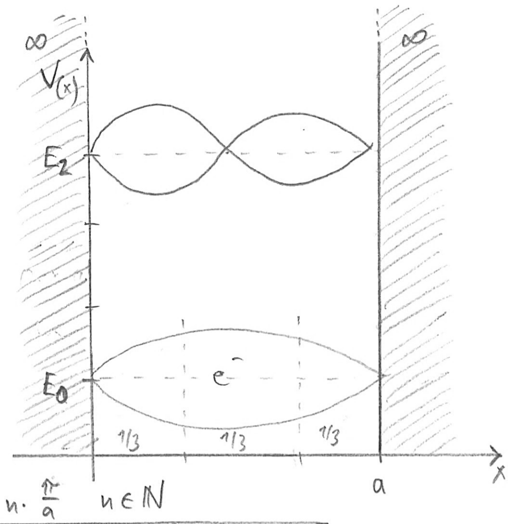
Modern Physics WS 21/22 Sören Birling

Problem Sheet 7



Ex. 7.1: Schrödinger equation: Infinitely deep potential well

a)

$$V_{(x)} = \begin{cases} 0 & 0 < x < a \\ \infty & \text{else} \end{cases} \qquad E_0 = 0{,}1\,\text{eV}$$

Recall Lecture 10: Schrödinger eq. for $0<x<a$

\+ boundary conditions $\Psi_{(x=0)} = 0 = \Psi_{(x=a)}$

$$\Rightarrow \boxed{\Psi_{n(x,t)} = \Psi_0 \sin(k_n x)\, e^{-i\frac{E_n}{\hbar}t}} \quad \text{with} \quad k_n = n\cdot\frac{\pi}{a} \quad n\in\mathbb{N}$$

$$|\Psi_{n(x,t)}|^2 = 1 \Rightarrow \Psi_0 = \sqrt{\frac{2}{a}} \quad \text{and} \quad \boxed{E_n = \frac{(\hbar k_n)^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2} \quad (\mathrm{I})$$

$$\Rightarrow a = \frac{\hbar\pi n}{\sqrt{2mE_n}}$$

$$a = \frac{\hbar\pi \overset{n=1}{n}}{\sqrt{2mE_0}} = 1{,}939\ \text{nm}$$

b)

$$|z|^2 = z^* z$$

$$P_{(e^- \text{ in left third})} = \int_0^{\frac{1}{3}a} \Psi^*_{1(x,t)} \Psi_{1(x,t)}\, dx = \underbrace{\Psi_0^* \Psi_0}_{\frac{2}{a}} \int_0^{\frac{1}{3}a} \sin^2\left(\frac{\pi}{a}x\right) dx = \underset{\dots}{(*)} = \frac{1}{3} - \frac{\sqrt{3}}{4\pi} \approx 19{,}55\,\%$$

(*) integral can be solved analytically by:

$$\frac{2}{a}\int_0^{a/3} \sin^2\left(\frac{\pi}{a}x\right)dx = \frac{2}{a}\int_0^{\pi/3} \sin^2(u)\frac{a}{\pi}\,du = \frac{2}{\pi}\cdot\frac{1}{2}\int_0^{\pi/3} du - \frac{2}{\pi}\cdot\frac{1}{2}\int_0^{\pi/3}\cos(2u)\,du$$

substitute $u = \frac{\pi x}{a} \rightarrow du = \frac{\pi}{a}dx$; $0 \rightarrow 0$, $\frac{a}{3} \rightarrow \frac{\pi}{3}$

$\sin^2(u) = \frac{1}{2} - \frac{1}{2}\cos(2u)$

$$= \frac{1}{\pi}\left[\frac{\pi}{3} - 0\right] - \frac{1}{\pi}\left[\frac{1}{2}\sin(2u)\right]_0^{\pi/3} = \frac{1}{3} - \frac{1}{2\pi}\left[\frac{\sqrt{3}}{2} - 0\right] = \frac{1}{3} - \frac{\sqrt{3}}{4\pi} \approx 19{,}55\%$$

c) first excited state energy?

$$E_2 = \underbrace{\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2}_{E_0}(2)^2 = 4\cdot E_0 = 0{,}4\,\text{eV}$$

Ex. 7.2: Harmonic oscillator

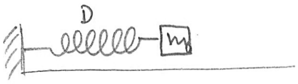
$$m_0 a = \sum \vec{F}$$

$$m_0 \ddot{x} + D x = 0$$

$$\ddot{x} + \underbrace{\frac{D}{m_0}}_{\omega^2} x = 0$$

a) $V_{(x)} = \frac{1}{2} D x^2 \quad D > 0$

$$\vec{F} = -\vec{\nabla} V_{(x)} = -Dx$$



$$\omega = 2\pi f = \sqrt{\frac{D}{m_0}}$$

b) Schrödinger equation: $\boxed{i\hbar \frac{\partial}{\partial t} \Psi_{(x,t)} = \hat{H} \Psi_{(x,t)}}$ with $\boxed{\hat{H} = -\frac{\hbar^2}{2m_0}\frac{\partial^2}{\partial x^2} + \frac{1}{2} D x^2}$

c) $E_0(D, m_0)$, $a_0(D, m_0)$?

grondstate wave-fct.: $\Psi_{0(x,t)} = A_0 e^{-\frac{x^2}{a_0^2}} e^{-\frac{iE_0 t}{\hbar}}$

into Schödinger eq.: $i\hbar\left(-\frac{iE_0}{\hbar}\right)\Psi_0 = -\frac{\hbar^2}{2m_0}\underbrace{\left(\frac{4x^2 - 2a_0^2}{a_0^4}\right)\Psi_0}_{} + \frac{1}{2} D x^2 \Psi_0$

$$\frac{\partial^2}{\partial x^2}\left(e^{-\frac{x^2}{a_0^2}}\right) = \frac{\partial}{\partial x}\left(e^{-\frac{x^2}{a_0^2}}\left(-\frac{2x}{a_0^2}\right)\right)$$

$$= e^{-\frac{x^2}{a_0^2}}\left(-\frac{2x}{a_0^2}\right)^2 + e^{-\frac{x^2}{a_0^2}}\left(-\frac{2}{a_0^2}\right)$$

$$E_0 = -\frac{\hbar^2}{2m_0}\left(\frac{4x^2 - 2a_0^2}{a_0^4}\right) + \frac{1}{2} D x^2$$

$$E_0 = \underbrace{\left[\frac{1}{2} D - \frac{2\hbar^2}{m_0 a_0^4}\right]}_{B} x^2 + \underbrace{\frac{\hbar^2}{m_0 a_0^2}}_{A}$$

(A) $x = 0$: $E_0 = \frac{\hbar^2}{m_0 a_0^2}$

(B) $\frac{1}{2} D - \frac{2\hbar^2}{m_0 a_0^4} = 0 \longrightarrow \frac{1}{a_0^2} = \frac{1}{2\hbar}\sqrt{D m_0}$ (I)

(I)

$$E_0 = \frac{\hbar^2}{2m_0\hbar}\sqrt{D m_0} = \frac{1}{2}\hbar\underbrace{\sqrt{\frac{D}{m_0}}}_{\omega} = \frac{1}{2}\hbar\omega$$

Ex. 7.3:

Mo: $Z = 42$ $\quad U = 35\,\mathrm{kV}$

Moseley's law: $(m \to n)$ $\boxed{\frac{hc}{\lambda} = R_y \left|\frac{1}{n^2} - \frac{1}{m^2}\right| \times (Z - \beta)^2}$

or $\frac{1}{\lambda} = R_\infty \ldots$

β: screening constant of nuclear charge

$R_y = 13{,}6\,\mathrm{eV}$

$R_\infty = 1{,}0974 \cdot 10^5\,\mathrm{cm}^{-1}$

K_α: $m = 2 \rightarrow n = 1$

K_β: $m = 3 \rightarrow n = 1$

$\beta = 1$

$$\lambda = hc\left[R_y\left|\frac{1}{n^2} - \frac{1}{m^2}\right| \cdot (Z - \beta)^2\right]^{-1}$$

L_α: $m = 3 \longrightarrow n = 2$

L_β: $m = 4 \longrightarrow n = 2$

$\beta = 7{,}4$

a) $\lambda_{K_\alpha} = \left\{\begin{matrix} m=2 \\ n=1 \\ \beta=1 \\ Z=42 \end{matrix}\right\} = 0{,}723\,\text{Å}$

both agree with figure! ✓

$\lambda_{K_\beta} = \left\{\begin{matrix} m=3 \\ \vdots \end{matrix}\right\} = 0{,}610\,\text{Å}$

b) $\lambda_{\text{cut-off}} = \frac{hc}{eU} = 0{,}354\,\text{Å}$ (figure ✓)

c) $\lambda_{L_\alpha} = \left\{\begin{matrix} m=3 \rightarrow n=2 \\ \beta = 7{,}4 \end{matrix}\right\} = 5{,}48\,\text{Å}$

$\lambda_{L_\beta} = \left\{\begin{matrix} m=4 \rightarrow n=2 \\ \beta = 7{,}4 \end{matrix}\right\} = 4{,}06\,\text{Å}$