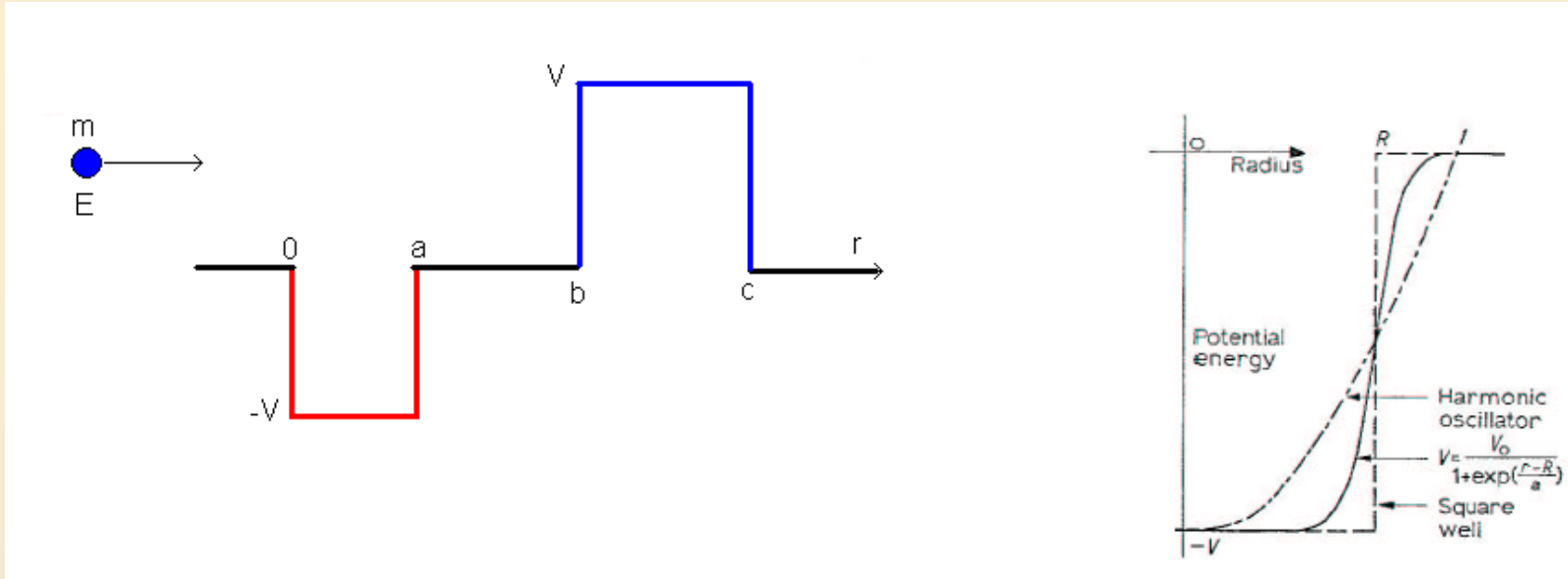


Kuantum Mekanikinin Temelleri



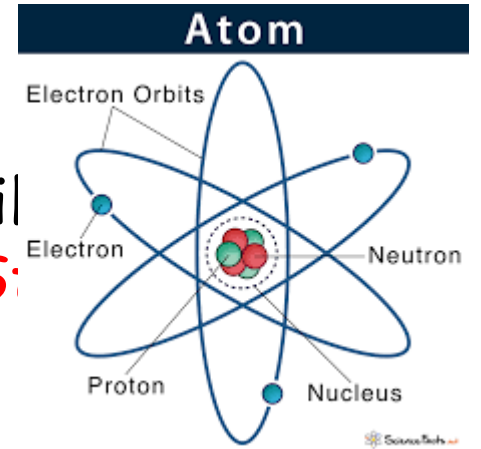
- Bu sistemde Fizik nedir?
- Niçin 3. sınıf KM dersinde Kare-Kuyu, bariyer vb potansiyelleri çözeriz?
- Niçin zamandan bağımsız Schrödinger denklemini kullanırız?
- vb

İsmail Boztosun, Prof. Dr.
Akdeniz Üniversitesi

Modern Fizik-Giriş

Black-Body Radiation, Photoelectric Effect, Compton Scattering

- 19YY sonunda birçok bilim insanı Fizikteki bir çok problemin çözüldüğünü düşünüyorlardı:
 - Yörüngesel hareketler anlaşılmıştı
 - Elektrik ve Manyetik Kanunlar biliniyordu.
 - Korunum prensipleri kurulmuştu
- Ancak, Atomda ki kararlı yörüngeler klasik ile açıklanamamıştı: **Kararlı Yörüngeler (Stable orbits)**
- "Modern" dönem - 20. Yüzyıl
 - Siyah Cisim Işıması, Fotoelektrik etki, Compton Saçılması: Kuantize/kesikli seviyeler ve enerji, dualite:dalga-parçacık



$$\nabla \cdot \mathbf{B} = 0$$

Gauss' Law of Magnetism

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \mu_0 \epsilon_0 \frac{\partial \mathbf{D}}{\partial t}$$

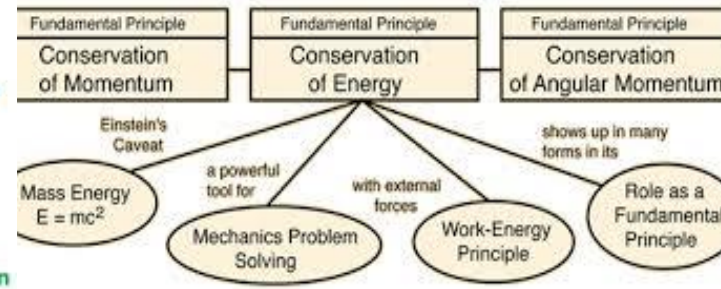
Ampere's Law

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}$$

Gauss' Law of Electricity

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

Faraday's Law of Induction



Kuantum Mekanikası Dönemi

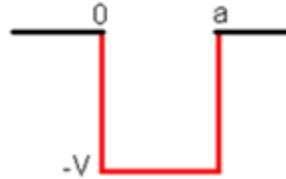
- Kuantum mekaniği, atom ve atom altı sistemlerin gözlenebilirlerini bulmak için operator tekniğini kullanan bir matematiksel kuramdır.
- Temelleri:
 - Kuantizasyon (Planck)
 - Karşılıklılık (Bohr, Ehrenfest teoremi)
 - Dualite / Belirsizlik (Fermi, Heisenberg)
 - Simetri / Dışarlama (Pauli)

Klasik ve Kuantum Mekanikçi Operatörleri

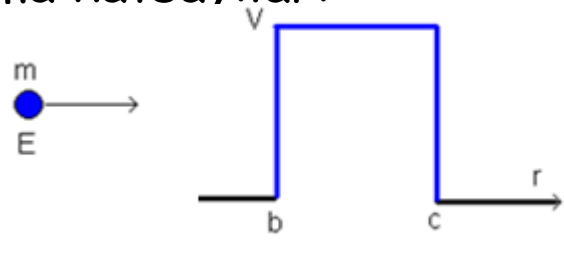
Klasik Fizik Operatörleri	Kuantum Mekanikçi Operatörleri
Konum: x, y, z	Konum Operatörü: $\hat{x} = x$
Momentum: $p = m v$	Momentum Operatörü: $\hat{p} = -i \hbar d/dx$
Enerji: $E = 1/2 m v^2 + U(x)$	Hamiltonyen Operatörü: $\hat{H} = p^2/2m + V(\hat{x})$
Kuvvet: $F = - dU/dx$	Schrödinger Denklemi: $\hat{H} \psi = E \psi$
Açısal Momentum: $L = r \times p$	Açısal Momentum Operatörleri: $\hat{L}_x, \hat{L}_y, \hat{L}_z$
Türev Operatörleri: $d/dx, d/dt$	Diferansiyel Operatörler: $-i \hbar d/dx$
Laplasyen: $\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$	Dalga Fonksiyonu Operatörleri: $\psi(x)$

Fizikte Sistemler

- Bağılıdır (enerji E , potansiyel $V(r)$ 'den küçük)
 - Gözlenebilir: Bağlanma enerjisi



- Saçılırlar (Enerji potansiyel $V(r)$ 'den büyük)
 - Gözlenebilir tesir kesiti,
 - geçme /yansıma katsayıları

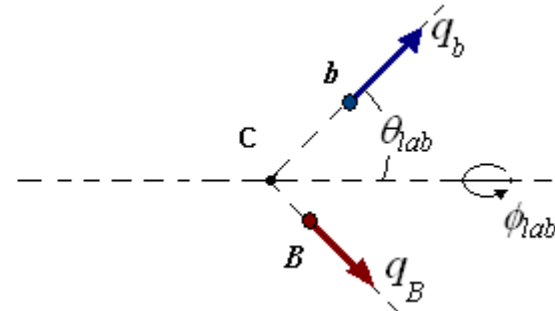
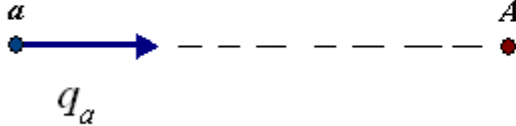
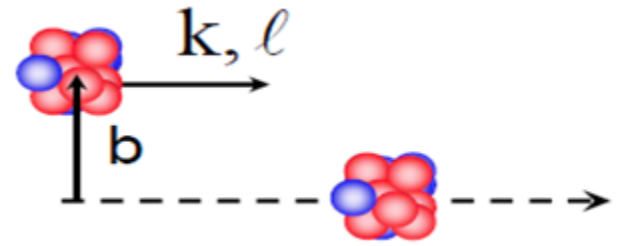


- Yarı Bağılı-Rezonsans (Enerji ve Potansiyel birbirine yakın)

Referans Sistemler

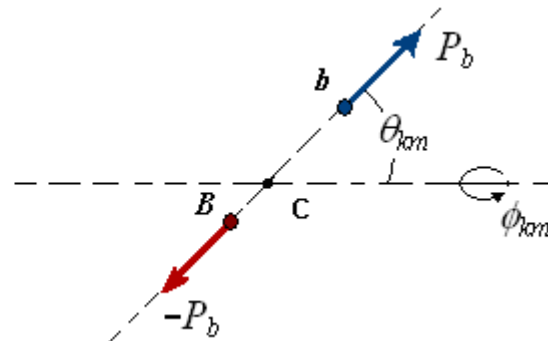
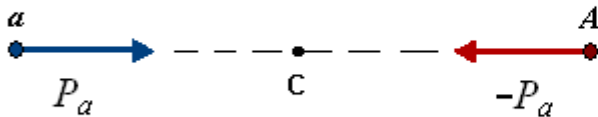
- Laboratuvar Referans Sistemi

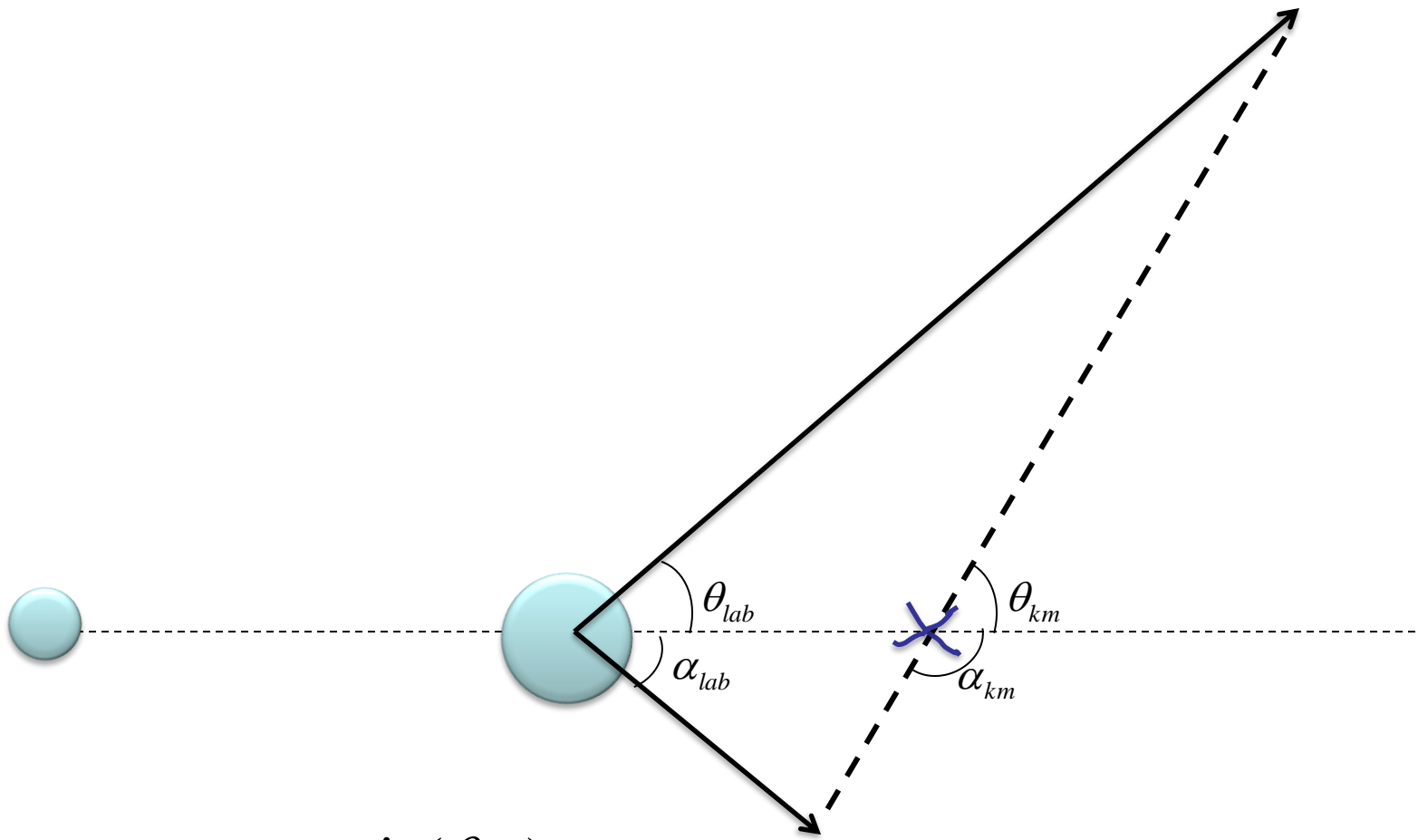
- Gelen parçacık her zaman bir hız/momentum/enerji sahiptir
- Hedef parçacık her zaman durgundur.



- Kütle Merkezi Koordinat Sistemi

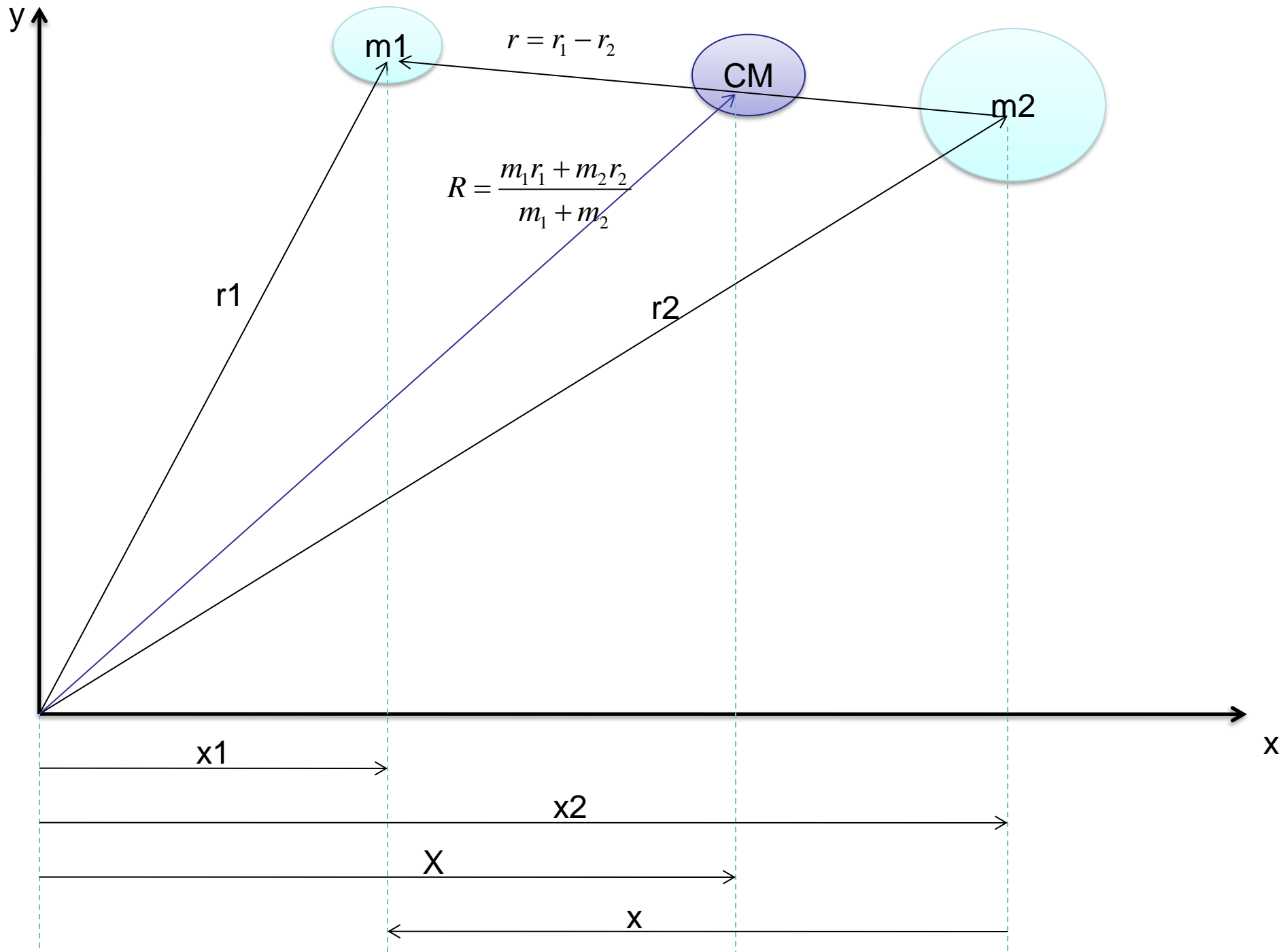
- Kütle merkezi sabit hızla hareket ediyor dolayısıyla Gelen ve Hedef parçacıklar hareketli





$$\tan(\theta_{lab}) = \frac{\sin(\theta_{cm})}{\cos(\theta_{cm}) + v_M / v_{cm}}$$

$$E_{CM} = \frac{m_2}{m_1 + m_2} E_{lab}$$



$$\left(-\frac{\hbar^2}{2m_1} \nabla_1^2 - \frac{\hbar^2}{2m_2} \nabla_2^2 + V(r_1, r_2) \right) \psi = E\psi$$

$$\nabla_i \psi = \frac{\partial \psi}{\partial x_i} + \frac{\partial \psi}{\partial y_i} + \frac{\partial \psi}{\partial z_i}$$

$$\left(-\frac{\hbar^2}{2[m_1 + m_2]} \nabla_R^2 - \frac{\hbar^2}{2[m_1 m_2 / (m_1 + m_2)]} \nabla_r^2 + V(r) \right) \psi = E\psi$$

$$-\frac{\hbar^2}{2M} \nabla_R^2 \psi - \left(\frac{\hbar^2}{2m} \nabla_r^2 + V(r) \right) \psi = E\psi$$

R

Center of Mass

r

Relative Motion

$$-\frac{\hbar^2}{2M} \nabla_R^2 \psi = \epsilon_0 \psi$$

$$-\left(\frac{\hbar^2}{2m} \nabla_r^2 + V(r) \right) \psi = \epsilon \psi$$

$$\frac{\partial \psi}{\partial x_1} = \frac{\partial \psi}{\partial X} \frac{\partial X}{\partial x_1} + \frac{\partial \psi}{\partial x} \frac{\partial x}{\partial x_1}$$

$$\frac{\partial X}{\partial x_1} = \frac{m_1}{m_1 + m_2}$$

$$\frac{\partial x}{\partial x_1} = 1$$

$$\frac{\partial \psi}{\partial x_1} = \frac{m_1}{m_1 + m_2} \frac{\partial \psi}{\partial X} + \frac{\partial \psi}{\partial x}$$

$$m = m_1 m_2 / (m_1 + m_2)$$

$$M = m_1 + m_2$$

İki Cisim Problemi: Schrodinger denkleminin efektif potansiyel için çözümü

İki Cisim Problemi

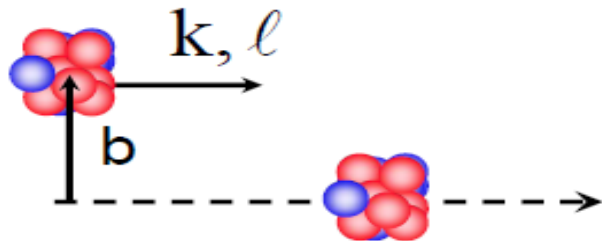
1. Lab Sisteminden KM Sistemine taşı
2. KM hareketini ayır
3. İndirgenmiş kütle bul

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

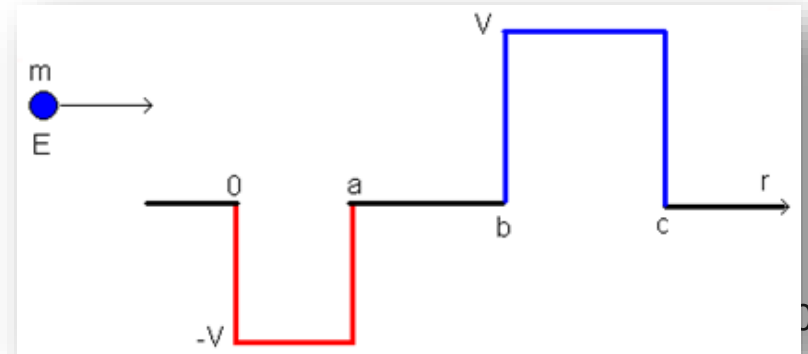
4. Potansiyeli tanımla $V(r)$
5. Sch. Denklemini bu $V(r)$ potansiyeli için çöz.

“İki cisim etkileşmesini, indirgenmiş kütleli tek bir cismin bu iki cisim arasındaki relative potansiyel ile yaptığı etkileşme şeklinde tanımlamadır.”

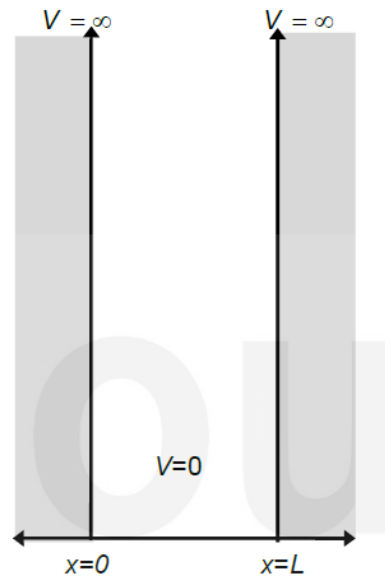
b =impact parameter



=



Zamandan Bağımsız Schrödinger Denklemi



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

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x) \quad 0 \leq x \leq L$$

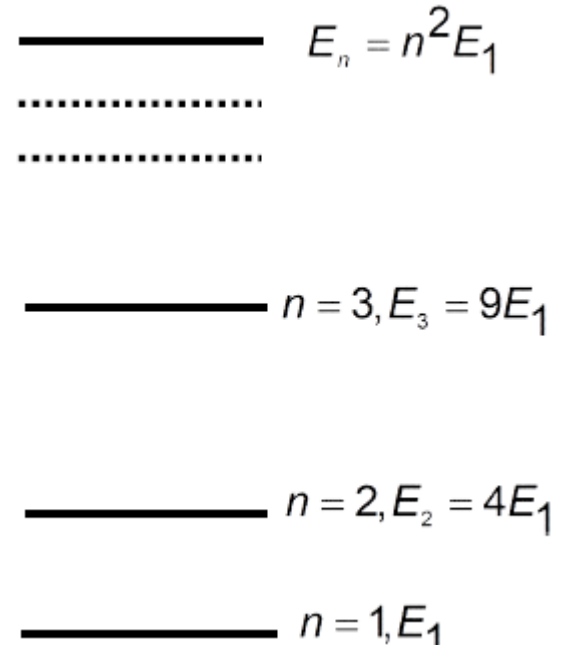
$$\psi(x=0) = \psi(x=L) = 0$$

$$k^2 = \frac{2mE}{\hbar^2} \quad \frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$$

$$\psi(x) = A \sin kx + B \cos kx$$

$$E_n = \frac{\hbar^2 k_n^2}{2mL^2} = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

$$n = 1, 2, 3, \dots$$



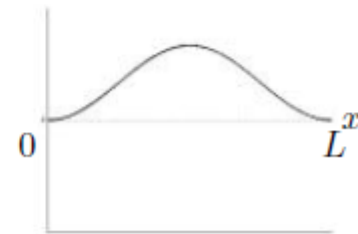
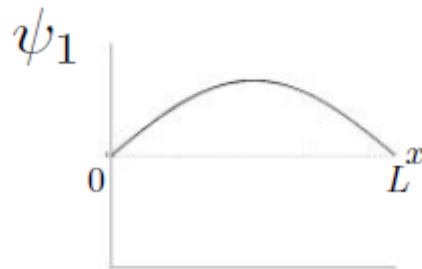
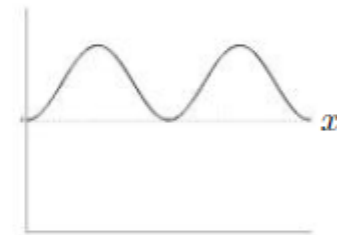
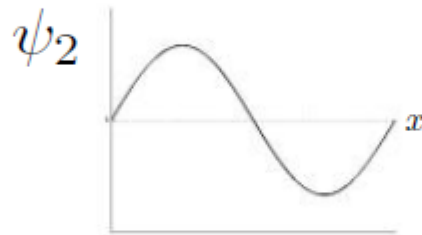
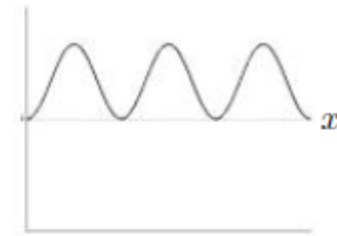
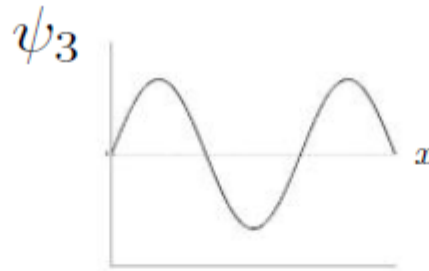
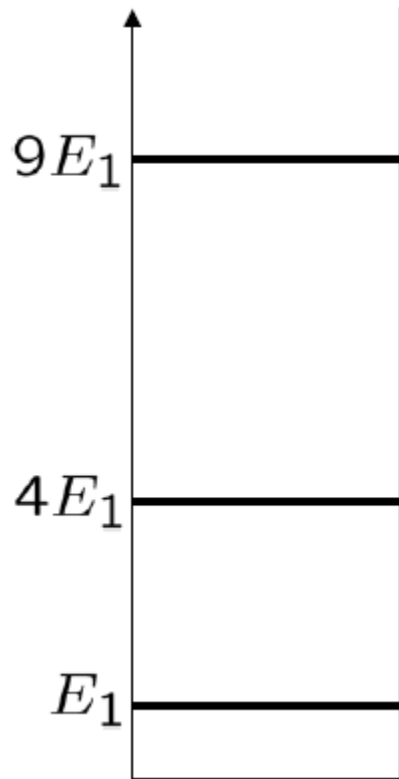
Sonsuz Kuyu Özdeğer ve Özfonksiyonları

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

$$n = 1, 2, 3, \dots$$

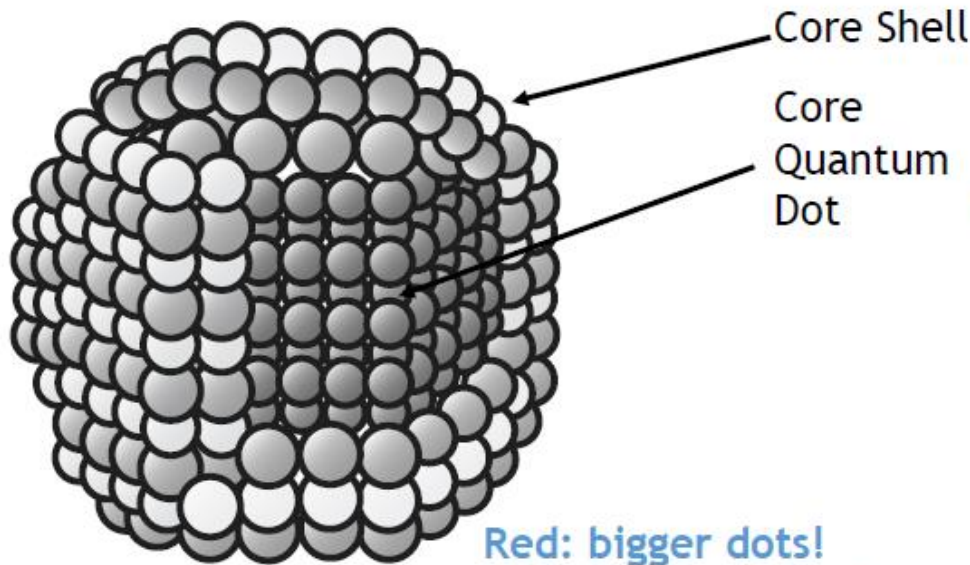
$$E_n = \frac{\hbar^2 k_n^2}{2mL^2} = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

$$n = 1, 2, 3, \dots$$



Semiconductor Nanoparticles

(aka: Quantum Dots)



Red: bigger dots!
Blue: smaller dots!

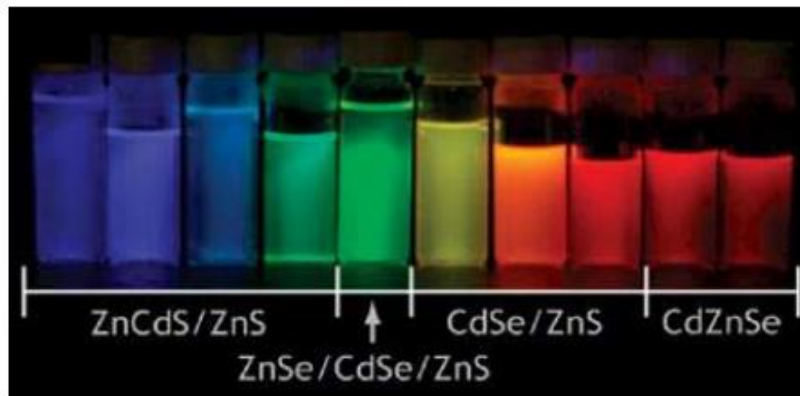
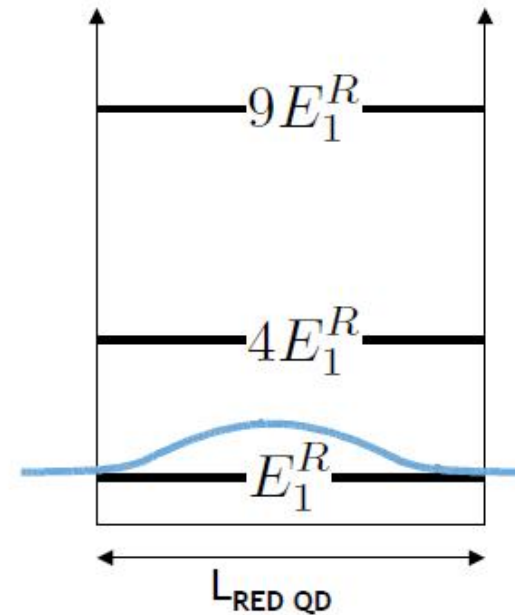
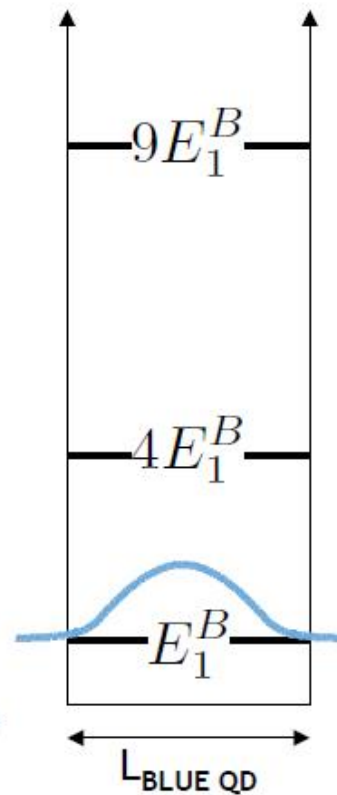


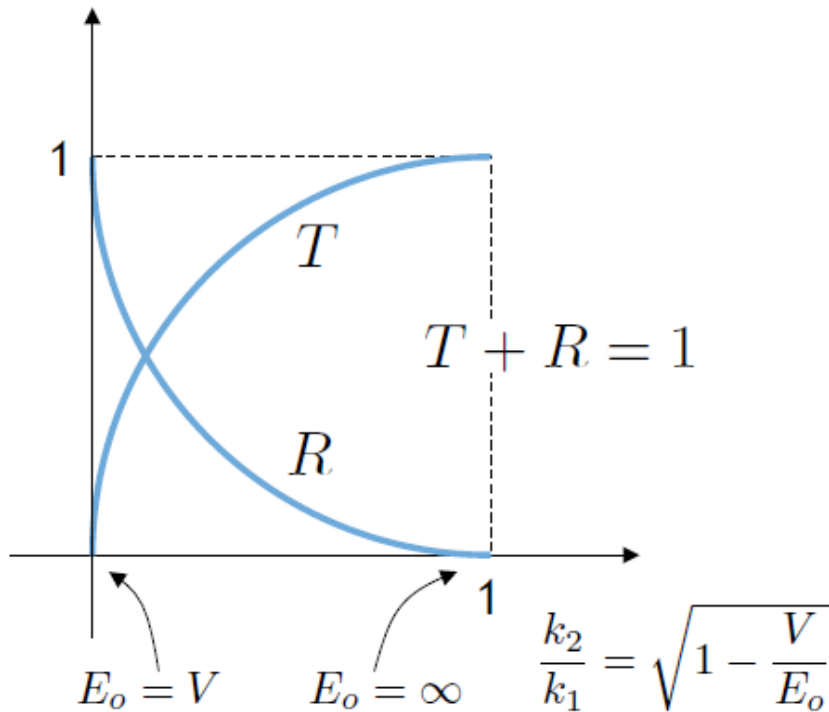
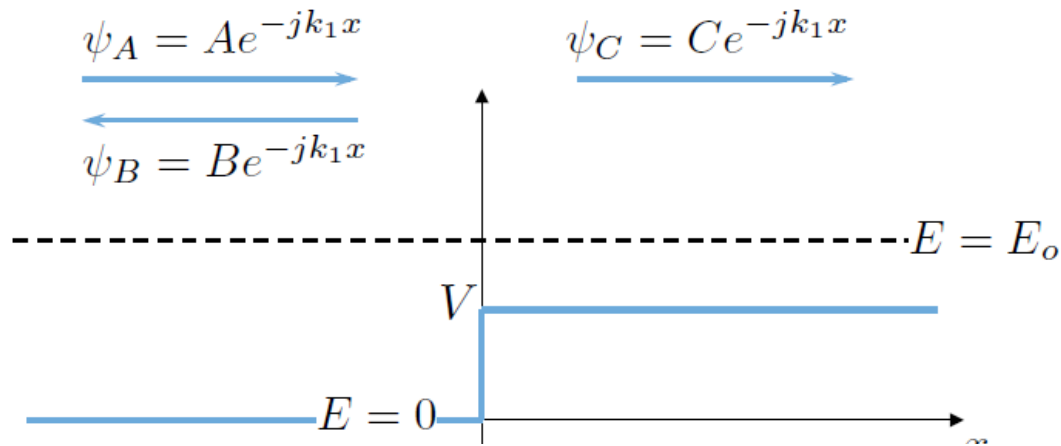
Photo by J. Halpert Courtesy of M. Bawendi Group, Chemistry, MIT

Determining QD energy using the Schrödinger Equation

$$E_1 = n^2 E_1 \quad E_1 = \frac{\hbar^2 k_1^2}{2m} = \frac{\hbar^2 \pi^2}{2mL^2}$$



Basamak Potansiyeli, $E > V(x)$



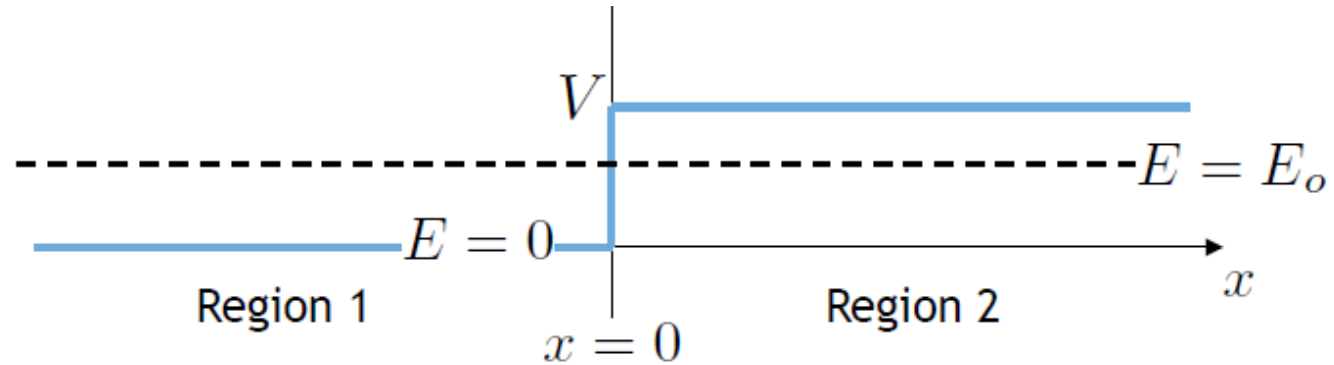
$$\text{Reflection} = R = \left| \frac{B}{A} \right|^2 = \left| \frac{k_1 - k_2}{k_1 + k_2} \right|^2$$

$$\text{Transmission} = T = 1 - R$$

$$= \frac{4k_1 k_2}{|k_1 + k_2|^2}$$

Basamak Potansiyeli, $E < V(x)$

CASE II : $E_o < V$



$$\frac{B}{A} = \frac{1 + j\kappa/k_1}{1 - j\kappa/k_1}$$

$$\frac{C}{A} = \frac{2}{1 - j\kappa/k_1}$$

$$\left\{ \begin{array}{l} A + B = C \\ A - B = -j \frac{\kappa}{k_1} C \end{array} \right. \leftarrow$$

$$R = \left| \frac{B}{A} \right|^2 = 1 \quad T = 0$$

Total reflection \rightarrow Transmission must be zero

Born and Distorted Wave Born Approximation

$$L_k(r)\psi(r) = U(r)\psi(r) \quad \text{where} \quad L_k(r) = \nabla^2 + k^2$$

Multiplying by $L_k^{-1}(r)$ and integrating all over the space we get

$$\psi(r) = \phi_k(r) + \int U(r')\psi(r')L_k^{-1}(r)\delta(r' - r)dr'$$

$\phi_k(r) = e^{ikr}$ is the free particle solution ($V=0$). Using Green functions:

$$L_k^{-1}(r)\delta(r' - r) = G_k(r - r') \quad G_k^+(r - r') = -\frac{1}{4\pi} \frac{e^{ik|r-r'|}}{|r - r'|}$$

$$\psi_k^+(r) = \phi_k(r) - \frac{1}{4\pi} \int \frac{e^{ik|r-r'|}}{|r - r'|} U(r')\psi_k^+(r')dr' \quad \frac{1}{r - r'} \approx \frac{1}{r} \quad k|r - r'| \approx kr - k.r'$$

$$\psi_k^+(r) = \phi_k(r) - \frac{e^{ikr}}{4\pi r} \int e^{-ik'.r'} U(r')\psi_k^+(r')dr'$$

Scattering Amplitude and Cross-section

$$f(\theta, \varphi) = -\frac{1}{4\pi} \int e^{-ik'.r'} U(r') \psi_k^+(r') dr'$$

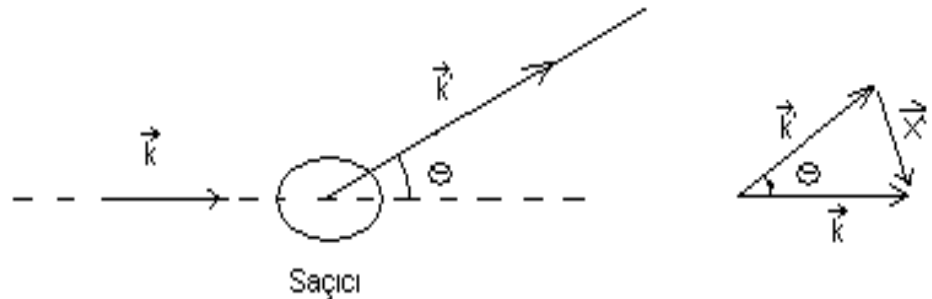
If we use plane wave for the $\psi_k^+(r)$ scattering amplitude in Born Approximation is:

$$f_{BA}(\theta, \varphi) = -\frac{1}{4\pi} \int e^{-ik'.r'} U(r') e^{ik.r'} dr'$$

$$q = k - k'; \quad f_{BA}(\theta, \varphi) = -\frac{1}{4\pi} \int U(r) e^{iqr} d^3r$$

For spherically symmetric potential $\int U(r) e^{iqr} d^3r = \frac{4\pi}{q} \int U(r) r \sin(qr) dr$

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2, \quad \sigma = \int \frac{d\sigma}{d\Omega} d\Omega$$



Distorted Wave Born Approximation

$U = U_1 + U_2$ such that $U_1 > U_2$

$$[\nabla^2 + k^2 - U_1(r)]\chi_1(k, r) = 0$$

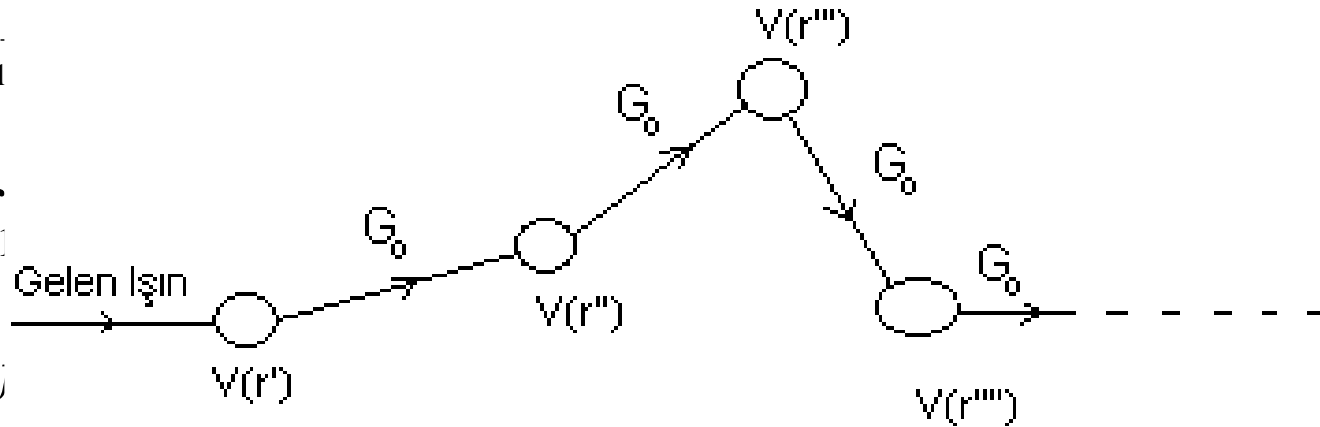
$$\chi_1(k, r) = \chi_1^-(k, r) + \chi_1^+(k, r)$$

Incoming and outgoing waves

$$\chi(k, r) \xrightarrow{r \rightarrow \infty} \chi_1$$

$$f(\theta, \varphi) = f_1$$

$$f_{DWBA}(\theta, \varphi) = f_1$$



$$(E - H_0)\psi = V\psi \quad \implies \psi = (E - H_0)^{-1}V\psi = G_0(E)V\psi$$

$$\psi = \phi + G_0V\phi + G_0VG_0V\phi + \dots$$

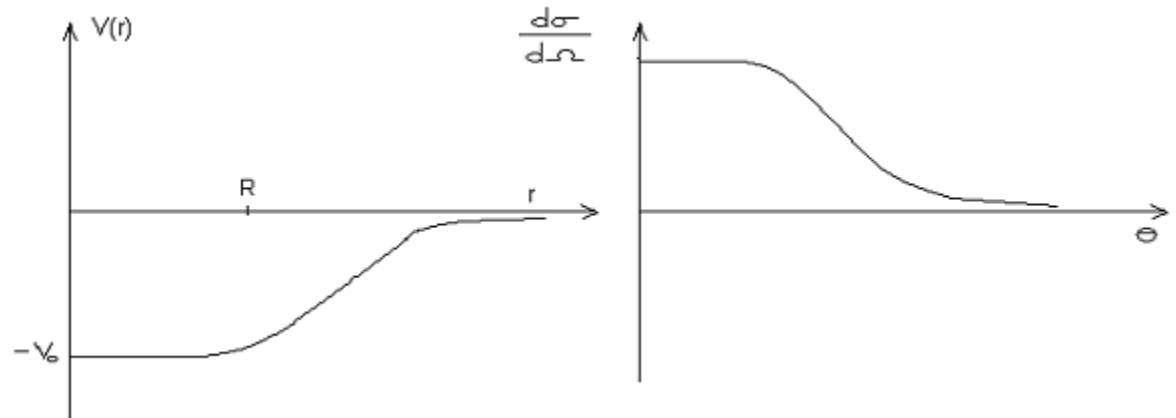
$$f(\theta, \varphi) = -\frac{m}{2\pi\hbar^2} \left[\int dr e^{-i\vec{k}' \cdot \vec{r}} V(r) e^{i\vec{k} \cdot \vec{r}} + \int dr \int dr' e^{-i\vec{k}' \cdot \vec{r}} V(r) G_0(r, r') V(r') e^{i\vec{k} \cdot \vec{r}'} + \int dr \int dr' \int dr'' + \dots \right]$$

Example: Gaussian Potential

$$V(r) = -V_0 e^{-\left(\frac{r}{R}\right)^2} \quad f(\theta) = \int_0^{\infty} V(r) \frac{\sin qr}{qr} 4\pi r^2 dr \quad q = 2k \sin\left(\frac{\theta}{2}\right)$$

$$f(\theta) = -V_0 \int_0^{\infty} e^{-\left(\frac{r}{R}\right)^2} \frac{\sin qr}{qr} 4\pi r^2 dr = -(2\pi)^{\frac{3}{2}} V_0 R^3 e^{-\frac{(qR)^2}{2}}$$

$$\frac{d\sigma}{d\Omega} = C e^{-(2kR)^2 \sin^2\left(\frac{\theta}{2}\right)}$$



Schrödinger equation II: Partial wave methods

We must solve:

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + \frac{2\mu}{\hbar^2} [E_{cm} - U_{\ell j}(r)] \right) u_{\ell j}(r) = 0$$

For bound states $E_{cm} < 0$ $\kappa_b = \sqrt{\frac{2\mu|E_{cm}|}{\hbar^2}}$

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - \frac{2\mu}{\hbar^2} U_{\ell j}(r) - \kappa_b^2 \right) u_{n\ell j}(r) = 0$$



Discrete
Spectrum

For scattering states $E_{cm} > 0$ $k = \sqrt{\frac{2\mu E_{cm}}{\hbar^2}}$

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - \frac{2\mu}{\hbar^2} U_{\ell j}(r) + k^2 \right) u_{k\ell j}(r) = 0$$



Continuous
Spectrum

General Solution:

$$U_l(r) = F_l(r) + iG_l(r) + S_l[G_l(r) - iG_l(r)]$$

$$F_l(r) = krj_l(kr) \quad \text{Bessel functions}$$

$$G_l(r) = -kr\eta_l(kr) \quad \text{Neumann functions}$$

$$f(\theta) = f_c(\theta) + \frac{1}{2ik} \sum_{l=0}^{l=\infty} (2l+1)(S_l - 1)e^{2i\sigma_l} P_l(\cos\theta) \quad \text{scattering amplitude}$$

$$\sigma_{el} = \frac{\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) |1 - S_\ell|^2$$



$$\sigma_{tot} = \sigma_{el} + \sigma_R$$

$$\sigma_R = \frac{\pi}{k^2} \sum_l (2l+1) [1 - |S_l|^2]$$

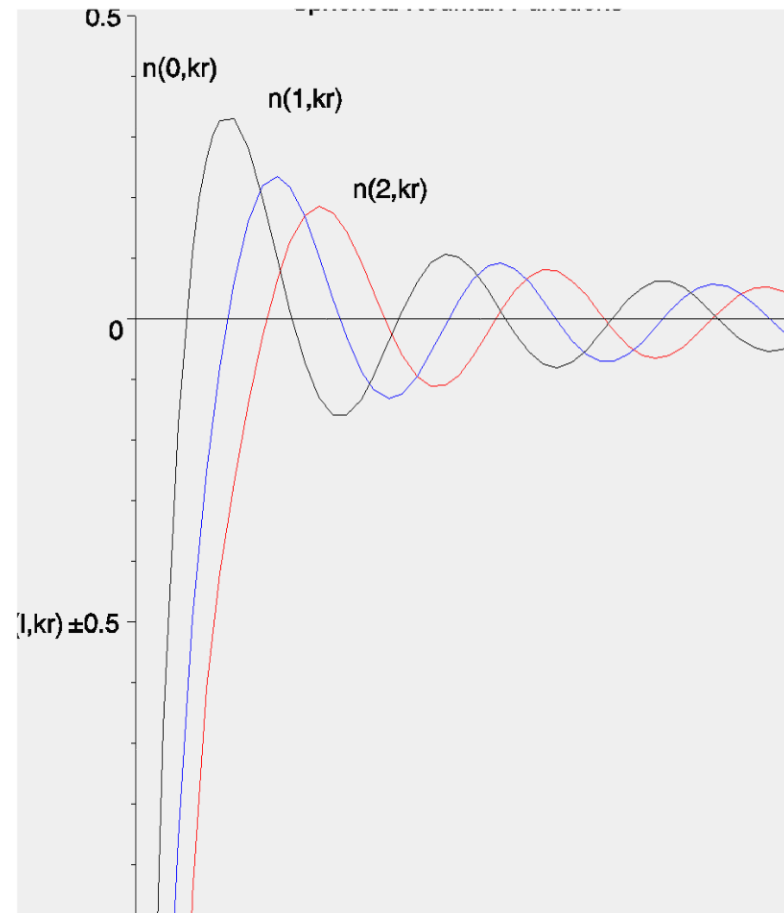
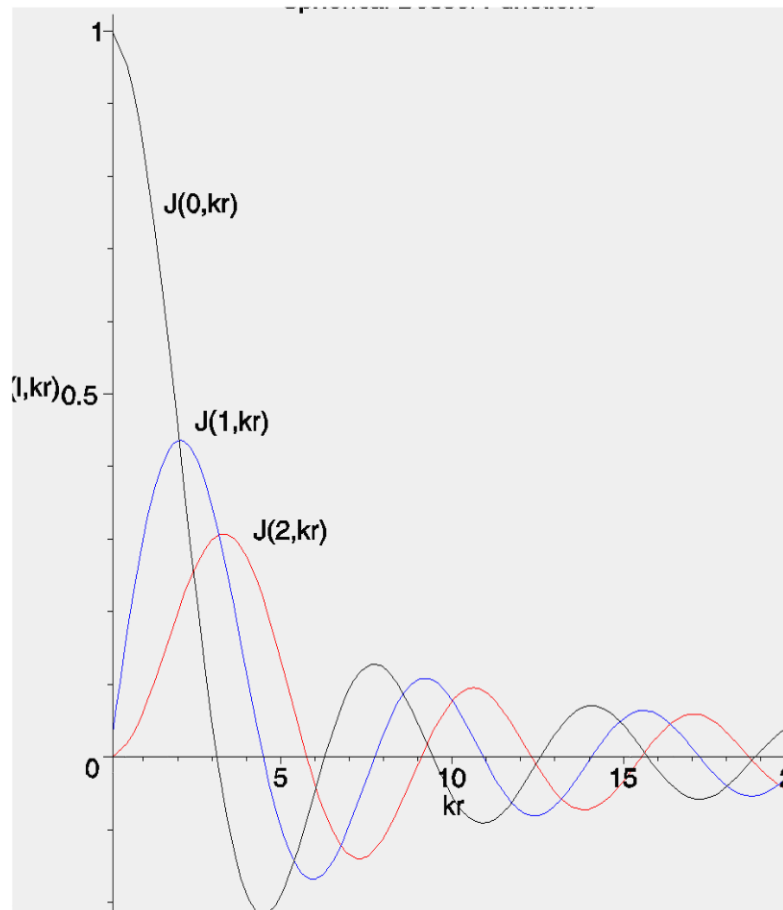
Bessel and Neumann functions

For small x $j_l(x) \rightarrow \frac{x^l}{(2l+1)!!}$

$n_l(x) \rightarrow -\frac{(2l-1)!!}{x^{l+1}}$

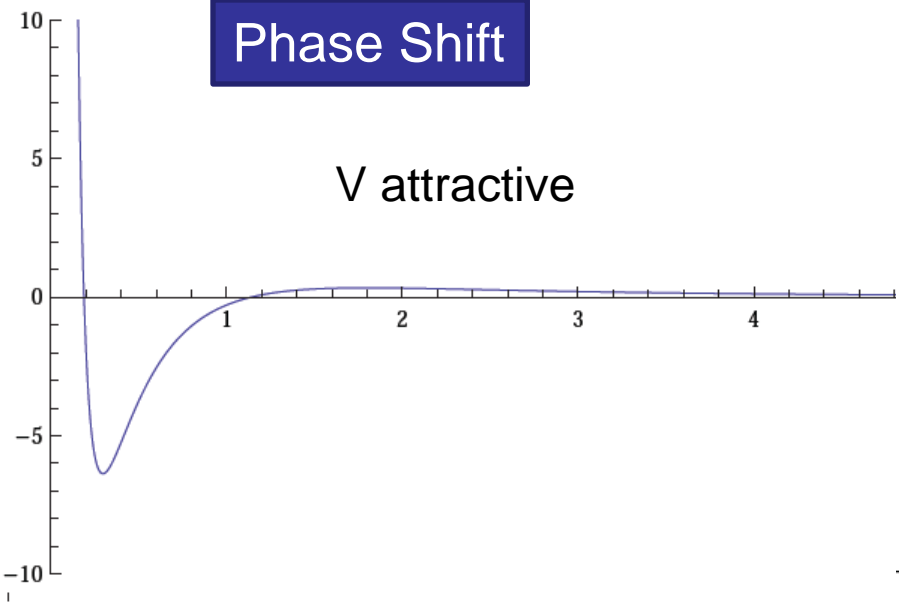
For large x $j_l(x) \rightarrow \frac{1}{x} \sin(x - l\pi/2)$

$n_l(x) \rightarrow -\frac{1}{x} \cos(x - l\pi/2)$

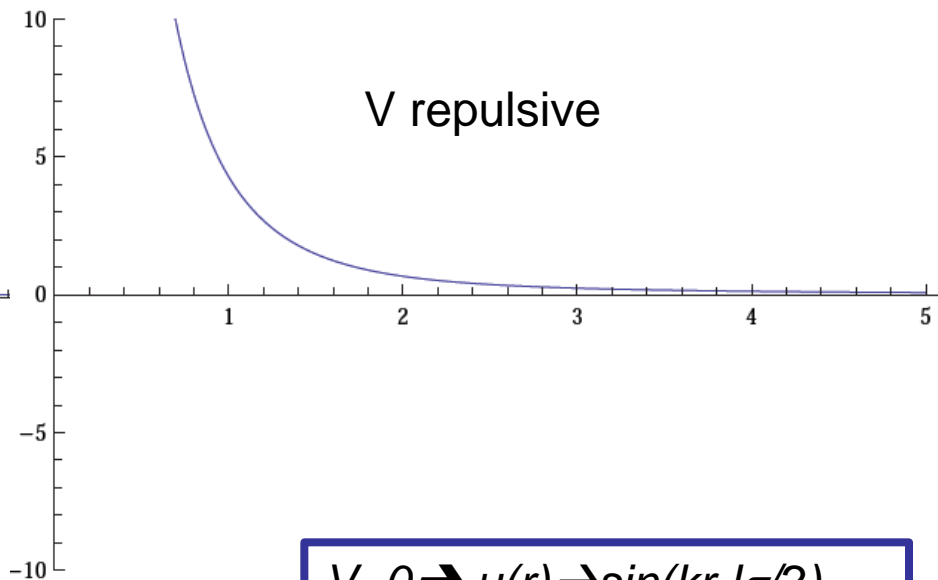


Phase Shift

V attractive

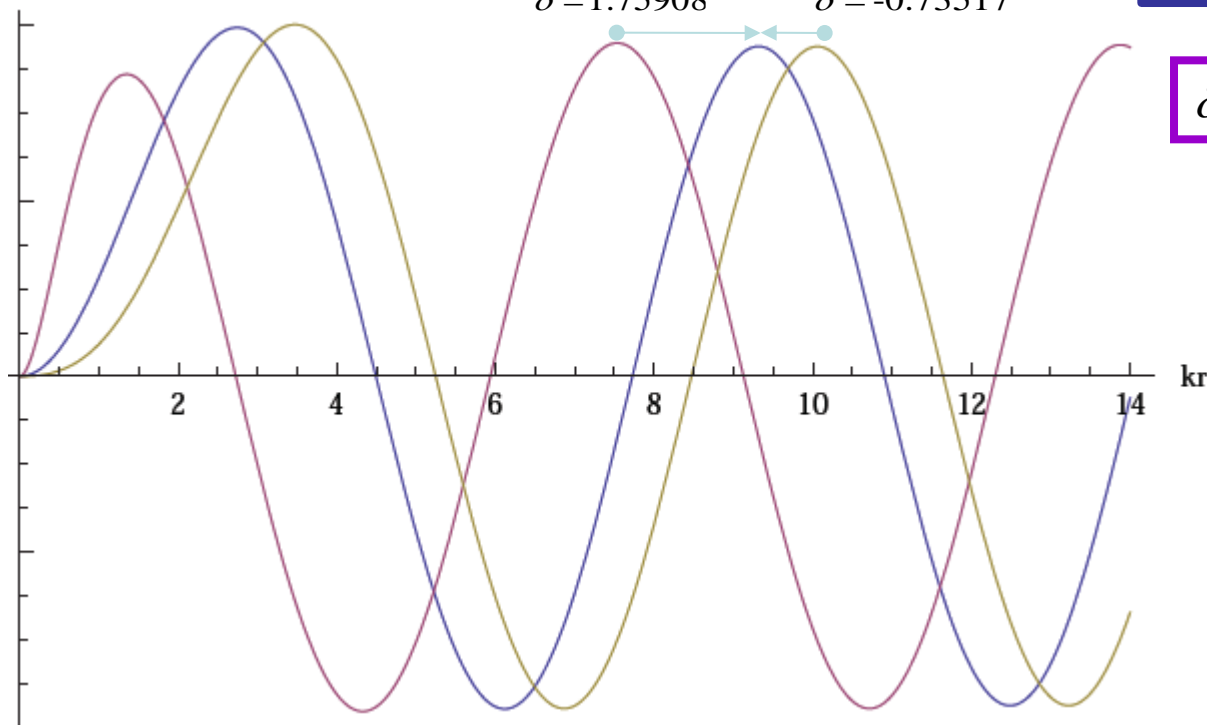


V repulsive



$$V=0 \rightarrow u(r) \rightarrow \sin(kr - l\pi/2)$$
$$\delta_l = 0$$

$$\delta = 1.75908$$
$$\delta = -0.73517$$



$$\delta_l > 0 \rightarrow V \text{ attractive}$$

$$V \neq 0 \rightarrow u(r) \rightarrow \sin(kr - l\pi/2 + \delta_l)$$

$$\delta_l < 0 \rightarrow V \text{ repulsive}$$

Teşekkürler