3.012 Bonding-Structure: Recitation 1

1 Wave-Particle Duality

Recall

- *de Broglie Relation:* $\lambda \times p = h$
- $h = 6.626 \times 10^{-34}\ J.s$
- $\hbar = h/(2\pi) = 1.054 \times 10^{-34}\ J.s$

Problem I (P12.10)

What speed does a H_2 molecule have if it as the same momentum as a photon of wavelength 280 nm?

2 Solving the Schrödinger Equation

Recall

- *Time-dependent Schrödinger Equation:*

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\overrightarrow{r},t) + V(\overrightarrow{r},t)\Psi(\overrightarrow{r},t) = i\hbar\frac{\partial\Psi}{\partial t}(\overrightarrow{r},t) \tag{1}$$

- *Stationary Schrödinger Equation (Eigenvalue Equation):*

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\overrightarrow{r}) + V(\overrightarrow{r})\Psi(\overrightarrow{r}) = E\psi(\overrightarrow{r}) \tag{2}$$

(useful when the potential V does not depend on time)

- *Laplacian:*

$$\nabla^2\psi = \begin{cases} \frac{d^2\psi}{dx^2}(x) & \textit{in 1D} \\ \frac{\partial^2\psi}{\partial x^2}(x,y) + \frac{\partial^2\psi}{\partial y^2}(x,y) & \textit{in 2D} \\ \frac{\partial^2\psi}{\partial x^2}(x,y,z) + \frac{\partial^2\psi}{\partial y^2}(x,y,z) + \frac{\partial^2\psi}{\partial z^2}(x,y,z) & \textit{in 3D} \end{cases} \tag{3}$$

Problem II

Which of the following statements are true? Explain.

- *Free Electron in 1D*: $V(x) = 0$

  (a1) $\psi(x) = 4e^{ikx}$ and $\psi(x) = 4e^{i5kx}$ (where k is a fixed wavevector) are solutions of the S.S.E. with the same energy

  (a2) $\psi(x) = 4\cos(kx) + 2e^{i\frac{\pi}{4}}\sin(kx)$ is a solution of the S.S.E.

  (a3) $\psi(x) = Ae^{ikx} + Be^{-2ikx}$ (where A and B are complex constants) is a solution of the S.S.E.

  (a4) $\psi(x) = A\sin(kx) + B\cos(kx)$ is a solution of the S.S.E.

  (a5) $\psi(x,t) = Ae^{i(kx-\omega t)} + Be^{i(-kx-\omega t)}$ is a solution of the time-dependent Schrödinger equation (T.D.S.E.) on the conditions that $E = \hbar\omega$ and $E = \frac{(\hbar k)^2}{2m}$

- *Free Electron in 2D*: $V(x,y) = 0$

  (b1) $\psi(x,y) = (4+2i)e^{i(2x+3y)}$ is a solution of the S.S.E.

  (b2) $\psi(x,y) = A\cos(k_x x)\sin(k_y y)$ (where k_x and k_y are fixed wavevectors) is a solution of the S.S.E.

- *Electron in a 1D Infinite Box (Infinite Square Well)*: $V(x) = \begin{cases} +\infty & \text{if } x < 0 \\ 0 & \text{if } 0 < x < a \\ +\infty & \text{if } a < x \end{cases}$

  (c1) The S.S.E. can be rewritten as:

$$\begin{cases} \frac{d^2\psi}{dx^2}(x) = 0 \text{ for } 0 < x < a \\ \psi(0) = 0 \\ \psi(a) = 0 \end{cases} \tag{4}$$

  (c2) $\psi(x) = i\sqrt{2}\cos(\frac{3\pi x}{a})$ is a solution of the S.S.E.

  (c3) $\psi(x) = A\sin(\frac{n\pi x}{a})$ (where n is integer) is a solution of the S.S.E. with energy $E = (\hbar^2 n^2\pi^2)/(2ma^2)$

  (c4) $\psi(x) = A\sin(\frac{n\pi x}{a})$ is a solution of the S.S.E. with energy $E = (h^2 n^2)/(8ma^2)$

- *Electron in a 2D Infinite Box*: $V(x, y) = \begin{cases} 0 & \text{if } 0 < x < a \text{ and } 0 < y < b \\ +\infty & \text{elsewhere} \end{cases}$

  (d1) $\psi(x, y) = A\sin(\frac{l\pi x}{a})\sin(\frac{m\pi y}{b})$ (where l and m are integers) is a solution of the S.S.E. with energy:

$$E = \frac{\hbar^2}{4m}\left(\frac{l^2}{a^2} + \frac{m^2}{b^2}\right) \tag{5}$$

- *General Properties of the Schrödinger Equation*

  (e1) If $\psi_a(x)$ and ψ_b are solutions of the S.S.E. with different energies E_a and E_b, $A\psi_a(x) + B\psi_b(x)$ is also a solution.

  (e2) If $\psi(\overrightarrow{r})$ is a solution of the S.S.E with energy E, $\Psi(\overrightarrow{r}, t) = \psi(\overrightarrow{r}) \times e^{-i\frac{Et}{\hbar}}$ is a solution of the T.D.S.E.

3 Electron Density, Probability, Normalization

Recall

- *The electron density* $n(\overrightarrow{r})$ *is related to the electronic wavefunction* $\psi(\overrightarrow{r})$*:* $n(\overrightarrow{r}) = \psi^*(\overrightarrow{r})\psi(\overrightarrow{r})$
- *In 1D, the probability of finding an electron in the spatial interval* $x_{min} < x < x_{max}$ *is given by the integral* $\int_{x_{min}}^{x_{max}} \psi^*(x)\psi(x)dx$ *(*ψ *must be normalized)*
- *Normality condition:* $\int_{+\infty}^{-\infty} \psi^*(x)\psi(x)dx = 1$
- $\int_0^a \sin^2(\frac{n\pi x}{a})dx = \frac{a}{2}$

Problem III

(a) Why is it necessary to impose the normality condition on the electron wavefunction?

(b) Normalize the wavefunctions $\psi_1(x) = A_1\sin(\frac{\pi x}{a})$ and $\psi_6(x) = A_2\sin(\frac{6\pi x}{a})$.

(c) Plot $\psi_1(x)$, $\psi_6(x)$ and the corresponding charge densities. What is the probability of finding an electron of wavefunction $\psi_1(x)$ in the spatial interval $0 < x < a/2$? Same question with $\psi_6(x)$ and the interval $a/3 < x < 2a/3$.

4 Spectrum

Recall

- *The eigenvalues and normalized eigenfunctions of a particle (mass m) in a 1D-box (width a) are* $E_n = (\hbar^2 n^2 \pi^2)/(2ma^2) = (h^2 n^2)/(8ma^2)$ *and* $\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})$ *(where n=1,2,3,4,...)*

Problem IV

What is the meaning of the following g aph?

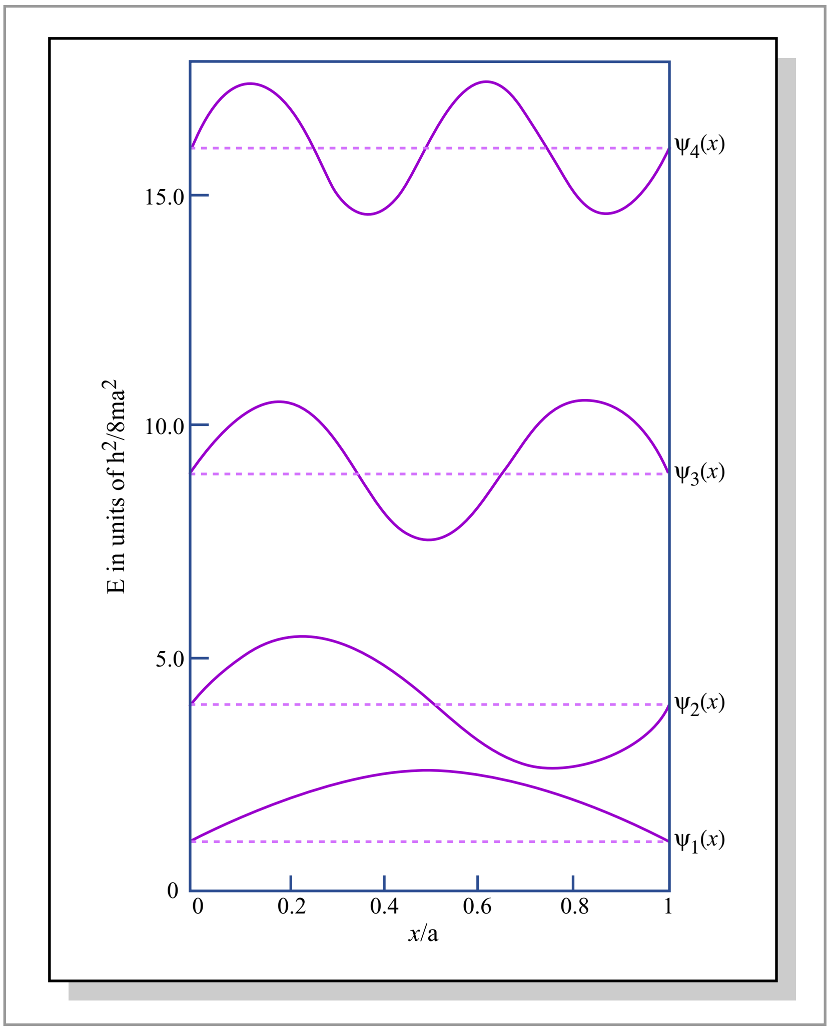

Figure by MIT OCW.