- Step potential
- Infinite box
- Finite box
- Harmonic oscillator

Free particle (V=0)

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

$$Solution: \quad \psi(x) = \exp(ikx)$$

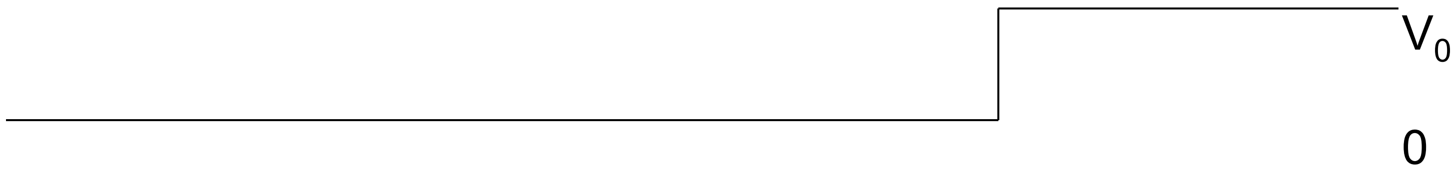
$$where \quad \frac{\hbar^2 k^2}{2m} = E$$

The complete solution is

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar} = e^{ikz-i(E/\hbar)t}$$

There are no constraints on E, any value is allowed at this point. This corresponds to a wave moving to the right. -k solutions are also valid.

Step Potential



- Sketch solutions for $E>V_0$ and $E<V_0$

Step potential

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

$$Solution: \quad For\ E > V_0$$

$$For\ x<0\ \psi(x)=A\exp(ik_1x)+B\exp(-ik_1x)$$

$$For\ x>0\ \psi(x)=C\exp(ik_2x)+D\exp(-ik_2x)$$

$$where \quad \frac{\hbar^2 k_1{}^2}{2m}=E \quad \frac{\hbar^2 k_2{}^2}{2m}=E-V_0$$

Boundary conditions

$$\psi(x\to 0^-)=\psi(x\to 0^+)$$

$$\frac{d\psi(x\to 0^-)}{dx}=\frac{d\psi(x\to 0^+)}{dx}$$

The wave is entering from the left.

Step Potential (E>V_0)

$$For\ x<0\ \ \psi(x) = A\exp(ik_1x) + B\exp(-ik_1x)$$

$$For\ x>0\ \ \psi(x) = C\exp(ik_2x) + D\exp(-ik_2x)$$

$$Wave\ \ from left:\ \ D=0$$

$$\psi:\ \ A+B=C$$

$$d\psi/dx:\ \ ik_1(A-B) = ik_2C$$

$$A = \frac{1}{2}(1+\frac{k_2}{k_1})C$$

$$B = \frac{1}{2}(1-\frac{k_2}{k_1})C$$

Normalization

- C can be normalized if the density of electrons is known, or the problem is limited by either
  - A large box
  - Periodic boundary conditions
- In general, though, what matters is the reflection coefficient R and transmission coefficient T

$$R = \frac{B^* B}{A^* A}$$

$$T = \frac{C^* C}{A^* A}$$

Step Potential (E<V$_0$)

$$For\ x < 0\ \ \psi(x) = A\exp(ikx) + B\exp(-ikx)$$

$$For\ x > 0\ \ \psi(x) = C\exp(-\kappa x) + D\exp(\kappa x)$$

$$Finite\ \ wave\ \ function.\ \ D = 0$$

$$\psi:\ \ A + B = C$$

$$d\psi / dx:\ \ ik(A - B) = -\kappa C$$

$$A = \frac{1}{2}(1 + \frac{i\kappa}{k})C$$

$$B = \frac{1}{2}(1 - \frac{i\kappa}{k})C$$

Infinite Well

Quantum Semiconductor Structures, Claude Weisbuch and Borge Vinter, Academic Press, 1991

ONE DIMENSIONAL CASE: $V_o = \infty$

$$-\left(\frac{\hbar^2}{2m}\right) d^2\psi/dz^2 = E\psi$$

Plug into here

Solve for E_n

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L_z}\right)^2 \quad n = 1, 2, 3 \ldots$$

Solution has to be of this form to terminate to zero at infinite walls

$$\psi_n = A\sin\frac{n\pi z}{L_z}$$

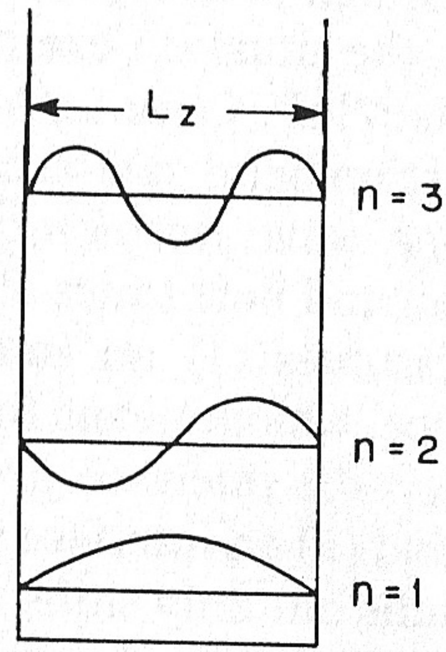


FIG. 5. Infinitely deep quantum-well energy levels and wave functions. (Reprinted with permission from Friedr. Vieweg & Sohn Verlagsgesellschaft mbH, R. Dingle, *Festkoerperprobleme* **15**, 21 (1975)).

Finite Well

Quantum Semiconductor Structures, Claude Weisbuch and Borge Vinter, Academic Press, 1991

$$\left(-\frac{\hbar^2}{2m^*(z)}\frac{\partial^2}{\partial z^2}+V_c(z)\right)\chi_n(z)=\varepsilon_n\chi_n(z)$$

Even Solution

$$\begin{aligned}\chi_n(z) &= A\cos kz, && \text{for } |z|<L/2\\ &= B\exp[-\kappa(z-L/2)], && \text{for } z>L/2 \\ &= B\exp[+\kappa(z+L/2)], && \text{for } z<-L/2\end{aligned}\qquad (2)$$

or

Odd Solution

$$\begin{aligned}\chi_n(z) &= A\sin kz, && \text{for } |z|<L/2,\\ &= B\exp[-\kappa(z-L/2)], && \text{for } z>L/2 \\ &= B\exp[+\kappa(z+L/2)], && \text{for } z<-L/2\end{aligned}\qquad (3)$$

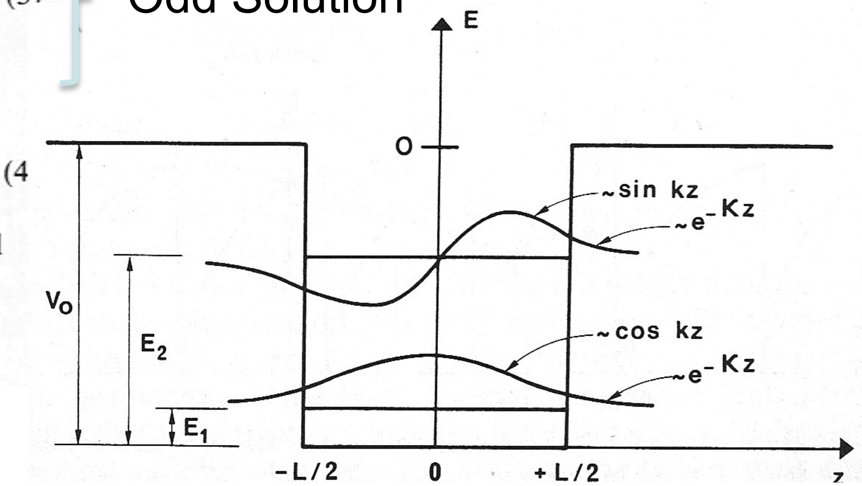
where

$$\varepsilon_n=\frac{\hbar^2k^2}{2m_A^*}-V_0,\qquad \varepsilon_n=-\frac{\hbar^2\kappa^2}{2m_B^*},\qquad -V_0<\varepsilon<0\qquad (4$$

For the solution of Eq. (2), the continuity conditions at $z=\pm L/2$ yield

$$A\cos(kL/2)=B$$

$$(k/m_A^*)\sin(kL/2)=\kappa B/m_B^*$$



Finite Well

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Solving for B in previous two equations and setting equal

$$(k/m_A^*)\tan(kL/2) = \kappa/m_B^* \quad (5)$$

Similarly, Eq. (3) yields

$$k/m_A^*\,\mathrm{cotan}(kL/2) = -\kappa/m_B^* \quad (6)$$

The equations can be solved numerically or graphically. A very simple graphical type of solution can be developed if $m_A^* \approx m_B^*$. Then, using Eq. (4), Eqs. (5) and (6) can be transformed into implicit equations in k alone:

$$\cos(kL/2) = k/k_0, \quad \text{for} \quad \tan kL/2 > 0 \quad (7)$$

$$\sin(kL/2) = k/k_0, \quad \text{for} \quad \tan kL/2 < 0 \quad (8)$$

where

$$k_0^2 = 2m^*V_0/\hbar^2 \quad (9)$$

These equations can be visualized graphically (Fig. 7). There is always one bound state. The number of bound states is

$$1 + \mathrm{Int}\left[\left(\frac{2m_A^* V_0 L^2}{\pi^2\hbar^2}\right)^{1/2}\right] \quad (10)$$

where Int[x] indicates the integer part of x.

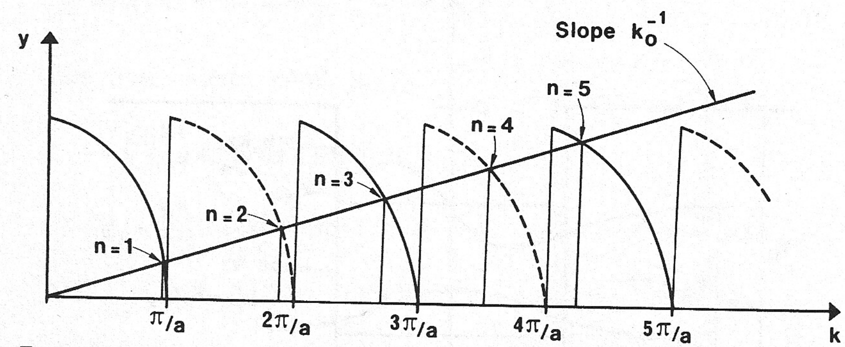

FIG. 7. Graphical solution for Eqs. (7) and (8). Solutions are located at the intersections of the straight line with slope k_0^{-1} with curves $y = \cos kL/2$ (with $\tan kL/2 > 0$; ——; even wave functions) or $y = \sin kL/2$ (with $\tan kL/2 < 0$; ---; odd solutions).