

17. Radial Current Density.

Problem 4.6. At instant $t = 0$ the electron behavior is described by the following wavefunction:

$$\Psi(r, 0) = A e^{-r^2/\alpha^2 + ikr} \quad (4.32)$$

Find the normalization constant, A , the most probable value r_{pr} , and the radial part of the probability current, j .

① Normalization

We are working here in spherical coordinates, so the normalization we have to use:

$$\int_V |\Psi|^2 dV = \int_V |\Psi|^2 r^2 \sin\theta dr d\theta d\varphi = 1 \quad r: 0 \rightarrow \infty, \theta: 0 \rightarrow \pi, \varphi: 0 \rightarrow 2\pi$$

$$\hookrightarrow |\Psi(r, 0)|^2 = \Psi^*(r, 0) \Psi(r, 0) = A^* e^{-r^2/\alpha^2 - ikr} \cdot A e^{-r^2/\alpha^2 + ikr} = |A|^2 e^{-2r^2/\alpha^2}$$

$$1 = \int_0^{2\pi} \int_0^\pi \int_0^\infty |\Psi(r, 0)|^2 r^2 \sin\theta dr d\theta d\varphi = 4\pi \int_0^\infty |\Psi(r, 0)|^2 r^2 dr = 4\pi \int_0^\infty |A|^2 r^2 e^{-2r^2/\alpha^2} dr$$

We solve the integral in general:

$$\textcircled{1} I(a) = \int_0^\infty e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}} \Rightarrow \frac{dI(a)}{da} = -\frac{\sqrt{\pi}}{4} a^{-3/2}$$

$$\textcircled{2} \frac{dI(a)}{da} = \frac{d}{da} \int_0^\infty e^{-ax^2} dx = \int_0^\infty \frac{d}{da} (e^{-ax^2}) dx = \int_0^\infty -x^2 e^{-ax^2} dx$$

From $\textcircled{1}$ and $\textcircled{2}$ we get and taking into account that in our case: $a = \frac{2}{\alpha^2}$

$$\int_0^\infty x^2 e^{-ax^2} dx = \frac{\sqrt{\pi}}{4} a^{-3/2} = \frac{\sqrt{\pi}}{4} \left(\frac{2}{\alpha^2}\right)^{-3/2}$$

Therefore:

$$1 = 4\pi |A|^2 \frac{\sqrt{\pi}}{4} \left(\frac{2}{\alpha^2}\right)^{-3/2} = |A|^2 \sqrt{\frac{\pi^3 \alpha^6}{8}} \Rightarrow |A| = \sqrt[4]{\frac{8}{\pi^3 \alpha^6}}$$

② r

We have to calculate: $P(r) dV = |\psi(r)|^2 dV$

Where the volume is of a sphere: $V = \frac{4\pi}{3} r^3 \Rightarrow dV = 4\pi r^2 dr$

$$P(r) dV = |\psi(r)|^2 4\pi r^2 dr = \underbrace{4\pi |A|^2 r^2}_{P(r)} e^{\underbrace{-2r^2/\alpha^2}_{=V}} dr \Rightarrow \text{The most probable value will be the maximum of } P(r)$$

$$\frac{dP(r)}{dr} = 0 \Rightarrow 4\pi |A|^2 \left[2r e^V + \frac{dV}{dr} r^2 e^V \right] = 0 \Rightarrow 4\pi |A|^2 r e^V \left[2 - \frac{4r^2}{\alpha^2} \right] = 0$$

$$\Rightarrow 1 - \frac{2r^2}{\alpha^2} = 0 \Rightarrow r = \pm \frac{\alpha}{\sqrt{2}} \quad \xrightarrow{\text{No negative distance}} \quad \boxed{r = \frac{\alpha}{\sqrt{2}}}$$

③ Probability Current

The expression is: $j = \frac{\hbar}{2mi} (\psi^* \nabla \psi - \psi \nabla \psi^*)$

$$\nabla \psi(r) = \frac{\partial \psi}{\partial r} = \frac{\partial}{\partial r} A \cdot e^{\underbrace{-r^2/\alpha^2 + ikr}_{=V}} = A \frac{dV}{dr} e^V = A v' e^V = A \left(-\frac{2r}{\alpha^2} + ik \right) e^V$$

$$\nabla \psi^* = A^* v'^* e^{V^*}$$

$$\psi = A e^V \rightarrow \psi^* = A^* e^{V^*} \rightarrow |\psi|^2 = |A|^2 e^{\text{Re}[V]}$$

$$\Rightarrow \psi^* \nabla \psi = A^* e^{V^*} \cdot A v' e^V = |A|^2 v' e^{(V+V^*)} = |A|^2 v' e^{\text{Re}[V]} = v' |\psi|^2$$

$$\Rightarrow \psi \nabla \psi^* = A e^V \cdot A^* v'^* e^{V^*} = |A|^2 v'^* e^{\text{Re}[V]} = v'^* |\psi|^2$$

$$j = \frac{\hbar}{2mi} (v' |\psi|^2 - v'^* |\psi|^2) = \frac{\hbar}{2mi} |\psi|^2 \cdot \text{Im}[v'] = \frac{\hbar}{2m} |\psi|^2 \cdot k$$

$$\boxed{j = \frac{\hbar k}{2m} \sqrt{\frac{8}{\pi^3 \alpha^6}} e^{-r^2/\alpha^2}}$$

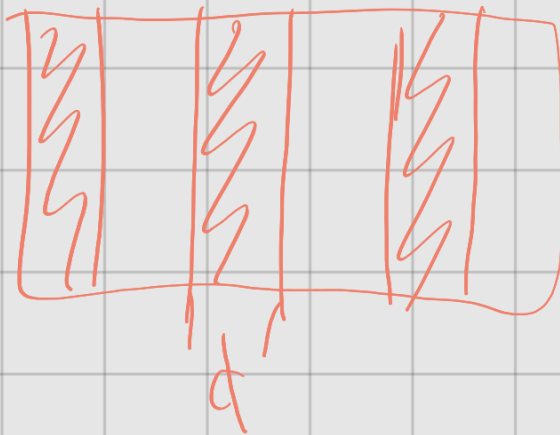
18.

The reflection and transmission coefficient of a dielectric slab of thickness “d” are:

$$r = \frac{(n^2 - 1)(e^{2ikdn} - 1)}{(n+1)^2 - (n-1)^2 e^{2ikdn}} \quad t = \frac{4n e^{ikdn}}{(n+1)^2 - (n-1)^2 e^{2ikdn}}$$

A non absorbing photonic crystal with $n=2$ (real) is made up of a periodic distribution of dielectric slabs whose thickness is $d = 0.1 a$ alternated by vacuum regions. The structure periodicity is a .

- Find the equation that describes the photonic band gap in terms of $\omega a/c$.
- Plot (Python, Mathematica, Matlab etc.) such an equation as a function of $\omega a/c$.
- Would an incident light beam with frequency such that $\omega a/c=3$ e $\omega a/c=4$ propagate or not?



19. Electrons may tunnel from a metal through the application of a suitable (constant) external electric field ε . After the application of the electric field ε the potential at the metal surface taken at $x=a$ reads as (see class notes)

$$V(x) = E_F + \Phi - e\mathcal{E}(x - a)$$

Assuming that the tunneling electrons originates from a single-electronic state, estimate the field strength ε (volt/cm) needed to draw (*tunneling*) current densities of the order of mA/cm² from a potassium sample surface.