Homework 6

PHYSICS 450
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1. For the infinite square well, the energies are defined by (2.30). The zero point energy is simply the $n = 1$ state,

$$E_1 = \frac{\pi^2 \hbar^2}{2ma^2} = \frac{\pi^2 \left(1.05 \times 10^{-34}\,\mathrm{J \cdot s}\right)^2}{2 \times 1\,\mathrm{g} \times (1\,\mu\mathrm{m})^2} = 5.5 \times 10^{-53}\,\mathrm{J}.$$

From that, its classical speed is

$$v = \sqrt{2E/m} = 3.3 \times 10^{-25}\,\mathrm{m \cdot s^{-1}} \approx 0.$$

2. For a mass of $m_e \approx 1 \times 10^{-30}\,\mathrm{kg}$ and well width $1\,\mathrm{nm}$,

$$\begin{aligned} E_1 &\approx 5.5 \times 10^{-20}\,\mathrm{J}. \\ v &\approx 3.31 \times 10^{5}\,\mathrm{m \cdot s^{-1}}. \end{aligned}$$

3. For the infinite square well in 3D of lengths L_x, L_y, and L_z, we can assume a (spatial) wavefunction of the form

$$\psi(x, y, z) = X(x)Y(y)Z(z)$$

and potential

$$V(x, y, z) = \begin{cases} 0 & 0 \le x \le L_x \wedge 0 \le y \le L_y \wedge 0 \le z \le L_z \\ \infty & \text{otherwise} \end{cases}.$$

Then, using the Schrödinger equation with this ansatz,

$$\begin{aligned} -\frac{\hbar^2}{2m}\nabla^2 \left[X(x)Y(y)Z(z)\right] + V(x, y, z)X(x)Y(y)Z(z) &= EX(x)Y(y)Z(z) \\ \implies \frac{-\hbar^2}{2m}\left[X''(x)YZ + XY''(y)Z + XYZ''(z)\right] + V(x, y, z)XYZ &= EXYZ \\ \implies \frac{-\hbar^2}{2m}\left[\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)}\right] &= E - V. \end{aligned}$$

Inside the well, $V = 0$,

$$\frac{-\hbar^2}{2m}\left[\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)}\right] = E.$$

As each term only depends on their respective variable, we can split the energies up as well, so

$$\begin{aligned} X''(x) &= -\frac{2mE_x}{\hbar^2}X(x) \\ \implies X(x) &= A\sin(k_x x) \\ k_x &= \frac{n\pi^2\hbar^2}{2mL_x} \end{aligned}$$

Doing this for the other dimensions y and z, the total wavefunction is

$$\psi(x,y,z) = A' \sin\left(\frac{n_x \pi^2 \hbar^2}{2mL_x} x\right) \sin\left(\frac{n_y \pi^2 \hbar^2}{2mL_y} y\right) \sin\left(\frac{n_z \pi^2 \hbar^2}{2mL_z} z\right),$$

where A' is the normalization constant, and $n_x, n_y, n_z = 1, 2, 3 \ldots$

Following (2.30), the energies are given by

$$\begin{aligned} E(n) &= E_x + E_y + E_z \\ &= \sum_i \frac{\hbar {k_i}^2}{2m} = \sum_i \frac{{n_i}^2 \pi^2 \hbar^2}{2m{L_i}^2} \\ &= \frac{\pi^2\hbar^2}{2m} \left(\frac{{n_x}^2}{{L_x}^2} + \frac{{n_y}^2}{{L_y}^2} + \frac{{n_z}^2}{{L_z}^2}\right). \end{aligned}$$

4. (a) The energy is NE_1,

$$E_{\text{isolated}} = NE_1 = \frac{N\pi^2\hbar^2}{2m_e a^2}.$$

(b) Since no two states can be occupied, each higher state will be in the $(n+1)$th state, so

$$\begin{aligned} E_{\text{metal}} &= E_1 + E_2 + \cdots + E_N \\ &= \frac{2N^3 + 3N^2 + N}{6} \frac{\pi^2\hbar^2}{2m_e N^2 a^2} \\ &= \frac{2N + 3 + 1/N}{6} \frac{\pi^2\hbar^2}{2m_e a^2}. \end{aligned}$$

(c) Taking the N-th order term only,

$$\begin{aligned} \Delta E &= E_{\text{isolated}} - E_{\text{metal}} \\ &= \frac{4N}{6} \frac{\pi^2\hbar^2}{2m_e a^2} \\ &= \frac{N\pi^2\hbar^2}{3m_e a^2}. \end{aligned}$$

Per atom,

$$\Delta E/N = \frac{\pi^2\hbar^2}{3m_e a^2}.$$

(d) For a typical atom separation of $a \approx 4\,\text{Å}$,

$$\begin{aligned} \Delta E/N &= \frac{\pi^2\hbar^2}{3m_e \times (4\,\text{Å})^2} \\ &\approx 1.56\,\text{eV}. \end{aligned}$$

5. Read Chapter 2.6.