

Highlights from ECE 235: Solid-state Physics

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Notes prepared mainly for exam preparations for ECE 235. Some basic results from modern physics are discussed, and many inks has been spilled on Schrodinger's equation. Schrodinger's equation is treated as a standard PDE and is solved via separation of variables in 1D and 3D, and with different potential functions. This class can be seen as a fun supplement to Math 322: Partial Differential Equations.

The final 1/3 of the class is on solid state physics, with an attention on PN junctions. However, the class is poorly organized after MT2 and the contents are ill-instructed. It is out of these reasons that I try to frame this note as a recap on Modern physics, and **an introduction to Schrodinger's equation**.

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1 EM wave

1.1 waves

- Traverse wave: oscillation \perp propagation
- Longitudinal wave: oscillation \parallel propagation
- $v = \lambda f$

1.2 EM wave function

$$\begin{cases} E_x = E_0 \sin(kz - \omega t) \\ B_y = B_0 \sin(kz - \omega t) \end{cases} \quad [1]$$

where $k = \frac{2\pi}{\lambda}$ (wave number), $\omega = 2\pi f = kc$ (dispersion relationship), B_0 : magnetic field amplitude, E_0 : electric field amplitude

1.3 EM Energy flux

Energy flux the energy transferred per unit area per unit time in the direction of wave propagation of an EM wave is defined by the Poynting vector

$$\vec{S} \equiv \frac{\vec{E} \times \vec{B}}{\mu_0}. \quad [2]$$

Where $\mu_0 = 1.25663706126e-6 (N \cdot A^{-2})$ is the vacuum permeability.

- Intensity of EM wave is the magnitude of the Poynting vector:

$$I = \langle S \rangle = \frac{E_0^2}{377\Omega} \quad [3]$$

where Ω is ohm. Very unorthodox I know, but hey we are in Engineering Hall.

- Specially, when EM wave is emitted from a point light source with power P ,

$$I = \frac{P}{4\pi r^2} = \frac{E_0^2}{377\Omega} \quad [4]$$

2 Double slit interference

Consider a double-slit setup, where the first dark line is at an angle θ from the central bright line with a distance Y . Distance from light source to screen is L . Then by trigonometry:

$$Y = L \tan \theta. \quad [5]$$

When considering constructive/destructive interference, given the separation between two slits is d the path difference between the two slits is

$$\begin{aligned} m\lambda &= d \sin \theta \text{ constructive} \\ \left(m + \frac{1}{2}\right)\lambda &= d \sin \theta \text{ destructive} \quad m = 0, 1, 2, \dots \end{aligned} \quad [6]$$

3 Photoelectric effect

- Energy of a photon

$$E_p = hf = \frac{hc}{\lambda} = \Phi + E_k \quad [7]$$

where Φ is the work function of the material, E_k is the kinetic energy of the emitted electron at the surface of the material. $h = 6.26e-34$ is the Planck constant, $c = 3e-8$ m/s is the speed of light, f is the frequency of the photon, and λ is the wavelength of the photon.

- Motion for Photoelectric effect:

$$E_{k,m} + (-e)V_m = E_{k,d} + (-e)V_d \quad [8]$$

Where $E_{k,m}$ is K.E at the metal surface, V_m is the voltage at the metal, $E_{k,d}$ is the K.E of the electron at the detector, and V_d is the voltage at the detector.

- stopping potential

$$eV_{\text{stop}} = \frac{hc}{\lambda} - \Phi \quad [9]$$

the minimum potential required to stop the emitted electron.

- Threshold frequency & wavelength: set $E_k = 0$:

$$\begin{aligned} \Phi &= hf_t = \frac{hc}{\lambda_t} \\ \Rightarrow f_t &= \frac{\Phi}{h}, \quad \lambda_t = \frac{hc}{\Phi} \end{aligned} \quad [10]$$

4 Blackbody radiation

- Stefan-Boltzmann law:

$$R = \sigma T^4. \quad [11]$$

Where R is the **power radiated per unit area**, or surface energy density of radiation. T is temperature in Kelvin, $\sigma = 5.67e-8 (W \cdot m^{-2} \cdot K^{-4})$ is the Stefan-Boltzmann constant.

- Wien's displacement law:

$$\lambda_{\text{max}} T = b \quad [12]$$

where $b = 2.89e-3 (m \cdot K)$ is the Wien's constant, and λ_{max} is the wavelength at which the blackbody **radiation is maximum**, and T is the temperature in Kelvin of the blackbody.

- Rayleigh-Jeans law:

$$\begin{aligned} R(\lambda) &= \frac{1}{4} cu(\lambda), \\ u(\lambda) &= 8\pi kT \lambda^{-4} \end{aligned} \quad [13]$$

Where R is radiation power per unit area, or energy density, u is the energy density of radiation, c is the speed of light, and $k = 8.617e-5 \text{ eV/K} = 1.38e-23 \text{ J} \cdot \text{K}^{-1}$ is the Boltzmann constant. This law is valid for long wavelength, but it diverges at short wavelength. **This equation is only good for long wavelength.**

- Planck's law:

$$u(\lambda) = \frac{8\pi hc \lambda^{-5}}{e^{hc/\lambda kT} - 1} \quad [14]$$

where $k = 1.38e-23 (\text{J} \cdot \text{K}^{-1})$ is the Boltzmann constant, h is the Planck constant, T is the temperature in Kelvin of the blackbody.

4.1 Energy of radiation

For an ideal blackbody, the energy radiated within a certain wavelength range is found by integrating Equation 14 over the range of wavelength.

$$U = \int_{\lambda_1}^{\lambda_2} u(\lambda) d\lambda \quad [15]$$

- It is often times easier to use mid-point approximation to handle the above integration:

$$U \approx u(\lambda) \Delta\lambda \quad [16]$$

Where $\lambda = \frac{\lambda_2 - \lambda_1}{2}$ is the mid-point of the wavelength range, and $\Delta\lambda$ is the width of the wavelength range.

5 Wavelike properties of particles

5.1 De broglie Hypothesis

$$f = \frac{E}{h}, \lambda = \frac{h}{p} \quad [17]$$

Where E is the total energy, p is the momentum, and λ is the wavelength of the particle. $h = 6.63e-34 \text{ J} \cdot \text{s}$ is the Planck constant.

- For a particle of zero rest energy,

$$E = pc = hf = \frac{hc}{\lambda}, \quad [18]$$

where p is the momentum of the particle.

- For a moving particle,

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} \quad [19]$$

5.2 Wavefunction for particles

$$\Psi(x, t) = A \sin(kx - \omega t) \quad [20]$$

or $Ae^{i(kx - \omega t)}$

- probability density of the particle is

$$p(x, t) = |\Psi|^2 \equiv \Psi^* \Psi \quad [21]$$

5.3 Uncertainty Principle

$$\Delta x \Delta p \geq \frac{\hbar}{2}, \quad \Delta E \Delta t \geq \frac{\hbar}{2} \quad [22]$$

Where x is position, p is momentum, E is energy, t is time, and $\hbar = \frac{h}{2\pi} = 1.05e-34 J \cdot s$ is the reduced Planck constant.

5.3.1 Min. Energy of Particle in a box

$$E = \frac{p^2}{2m} \geq \frac{\hbar^2}{2mL^2} \quad [23]$$

6 Schrodinger's equation

6.1 Time-dependent Schrodinger's equation in 1D

1D Schrodinger's equation in position basis:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x, t) + V(x, t) \Psi(x, t) = i\hbar \frac{\partial}{\partial t} \Psi(x, t) \quad [24]$$

6.2 Time-independent Schrodinger's equation in 1D

Via separation of variable, set $\Psi(x, t) = \psi(x)\varphi(t)$, and noticing $f = \frac{E}{\hbar}$, we have

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x) = E\psi(x) \quad [25]$$

time variation of wavefunction: $\varphi(t) = e^{-iEt/\hbar}$

- Probability density is thus simplified to

$$p(x) = |\Psi(x, t)|^2 = |\psi(x)|^2 \quad [26]$$

- Normalization condition:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1 \quad [27]$$

7 Potential Barrier

7.1 Potential Well

7.1.1 Infinite potential well- particle in a box $E < V_0$

- For a particle in a box of length L , where $V(x) = 0$ for $0 < x < L$, and $V(x) = \infty$ otherwise, the wavefunction inside box is found by

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) = E\psi(x) \quad [28]$$

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

Noticing boundary values, the following is obtained:

$$E_n = \frac{\hbar^2 k_n^2}{2m} = n^2 \frac{\hbar^2 \pi^2}{2mL^2} = n^2 E_1 \quad [29]$$

where $k = 2\frac{\pi}{\lambda}$; $k^2 = \left(\frac{p}{\hbar}\right)^2 = \frac{2mE}{\hbar^2}$

- Notably, $\lambda_n = 2\frac{L}{n}$; and the energy levels can be also expressed in terms of hc and mc^2 :

$$E_1 = \frac{(hc)^2}{8mc^2 L^2}; \quad E_n = \frac{n^2 (hc)^2}{8mc^2 L^2} \quad [30]$$

These results are true for any potential well with $V(x) = 0$ inside the well.

- Normalization condition in box of length L :

$$\int_0^L |\psi(x)|^2 dx = 1 \quad [31]$$

7.1.2 Finite Square Well ($E < V_0$)

Consider Finite Square well with constant potential $V_0 > E$.

- Inside the well, The Schrodinger's eqn becomes

$$\psi'' = \frac{(E - V_0)2m}{-\hbar^2} \psi \equiv \alpha^2 \psi \quad [32]$$

and is solved with boundary conditions as

$$\psi_2(x) = A_1 \sin(kx) + A_2 \cos(kx) \quad [33]$$

- Outside well:

$$\psi_1(x) = B_1 e^{kx}; \quad \psi_3(x) = C_2 e^{-kx} \quad [34]$$

with

$$k = \frac{\sqrt{2m(V_0 - E)}}{\hbar}. \quad [35]$$

7.2 Step potential: Transmission & Reflection

7.2.1 When $E > V_0$,

Now consider finite step potential $V(x) = V_0 H(x)$, $E > V_0$. The wave equation is solved as

$$\begin{aligned} \psi_1(x) &= A e^{ik_1 x} + B e^{-ik_1 x}; \\ \psi_2(x) &= C e^{ik_2 x} \end{aligned} \quad [36]$$

with $k_1 = \frac{\sqrt{2mE}}{\hbar}$, $k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$ Boundary condition further gives

$$\begin{aligned} B &= \frac{k_1 - k_2}{k_1 + k_2} A; \\ C &= \frac{2k_1}{k_1 + k_2} A. \end{aligned} \quad [37]$$

We are thus motivated to define Reflection and Transmission coefficients as

$$\begin{aligned} R &= \left| \frac{B}{A} \right|^2 = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}; \\ T &= \frac{k_2 |C|^2}{k_1 |A|^2} = \frac{4k_1 k_2}{(k_1 + k_2)^2}; \\ R + T &= 1. \end{aligned} \quad [38]$$

They are the probability of reflection and transmission respectively.

7.2.2 When $E < V_0$,

we have $R = 1$ and thus no transmission. This is the case for a particle in a finite square well. Before potential step:

$$\begin{aligned} \psi_1(x) &= Ae^{ik_1 x} + Be^{-ik_1 x}; \\ \psi_2(x) &= Ce^{-\alpha x} \end{aligned} \quad [39]$$

where $\alpha = \frac{\sqrt{2m(V_0-E)}}{\hbar}$ and $k_1 = \frac{\sqrt{2mE}}{\hbar}$

7.3 Box potential: Tunneling

- consider $E < V_0$: Transmission: $T = Ge^{-2\alpha L}$; $G = 16 \frac{E}{V_0} \left(1 - \frac{E}{V_0}\right)$ Particle can tunnel through the box potential before exponential decay to zero inside the box.

8 Expectations & Operators

- expectation

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} \psi^* f(x) \psi dx \quad [40]$$

.

- for infinite square well: $\langle x^2 \rangle = \frac{L^2}{3} - \frac{L^2}{2n^2\pi^2}$
- Momentum operator: $\hat{p}_q = \frac{\hbar}{i} \partial_q$, Hamiltonian operator: $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$.

.

$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} \psi^* \left(\frac{\hbar}{i} \right) \partial_x \psi dx \quad [41]$$

9 Schrodinger's equation in 3D

- time independent:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \quad [42]$$

9.1 Infinite square well in 3D

Separation of variables:

$$\psi(\mathbf{x}) = \psi(x) \psi(y) \psi(z) \quad [43]$$

and Schrodinger's eqn is solved as

$$\psi(\mathbf{x}) = A \sin(k_1 x) \sin(k_2 y) \sin(k_3 z) \quad [44]$$

and we find descriptions on energy level by plugging this solution back:

$$E_{n_1 n_2 n_3} = \frac{\hbar^2 \pi^2}{2mL^2} (n_1^2 + n_2^2 + n_3^2) \quad [45]$$

or, when well is not cubic:

$$E_{n_1 n_2 n_3} = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_1^2}{L_x^2} + \frac{n_2^2}{L_y^2} + \frac{n_3^2}{L_z^2} \right). \quad [46]$$

Where n is a quantum number $n \in \{1, 2, 3, \dots\}$. Ground state: $n_1 = n_2 = n_3 = 1$

- when potential is cubic, notice degeneracy in energy levels. For example, the first energy state:

$$E_{112} = E_{121} = E_{211} \quad [47]$$

9.2 Scho's equation in spherical coordinates: atomic model, and quantum numbers

Due to ugliness of Spherical Laplacian, and out of our respect to Engineering, we will skip the explicit Schrodinger's Eqn in spherical coord.

Separation of variables:

$$\psi(r, \theta, \varphi) = R(r) f(\theta) g(\varphi) \quad [48]$$

- Solving partially using spherical harmonics:

$$\begin{aligned} Y_{lm}(\theta, \varphi) &= f_{lm}(\theta) g_m(\varphi), \\ g_m(\varphi) &= e^{im\varphi} \end{aligned} \quad [49]$$

A list of Y_{lm} can be found in text p.274

- The radial part can be solved by Legendre polynomials:

$$\begin{aligned} R_{nl}(r) &= A_{nl} e^{-r/a_0} r^l \mathcal{L}_{nl}^{r/a_0}, \\ a_0 &= \frac{\hbar^2}{ke^2 \mu} \end{aligned} \quad [50]$$

9.2.1 quantization of angular momentum

Angular momentum of a particle satisfying 3d Scho's eqn is

$$\begin{aligned} \mathbf{L} &= \mathbf{r} \times \mathbf{p} \Rightarrow \\ |\mathbf{L}| &= \hbar\sqrt{l(l+1)}, \quad L_z = m_l \hbar \end{aligned} \quad [51]$$

Where $l = 0, 1, 2, \dots, (n-1)$, and $m_l = 0, \pm 1, \pm 2, \dots, \pm(l-1), \pm l$ are quantum numbers.

9.3 Atomic energy level

Using solution of $R_{nl}(r)$ and $f_{lm}(\theta)g_m(\varphi)$ on a Hydrogen atom, and using the potential due to nucleus being $V(r) = -Zke^2/r$, we can find the energy levels of an atom as

$$E_n = -\frac{\mu}{2n^2} \left(\frac{Zke^2}{\hbar} \right)^2 = -\frac{Z^2 E_1}{n^2} \quad [52]$$

- For a hydrogen atom with $Z = 1$, $E_1 = \frac{1}{2} \frac{ke^2}{\hbar} \mu = 13.6 \text{ eV}$.

9.4 Quantum numbers

- Principal quantum number $n = 1, 2, 3, \dots$
- Azimuthal quantum number $l = 0(s), 1(p), 2(d), 3(f), \dots, (n-1)$
- Magnetic quantum number $m_l = 0, \pm 1, \pm 2, \dots, \pm(l-1), \pm l$
- Spin quantum number $m_s = \pm \frac{1}{2}$

9.4.1 Puali exclusion principle & Hund's rule

- Puali: No two electrons in an atom can have the same set of quantum numbers.
- Hund: Maximize unpaired elctrons: fill each m_l in increasing order with $m_s = +\frac{1}{2}$, and then with $m_s = -\frac{1}{2}$.

Example: on 2p shell: $\{n, l, m_l, m_s\} = \{2, 1, -1, 1/2\}, \{2, 1, 0, 1/2\}, \{2, 1, 1, 1/2\}, \{2, 1, -1, -1/2\}, \{2, 1, 0, -1/2\}, \{2, 1, 1, -1/2\}$.

10 Solids States

10.1 Energy bands

Many atoms couples together to form a solid, and the energy levels of a solid can be described by the energy bands.

What matters the most, under the scope of this exam, is the following:

- Valance band: The highest energy band occupied by electrons at 0K. Electrons here are considered to be bounded.
- Conduction band: The lowest energy band unoccupied by electrons at 0K. Electrons here are considered to be free moving and contributes to conductivity.
- Band gap: $E_g = E_c - E_v$, discribes the energy difference between the valance band and the conduction band. This is the difficulty for an electron to move from valance band to conduction band, and for an atom to be conductive.
 - Insulator: $E_g > 4\text{eV}$,
 - Semiconductor: $0 < E_g < 4\text{eV}$,
 - Metal: $E_g = 0 \text{ eV}$.

10.2 Fermi distribution

$$f(E) = \frac{1}{e^{(E-E_f)/(kT)} + 1} \quad [53]$$

where E_f is the Fermi energy, $k = 8.617e-5$ eV/K is the Boltzmann constant, and T is the temprature in Kelvin.

- This distribution describes the probability of an electron to be found at energy level E at temprature T , given the Fermi energy E_f .

11 Appendix

1. Useful integral for probability of wavefunction

$$\int_{-\infty}^{\infty} e^{-a(x+b)^2} dx = \sqrt{\frac{\pi}{a}} \quad [54]$$

1. Useful constants:

- $hc = 1240$ eV nm.
- For an electron: $mc^2 = 0.511\text{MeV} = 5.11e5$ eV