3D Particle in a Box

many degenerate states

Now count large # of particles

$$E_n = \frac{1}{2m}\left(\frac{\pi\hbar}{a}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

$$\psi(x) \sim e^{ikx} \longrightarrow \psi(x,y,z) \sim e^{i(k_x x + k_y y + k_z z)} = e^{i(\vec{k}\cdot\vec{r})}$$

periodic boundary conditions $\psi(q_i + L) = \psi(q_i)$

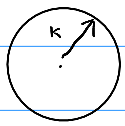
$$e^{ik_x L} = e^{ik_y L} = e^{ik_z L} = 1$$

$$k_x = \frac{2\pi n_x}{L} \quad k_y = \frac{2\pi n_y}{L} \quad k_z = \frac{2\pi n_z}{L}$$

$$E = \frac{p^2}{2m} = \frac{(\hbar\vec{k})^2}{2m} = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2) = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

Equipotential Surface = sphere $N = \left(\frac{L^3}{(2\pi)^3}\right) \cdot \frac{4}{3}\pi k^3$

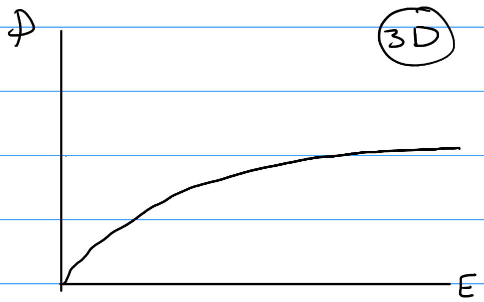
$$E = \frac{\hbar^2 k^2}{2m}$$

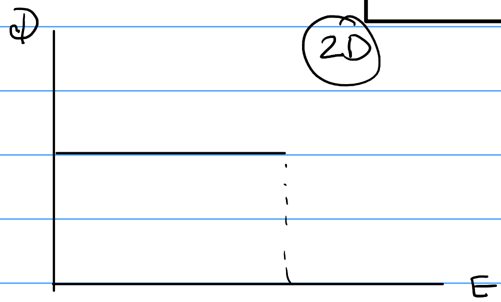


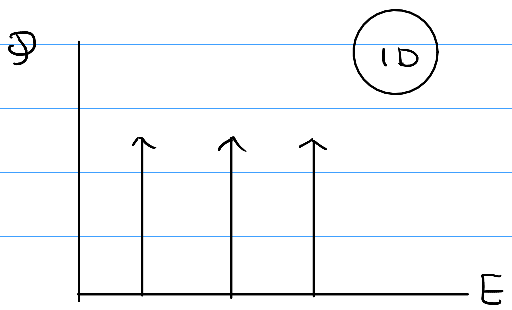
In HW 6 2.35 !

Density of states $\longrightarrow$ Large # particle limit

$$D(E) = \frac{dN}{dE} \longrightarrow N = L^3 (2m)^{3/2} E^{3/2} \cdot \frac{1}{8\pi^2\hbar^3} \longrightarrow \boxed{\frac{dN}{dE} = \frac{m^{3/2} E^{1/2} L^3}{\sqrt{2}\,\pi^2\hbar^3}}$$







Revisiting the Simple Harmonic Oscillator

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi(x)$$

let $y = \sqrt{\frac{m\omega}{\hbar}}\,x$

$$\rightarrow \quad \frac{d^2\phi(y)}{dy^2} + \left(\frac{2E}{\hbar\omega} - y^2\right)\phi(y) = 0$$

- Solve $h(y)$ via power series

$\phi(y) = h(y)\,e^{-y^2/2} \longrightarrow$ solve $h(y)$ by power series

$$h(y) = \sum_{j=1}^{\infty} a_j y^{2j} + \sum_{j=0}^{\infty} a_j y^{2j+1}$$

$$\boxed{a_{n+2} = \frac{\left[2n - \left(\frac{2E}{\hbar\omega} - 1\right)\right]a_n}{(n+1)(n+2)}}$$

- quantization is realized by termination of the series after k terms

for even states: $\frac{2E}{\hbar k} = (4k+1) \qquad E = (2k + \frac{1}{2})\hbar\omega$

$k = 0, 1, 2, \dots$

$k=0 \quad E = \hbar\omega/2 \qquad \phi_0 = a_0$

$k=1 \quad E = 5\hbar\omega/2 \qquad \phi_0 = A_0(+2y^2)e^{-y^2/2}$

$\frac{2E}{\hbar\omega} = 4k+3 \longrightarrow E = (2k + \frac{3}{2})\hbar\omega$

$k=0 \quad E = 3/2\,\hbar\omega \qquad \phi = a_0 y e^{-y^2/2}$

$k=1 \quad E = 7/2\,\hbar\omega \qquad \phi = a_0\,y(1 + \frac{2}{3}y^2)e^{-y^2/2}$

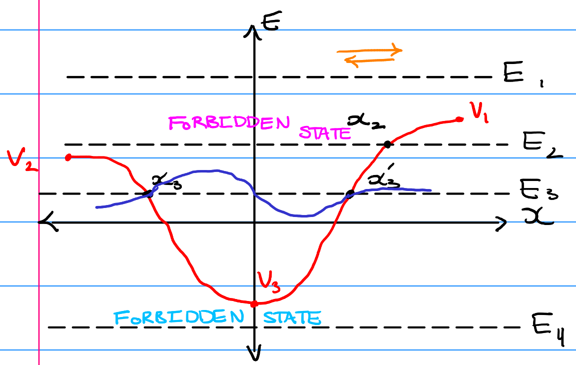
$$\boxed{\phi_n(y) = \left(\frac{\sqrt{m\omega/\hbar\pi}}{n!\,2^n}\right)^{1/2} h_n(y)\,e^{-y^2/2} \qquad E_n = (n + \frac{1}{2})\hbar\omega}$$

The series' coefficients $\longrightarrow$ generate Hermite Polynomials

General Features of Quantum states

- Bound States E_n, ϕ_n

ex. particle in a box and HO's



① $E_1 > V_1$ $\quad E - V(x) > 0$

cont. ⟵ left going wave

⟶ right " "

② $V_1 > E_2 > V_2$

Turning point

oscillatory $\quad x < x_2 \quad E_2 - V > 0$

exponential decay $\quad x > x_2 \quad E_2 - V < 0$

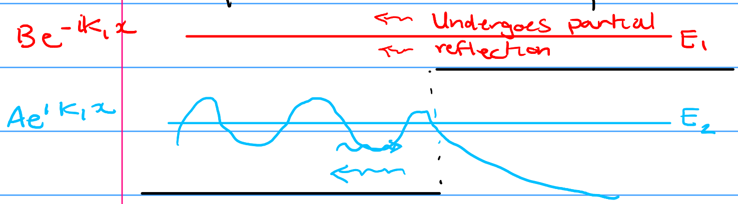
③ $V_2 > E_3 > V_3$

Two turning points

④ $E < V_3 \quad KE < 0$

Forbidden $E < V_3$ for all x

Example — Potential Step



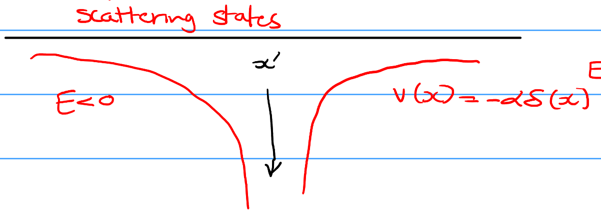
$$R = \frac{|B|^2}{|A|^2} \qquad T = \frac{k_2}{k_1}\frac{|C|^2}{|A|^2}$$

$$T = \frac{k_2}{k_1}\frac{|C|^2}{|A|^2} = \frac{4k_1k_2}{(k_1+k_2)^2} \qquad \frac{k_2}{k_1} = \sqrt{1 - \frac{V_0}{E}}$$

Example — Delta Function potential

$$V = -V_0\delta(x - x')$$

The

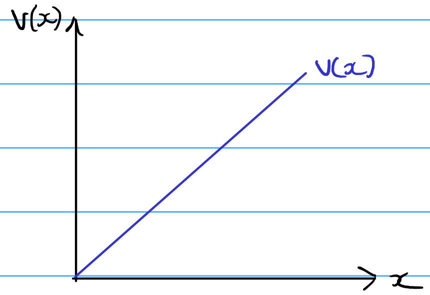


Sakurai 2.29 for HW#6

- only one bound state allowed $\quad E = -\frac{m\alpha^2}{2\hbar^2}$

$$\boxed{\phi(x) = \begin{cases} \sqrt{\frac{m\alpha}{\hbar}}\, e^{-\frac{m\alpha}{\hbar^2}x} & x \geq x' \\ \sqrt{\frac{m\alpha}{\hbar}}\, e^{+\frac{m\alpha}{\hbar^2}x} & x \leq x' \end{cases}}$$

Example — Linear Potential



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

ℓ

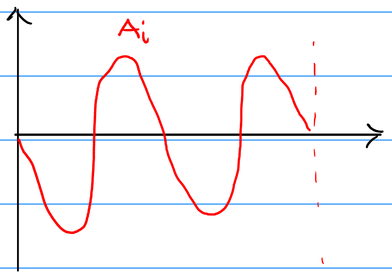
$$-\frac{d^2\psi}{dz^2} + z\psi = 0 \longrightarrow$$ soln. Airy functions

$z = y - \varepsilon$

$\psi(z) = a\,A_i(z) + b\,B_i(z)$ $\quad B_i(z) \to \infty$ for large z

$\psi(z) = a\,A_i(z)$

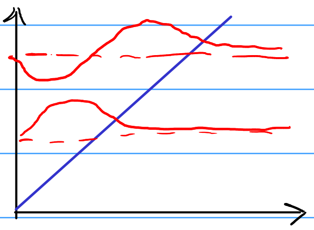
$\psi(x=0) = 0 \quad A_i(z = -\varepsilon) = 0$



Zeroes: $z = -2.338, -4.088, -5.521$

$\varepsilon = 2.338, 4.088, 5.521$

$E_1 = \varepsilon E_0$



neutron mass $m_n = 1.67e{-27}$ kg

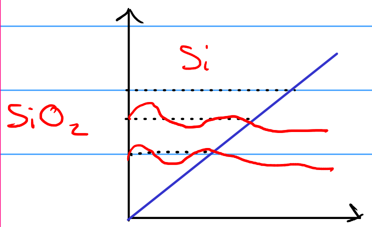
$l_0 = \left(\frac{\hbar^2}{2m^2 g}\right)^{1/3} \approx 5.88\ \mu m$

recall that $y = \frac{x}{l_0} - \varepsilon$

$x_1 = 2.338\, l_0 \approx 14\ \mu m$

$x_2 = 4.088\, l_0 \approx 24\ \mu m$

Other examples —— triangular potential in heterostructures



WKB Method

(Wentzel – Kramers – Brillouin)

- semi – classical approximation for systems w/ slowly-varying potential

$V(x)$ is roughly constant over the deBroglie wavelength $\lambda = h/p$

$$\frac{d^2\psi}{dx^2} = -\frac{p^2}{\hbar^2}\psi(x) \qquad p \equiv \sqrt{2m(E - V(x))}$$

$$\frac{d^2}{dx^2}A = A(x)\left[\left(\frac{d\phi(x)}{dx}\right)^2 - \frac{p^2}{\hbar^2}\right] \quad ①$$

$$\frac{d}{dx}\left(A(x)^2\frac{d\phi(x)}{dx}\right) = 0 \quad ②$$

② $A^2\phi' = \text{const}$

$$A(x) = \frac{c}{\sqrt{\phi'(x)}} \quad ③$$

$$\frac{d^2A}{dx^2} = A(x)\left[\left(\frac{d\phi(x)}{dx}\right)^2 - \frac{p^2}{\hbar^2}\right] \quad ④$$

Similar to the SE

$$\frac{d^2A}{dx^2} \approx 0$$

$$\left(\frac{d\phi}{dx}\right)^2 = \frac{p^2}{\hbar^2} \quad \xrightarrow{\text{Hand-wavy algebra}} \quad \psi_{WKB}(x) = \frac{c}{\sqrt{k(x)}}\exp\left(\pm i\int k(x)\,dx\right)$$

Caveat — careful around turning points $\rightarrow$ $\psi_{WKB} \rightarrow \infty$ diverges

↳ Solution: "patch" wave function w/ Airy functions

- i.e. Modified WKB wave functions