3.024 Electrical, Optical, and Magnetic Properties of Materials Spring 2012
Recitation 4 Notes

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1. Quantum Mechanics Review

From quantum mechanics, we have learned that there exists a duality between particles and waves. This duality means that at length scales where the wavelength of the particle and size of the particle are comparable, classical physics breaks down and the laws of physics at these lengths scales comes from the 6 postulates of Quantum Mechanics:

I. There exists a wave function (x, t) that describes a quantum mechanical particle's evolution in space-time with the following properties: Single Valued, Square Integrable, Nowhere Infinite, Continuous, Piecewise Continuous 1st Derivative

II. $\psi^*(x)\psi(x)$ is the probability density of finding the particle. This means that $\psi^*(x)\psi(x)dx$ is the probability of finding the particle in a given interval dx. Since the particle must be somewhere:

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

III. Observables are described as eigenvalues a of operators $\hat{A}$ that are Hermitian. This means all measurable quantities are eigenvalues of these operators on the eigenstates of the system. The expected or average value of $\hat{A}$ is then $\langle\psi|\hat{A}|\psi\rangle = \int_{-\infty}^{\infty} \psi^*(x)\hat{A}\psi(x)dx$

IV. If a system is in some state (x), and the normalized wave functions $\psi_n(x)$ are known with eigenvalues a_n, then the probability of observing the eigenvalue a_n is given by

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

and $(x) = \sum_n c_n\psi_n(x)$

V. If a measured eigenvalue a_n is observed for a system originally in the state (x), then after the measurement the system will be in the state $\psi_n(x)$ that is the eigenstate corresponding to a_n. This is called wave function collapse.

VI. The time evolution of a system is given by the Schrodinger equation.

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

When $(x, t) = \psi(x)\phi(t)$ and there is no time dependence in the potential energy, the Schrodinger equation reduces to the following:

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

a. Free Electron Scattering Problems

A free electron is described by a plane wave function with $V(x) = 0$. Here we denote $u(x)$ as the wave function of the free electron.

$$\hat{H}u(x) = Eu(x)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u(x)}{\partial x^2} = Eu(x)$$

$$u(x) = Ae^{ikx} + Be^{-ikx}$$

is the general solution.

$$\text{with } k = \frac{\sqrt{2mE}}{\hbar}$$

In this system, the momentum commutes with the Hamiltonian, meaning that the system is described completely by knowing the momentum and energy.

The particle is considered moving to the right if the value of the momentum is positive and to the left if it is negative.

Thus the first term in the general solution is a rightward traveling electron.

$$\hat{p}e^{ikx} = \left(-i\hbar\frac{\partial}{\partial x}\right)e^{ikx} = -i\hbar ike^{ikx} = \hbar ke^{ikx} \rightarrow p = \hbar k$$

Similarly the second term in the general solution is a leftward traveling electron.

$$\hat{p}e^{-ikx} = \left(-i\hbar\frac{\partial}{\partial x}\right)e^{-ikx} = i\hbar ike^{ikx} = -\hbar ke^{ikx} \rightarrow p = -\hbar k$$

If $V(x) = V_0$ on a given range, the oscillatory solution of the electron will change to have a lower amplitude as $V_0 \rightarrow E$.

When $V_0 = E$:

$$\hat{H}u(x) = Eu(x)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2 u(x)}{\partial x^2} = (E - V_0)u(x)$$

$$\frac{\partial^2 u(x)}{\partial x^2} = 0$$

$$u(x) = Ax + B$$

Thus the wave function in this region is linear.

If $V(x) > V_0$, k is no longer real and the general solution are real exponentials.

$$u(x) = Ae^{kx} + Be^{-kx}$$

Depending on the boundary conditions of a particular set of potentials a free electron might encounter, the overall wave function of the electron will be some piecewise combination of these basic wave functions with 2 sets of equations for each point at which there is a step up or down in potential energy.

b. Particle-in-a-box

$$V(x) = \begin{cases} \infty & x\epsilon\left(-\infty, -\frac{d}{2}\right) \cup \left(\frac{d}{2}, \infty\right) \\ 0 & x\epsilon\left[-\frac{d}{2}, \frac{d}{2}\right] \end{cases}$$

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{d}}\cos\left(\frac{n\pi x}{d}\right) & n\ odd \\ \sqrt{\frac{2}{d}}\sin\left(\frac{n\pi x}{d}\right) & n\ even \end{cases}$$

or

$$V(x) = \begin{cases} \infty & x\epsilon(-\infty, 0) \cup (L, \infty) \\ 0 & x\epsilon[0, L] \end{cases}$$

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2\left(\frac{n\pi}{d}\right)^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2md^2} = \frac{h^2 n^2}{8md^2}$$

Closest real system this reflects: Quantum Dot

c. Harmonic Oscillator

$$V(x) = \frac{1}{2}Kx^2 = \frac{1}{2}m\omega^2 x^2$$

$$\psi_n(x) = \sqrt{\frac{1}{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2} H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right)$$

Where the Hermite polynomials are defined recursively as:

$$H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}\left(e^{-x^2}\right)$$

$$E_n = \hbar\omega\left(\frac{1}{2} + n\right)$$

Real system to which this applies: Atomic bond between two atoms

d. Hydrogen Atom

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$$

$$u_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi)$$

$$= e^{-\frac{r}{na_0}}\sqrt{\left(\frac{2}{n}\right)^3 \frac{(n-l-1)!}{2n(n+l)!}}\left(\frac{r}{na_0}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)$$

$$* \begin{cases} (-1)^m \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta)e^{im\phi} & m \geq 0 \\ \sqrt{\frac{2l+1}{4\pi}\frac{(l+m)!}{(l-m)!}} P_l^{-m}(\cos\theta)e^{im\phi} & m < 0 \end{cases}$$

Here $L_z^y(x)$are the associated Laguerre polynomials and $P_z^y(x)$ are the associated Legendre polynomials.
The eigenvalues of the energy, angular momentum, & *z*-component angular momentum:

$$E_n = -\frac{E_I}{n^2}$$
$$L_l^2 = l(l+1)\hbar^2$$
$$L_{zm} = m\hbar$$

Real system to which this applies: Electron in hydrogen atom

f. Conservation & Ehrenfest Theorem

A quantity is conserved if its expected value does not change with time.
Mathematically, this is characterized by the Ehrenfest Theorm.

$$\frac{d\langle\hat{A}\rangle}{dt} = \frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle + \langle\frac{\partial\hat{A}}{\partial t}\rangle$$

If $\frac{d\langle\hat{A}\rangle}{dt} = 0$ then the observable to which $\hat{A}$ corresponds is conserved.
This means by the Ehrenfest Theorem that is the following two conditions hold, $\hat{A}$ corresponds to a conserved observable.

$$[\hat{A},\hat{H}] = 0$$
$$\langle\frac{\partial\hat{A}}{\partial t}\rangle = 0$$

e.g. 1 Momentum Conservation & Potential Energy Position Dependence
Given $V(x) = V_0 f(x)$
Is momentum conserved for a particle in this potential?

$$[\hat{p},\hat{H}]\psi = \hat{p}\hat{H}\psi(x) - \hat{H}\hat{p}\psi(x)$$

$$[\hat{p},\hat{H}]\psi = \left(-i\hbar\frac{\partial}{\partial x}\right)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0 f(x)\right)\psi(x) - \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0 f(x)\right)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x)$$

$$[\hat{p},\hat{H}]\psi = -i\hbar\left(\frac{\partial}{\partial x}\right)\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V_0 f(x)\psi(x)\right) - \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0 f(x)\right)\left(\frac{\partial\psi(x)}{\partial x}\right)$$

$$[\hat{p},\hat{H}]\psi = -i\hbar\left(-\frac{\hbar^2}{2m}\frac{\partial^3\psi(x)}{\partial x^3} + V_0\frac{\partial}{\partial x}\left(f(x)\psi(x)\right)\right) - \left(-\frac{\hbar^2}{2m}\frac{\partial^3\psi(x)}{\partial x^3} + V_0 f(x)\frac{\partial\psi(x)}{\partial x}\right)$$

$$[\hat{p},\hat{H}]\psi = -i\hbar\left(V_0\psi(x)\frac{\partial f(x)}{\partial x} + V_0 f(x)\frac{\partial\psi(x)}{\partial x} - V_0 f(x)\frac{\partial\psi(x)}{\partial x}\right)$$

$$[\hat{p},\hat{H}]\psi = -i\hbar V_0\frac{\partial f(x)}{\partial x}\psi(x)$$

$$[\hat{p},\hat{H}] = -i\hbar V_0 \frac{\partial f(x)}{\partial x} \neq 0$$

This implies that if a potential has a nonzero derivative with position, momentum for the particle will not be conserved.

2. Periodic Potentials Preview
   a. Bloch Theorem
      For periodic potentials, the wave functions of particles take on the following form.

$$f_{n\vec{k}}\left(\vec{r}+\vec{R}\right) = f_{n\vec{k}}\left(\vec{r}\right)$$
$$u_{n,\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} f_{n\vec{k}}\left(\vec{r}\right)$$

or

$$u_{n,\vec{k}}\left(\vec{r}+\vec{R}\right) = e^{i\vec{k}\cdot\vec{R}} u_{n,\vec{k}}(\vec{r})$$

   b. Reciprocal Lattice Vectors

$$\vec{b}_1 = \frac{2\pi(\vec{a}_2\times\vec{a}_3)}{\left(\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)\right)} \quad \vec{b}_2 = \frac{2\pi(\vec{a}_3\times\vec{a}_1)}{\left(\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)\right)} \quad \vec{b}_3 = \frac{2\pi(\vec{a}_1\times\vec{a}_2)}{\left(\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)\right)}$$

e.g. 2 Rectangular Lattice

Find the reciprocal lattice vectors for the following rectangular real space lattice:

$$\vec{a}_1 = a\begin{bmatrix}1\\0\\0\end{bmatrix} \vec{a}_2 = b\begin{bmatrix}0\\1\\0\end{bmatrix} \vec{a}_3 = c\begin{bmatrix}0\\0\\1\end{bmatrix}$$

$$\vec{a}_2\times\vec{a}_3 = \det\begin{vmatrix}\hat{\imath} & \hat{\jmath} & \hat{k}\\0 & b & 0\\0 & 0 & c\end{vmatrix}$$

$$\vec{a}_2\times\vec{a}_3 = (b\cdot c - 0\cdot 0)\hat{\imath} - (0\cdot c - 0\cdot 0)\hat{\jmath} + (0\cdot 0 - 0\cdot b)\hat{k}$$

$$\vec{a}_2\times\vec{a}_3 = bc\begin{bmatrix}1\\0\\0\end{bmatrix}$$

$$\vec{a}_3\times\vec{a}_1 = \det\begin{vmatrix}\hat{\imath} & \hat{\jmath} & \hat{k}\\0 & 0 & c\\a & 0 & 0\end{vmatrix}$$

$$\vec{a}_3\times\vec{a}_1 = (0\cdot 0 - 0\cdot c)\hat{\imath} - (0\cdot 0 - a\cdot c)\hat{\jmath} + (0\cdot 0 - a\cdot 0)\hat{k}$$

$$\vec{a}_3\times\vec{a}_1 = ac\begin{bmatrix}0\\1\\0\end{bmatrix}$$

$$\vec{a}_1\times\vec{a}_2 = \det\begin{vmatrix}\hat{\imath} & \hat{\jmath} & \hat{k}\\a & 0 & 0\\0 & b & 0\end{vmatrix}$$

$$\vec{a}_1\times\vec{a}_2 = (0\cdot 0 - b\cdot 0)\hat{\imath} - (a\cdot 0 - 0\cdot 0)\hat{\jmath} + (a\cdot b - 0\cdot 0)\hat{k}$$

$$\vec{a}_1\times\vec{a}_2 = ab\begin{bmatrix}0\\0\\1\end{bmatrix}$$

$$\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3) = (a\cdot bc) + (0\cdot 0) + (0\cdot 0) = abc$$

$$\vec{b}_1 = \frac{2\pi(\vec{a}_2 \times \vec{a}_3)}{\left(\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)\right)} = \frac{2\pi bc}{abc}\begin{bmatrix}1\\0\\0\end{bmatrix} = \frac{2\pi}{a}\begin{bmatrix}1\\0\\0\end{bmatrix}$$

$$\vec{b}_2 = \frac{2\pi(\vec{a}_3 \times \vec{a}_1)}{\left(\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)\right)} = \frac{2\pi ac}{abc}\begin{bmatrix}0\\1\\0\end{bmatrix} = \frac{2\pi}{b}\begin{bmatrix}0\\1\\0\end{bmatrix}$$

$$\vec{b}_3 = \frac{2\pi(\vec{a}_1 \times \vec{a}_2)}{\left(\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)\right)} = \frac{2\pi ab}{abc}\begin{bmatrix}0\\0\\1\end{bmatrix} = \frac{2\pi}{c}\begin{bmatrix}0\\0\\1\end{bmatrix}$$