Exam Major Concepts Review

Classical Hamiltonian Mechanics

$$H = T + V = E$$

$$T = \sum_i \frac{p_i^2}{2m_i}$$

$$V = V(x_i)$$

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial x_i} = -\frac{\partial V}{\partial x_i}$$

$$\frac{dx_i}{dt} = \frac{\partial H}{\partial p_i} = \frac{\partial T}{\partial p_i}$$

2nd Order Ordinary Differential Equation General Solution

$$\ddot{x} + \omega^2 x = 0 \rightarrow x(t) = Ae^{i\omega t} + Be^{-i\omega t}$$

Euler's Formula

$$e^{\pm i\theta} = \cos\theta \pm i \sin\theta$$

Classical Free Particle $E = \frac{p^2}{2m}$

Massless Wave $E = \hbar\omega = h\nu$

De Broglie Particle-Wave $p = \hbar k = \frac{h}{\lambda}$

I.

(x, t)

$$\int_{-\infty}^{\infty} \psi_n^*(x)\psi_m(x)dx = \begin{cases} 1 & n = m \\ 0 & n \neq m \end{cases}$$

$(x, t) \neq \infty$

If $\psi(x) = \begin{cases} \psi_I(x) & x\epsilon(-\infty, a] \\ \psi_{II}(x) & x\epsilon[a, \infty) \end{cases}$

$$\psi_I(a) = \psi_{II}(a)$$

$$\frac{\partial \psi_I}{\partial x}(a) = \frac{\partial \psi_{II}}{\partial x}(a)$$

II.

Probability Density $\rho(x) = \psi^*(x)\psi(x)$

$$P(a \leq x \leq b) = \int_a^b \psi^*(x)\psi(x)dx$$

$$1 = \int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx$$

III.

$$\langle\psi|\hat{A}|\psi\rangle = \int_{-\infty}^{\infty} \psi^*(x)\hat{A}\psi(x)dx$$

$$\hat{A}\psi_n(x) = a_n\psi_n(x)$$

IV.

$$\text{Total State} \quad (x) = \sum_n c_n \psi_n(x)$$

$$P(a_n) = |\langle \quad (x)|\psi_n(x)\rangle|^2 = \left| \int_{-\infty}^{\infty} \quad ^*(x)\psi_n(x)\, dx \right|^2 = |c_n|^2$$

V.

$$\text{If } \hat{A} \quad (x) = a_n \psi_n(x) \rightarrow \quad (x) = \psi_n(x)$$

VI.

$$\hat{H} \quad (x,t) = i\hbar \frac{\partial \quad (x,t)}{\partial t}$$

$$(x,t) = \psi(x)\phi(t)$$

$$\phi(t) = e^{-i\frac{E}{\hbar}t}$$

$$\hat{H}\psi(x) = E\psi(x)$$

Operators

1D Position $\hat{x} \rightarrow x$

3D Position $\hat{r} \rightarrow \vec{r} = x\hat{\imath} + y\hat{\jmath} + z\hat{k}$

1D Momentum $\hat{p}_x \rightarrow -i\hbar \frac{\partial}{\partial x}$

3D Momentum $\hat{p}_x \rightarrow -i\hbar\nabla = -i\hbar\left(\hat{\imath}\frac{\partial}{\partial x} + \hat{\jmath}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}\right)$

1D Hamiltonian $\hat{H} \rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

3D Hamiltonian $\hat{H} \rightarrow -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(\vec{r})$

Systems Studied

Particle-In-A-Box
Quantum Simple Harmonic Oscillator
Hydrogen Atom
Free Electrons
Electron in a Crystal Periodic Potential

Conservation

$$\text{If } \frac{d\langle\hat{A}\rangle}{dt} = 0, \hat{A} \rightarrow \text{Conserved Observable}$$

Ehrenfest Theorem

$$\frac{d\langle\hat{A}\rangle}{dt} = \frac{\langle[\hat{A},\hat{H}]\rangle}{i\hbar} + \langle\frac{\partial\hat{A}}{\partial t}\rangle$$

Real Material Effects of Element Choice (Periodic Table Trends)

N = Atomic Number

$$N \uparrow \rightarrow V \downarrow, a \uparrow, K \downarrow, m \uparrow$$

Free Electrons

$V(x) = 0 \rightarrow p$ & E are both conserved.

Eigenstates are given by energy E (magnitude) and momentum in k (direction)

$$\psi_{E,k}(x) = Ce^{\pm ikx} = Ce^{\pm i\frac{p}{\hbar}x} = Ce^{\pm i\frac{\sqrt{2mE}}{\hbar}x}$$

If the total wave function of a system is a sum of different momentum eigenstates:

$$(x) = \sum_p c_p\, e^{i\frac{p}{\hbar}x}$$

The average value of momentum is then given as:

$$\langle p\rangle = \sum_p pc_p^2 = \sum_k \hbar k c_k^2$$

The average value of energy is similarly given as:

$$\langle E\rangle = \sum_E Ec_E^2 = \sum_k \frac{\hbar^2 k^2}{2m} c_k^2$$

Bloch Theorem

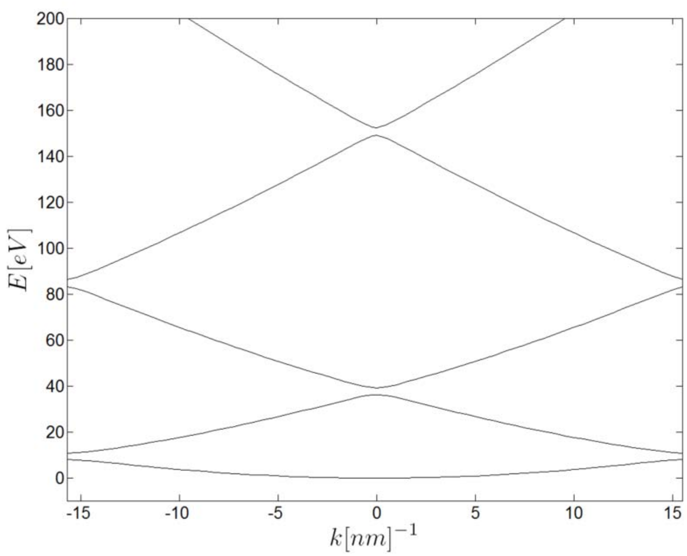
$$u(x) = e^{ikx} f(x)$$
$$f(x+a) = f(x)$$

Band Diagrams

Plots of E vs k for electrons

Plot below shows 1st 5 bands for

$$V(x) = 2V_0 \sum_{n=1}^{4} \cos ngx \text{ with } V_0 = 1.5 \text{ eV and } a = 0.2 \text{ nm}$$



If $V(x) = 2V_0 \cos gx$ to a 2nd order Central Matrix Equation approximation

$$E_\pm\left(\left|\frac{g}{2}\right| = \left|\frac{\pi}{a}\right|\right) = \frac{\hbar^2 g^2}{8m} \pm V_0 = \frac{\hbar^2\pi^2}{2ma^2} \pm V_0 \rightarrow E_g = 2V_0$$

3.024 Electronic, Optical and Magnetic Properties of Materials
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