

Condensed Matter Physics
from the context of the courses
PHY 491: Solid State Physics

Kaedon Cleland-Host

December 11, 2022

Contents

0.1	The SI System	1
0.2	Why Study Condensed Matter	2
1	Atoms and Molecules	3
1.1	Hydrogen Like Systems	3
1.1.14	Radial Component of Hydrogen	4
1.1.18	Angular Component of Hydrogen	4
1.2	Electron Configurations	5
1.2.1	Pauli exclusion principle	5
1.2.2	Hund's rules	5
1.2.4	Magnetism	5
1.3	Diatomic Molecules	5
1.3.4	Linear Combinations of Atomic Orbitals	6
2	Crystal Structures	7
2.1	Lattice and Basis	7
2.2	Reciprocal Space	8
2.3	X-Ray Scattering	9
2.3.9	Experimental X-Ray Scattering	9
3	Electrons in Crystals	10
3.1	Tight Binding Model	10
3.2	Nearly Free Electron Model	10

0.1 The SI System

In physics it's often important to have precisely defined units for the purposes of making very accurate measurements or simply having a coherent unit system. It's possible to derive all necessary units from five measurements of **length, mass, time, current, and temperature**. The standard SI units for these properties are listed below:

Type	Unit	Definition
Length	Meter(m)	Length of distance light in a vacuum travels in $\frac{1}{299792458}$ seconds
Mass	Kilogram(kg)	Defined by fixing the Planck's constant $h = 6.62607015 \times 10^{-34} kg \cdot m^2 s^{-1}$
Time	Second(s)	Defined by fixing the ground-state hyperfine transition frequency of the caesium-133 atom, to be $9192631770 s^{-1}$
Current	Ampere(A)	Defined by fixing the charge of an electron as $1.602176634 \times 10^{-19} A \cdot s$
Temperature	Kelvin(K)	Defined by fixing the value of the Boltzmann constant k to $1.380649 \times 10^{-23} kg \cdot m^2 s^{-2} K^{-1}$

Common prefixes are listed below:

Prefix	Symbol	Definition
mega	M	10^6
kilo	k	10^3
milli	m	10^{-3}
micro	μ	10^{-6}
nano	n	10^{-9}
pico	p	10^{-12}
femto	f	10^{-15}

Additionally, the following are defined constants:

Symbol	Definition
\hbar	$\hbar = \frac{h}{2\pi} \approx 1.0546 \times 10^{-34} kg \cdot m^2 s^{-1}$

0.2 Why Study Condensed Matter

Condensed matter physics is the most broad field of physics that has a large overlap with other fields such as atomic physics, quantum physics, chemistry, and biology. Condensed matter physics describes anything that is "condensed" this includes any solid material, such as metals, glass, wood and electronics. As such it is very important in our world. Condensed matter is simultaneously very fundamental describing microscopic sources for material properties such as superconductivity, charge density waves, topological insulators. These phenomenon can't be described by reductionism and many properties only emerge when you consider larger systems that cannot be solved using fundamental laws alone.

Chapter 1

Atoms and Molecules

1.1 Hydrogen Like Systems

Many systems in condensed matter are similar to the hydrogen atom system and so it is often useful to use the solutions to the basic hydrogen atom Hamiltonian to model these systems.

Definition 1.1.1. The **simple hydrogen atom Hamiltonian** is given by

$$\mathcal{H} = \underbrace{\frac{P_n^2}{2m_n}}_{\substack{\text{Nucleus} \\ \text{Kinetic Energy}}} + \underbrace{\frac{P_e^2}{2m_e}}_{\substack{\text{Electron} \\ \text{Kinetic Energy}}} - \underbrace{\frac{Ze^2}{4\pi\epsilon_0|\vec{x}_e - \vec{x}_n|}}_{\substack{\text{Electrostatic} \\ \text{Potential}}} \quad (1.1.1)$$

This simplified Hamiltonian ignores relativity, spin, and magnetism.

Definition 1.1.2. **Center of mass coordinates** for the hydrogen atom are defined by

$$\begin{aligned} \vec{X} &= \frac{m_e\vec{x}_e + m_n\vec{x}_n}{m_e + m_n} && \text{center of mass} \\ \vec{r} &= \vec{x}_e - \vec{x}_n && \text{relative coordinate} \end{aligned} \quad (1.1.2)$$

Corollary 1.1.3. The simple hydrogen atom Hamiltonian in center of mass coordinates is

$$\mathcal{H} = \underbrace{-\frac{\hbar^2}{2(m_e + m_n)}\nabla_X^2}_{\mathcal{H}_k} - \underbrace{\frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{Ze^2}{4\pi\epsilon_0|\vec{r}|}}_{\mathcal{H}_r} \quad (1.1.3)$$

Proposition 1.1.4. The Hamiltonians \mathcal{H}_k and \mathcal{H}_r are compatible observables.

$$[\mathcal{H}_k, \mathcal{H}_r] = 0, \quad [\mathcal{H}_k, \mathcal{H}] = 0, \quad [\mathcal{H}_r, \mathcal{H}] = 0 \quad (1.1.4)$$

Proposition 1.1.5. The Hamiltonian \mathcal{H}_r can be further separated in terms of radial and angular dependence.

$$\mathcal{H}_r = \underbrace{\frac{\hbar^2 L^2}{2\mu|\vec{r}|^2}}_{\substack{\text{Tangential} \\ \text{Kinetic} \\ \text{Energy}}} - \underbrace{\frac{\hbar}{2\mu}\frac{P_r^2}{\hbar^2}}_{\substack{\text{Radial} \\ \text{Kinetic} \\ \text{Energy}}} - \underbrace{\frac{Ze^2}{4\pi\epsilon_0|\vec{r}|}}_{\substack{\text{Electrostatic} \\ \text{Potential}}} \quad (1.1.5)$$

The solution to the Hamiltonian \mathcal{H}_r can be written in terms of independent radial and angular components.

$$n = 1, 2, 3, 4, 5, \dots$$

$$\ell = 0, 1, 2, 3, \dots, n-1 \quad (1.1.6)$$

$$m_\ell = -\ell, -\ell+1, \dots, -1, 0, 1, \dots, \ell-1, \ell$$

$$\psi_{n\ell m}(r, \theta, \phi) = U_n^\ell(r)Y_\ell^m(\theta, \phi) \quad (1.1.7)$$

Result 1.1.8. For the solution to the hydrogen atom $\psi_{n\ell m}(r, \theta, \phi)$, the following eigenvalue equations hold:

$$\mathcal{H}\psi_{n\ell m}(r, \theta, \phi) = -\frac{Z Ryd}{n^2}\psi_{n\ell m}(r, \theta, \phi) \quad (1.1.8)$$

$$L^2\psi_{n\ell m}(r, \theta, \phi) = \ell(\ell+1)\hbar^2\psi_{n\ell m}(r, \theta, \phi) \quad (1.1.9)$$

$$L_z\psi_{n\ell m}(r, \theta, \phi) = m\hbar\psi_{n\ell m}(r, \theta, \phi) \quad (1.1.10)$$

Definition 1.1.11. The **Bohr radius** is the average radius for the first energy level of the hydrogen atom given by

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{\mu Ze^2} \quad (1.1.11)$$

Definition 1.1.12. The **Rydberg constant** is the first energy level of hydrogen given by

$$Ryd = \frac{\hbar^2}{2a_0^2\mu} = \frac{e^2}{8\pi\epsilon_0 a_0} \quad (1.1.12)$$

Result 1.1.13. The **energy eigenvalues of hydrogen** are

$$E_n = -\frac{Z^2\hbar^2}{2a_0^2\mu} \frac{1}{n^2} = -\frac{Z^2 Ryd}{n^2} \quad (1.1.13)$$

1.1.14 Radial Component of Hydrogen

Definition 1.1.15. The **Laguerre polynomials** $L_q(z)$ are polynomials of degree q defined by

$$L_q(z) = e^z \frac{d^q}{dx^q} (z^q e^{-z}) \quad (1.1.15)$$

Definition 1.1.16. The **associated Laguerre polynomials** are polynomials of degree $q - p$ defined by

$$L_q^p(z) = \frac{d^p}{dx^p} L_q(x) \quad (1.1.16)$$

Result 1.1.17. The **radial component** $Y_\ell^m(\theta, \phi)$ has eigenvalues with eigenstates given by

$$U_n^\ell(r) = -\sqrt{\left(\frac{2Z}{na_0} \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}\right)^3} e^{-Zr/na_0} \left(\frac{2Zr}{na_0}\right)^\ell L_{n+\ell}^{2\ell+1}(2Zr/na_0) \quad (1.1.17)$$

1.1.18 Angular Component of Hydrogen

Definition 1.1.19. The **Legendre polynomials** denoted $P_\ell(z)$ are polynomials of degree ℓ that appear in spherically symmetric systems. They are defined with Rodrigues' formula given by

$$P_\ell(z) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{dz^\ell} (z^2 - 1)^\ell \quad (1.1.19)$$

Definition 1.1.20. The **associated Legendre polynomials** denoted $P_\ell^m(z)$ are polynomials calculated from the Legendre polynomials. They are equivalently defined by the following formulas

$$\begin{aligned} P_\ell^m(z) &= (-1)^m (1-z^2)^{m/2} \frac{d^m}{dz^m} P_\ell(z) \\ &= \frac{(-1)^m}{2^\ell \ell!} (1-z^2)^{m/2} \frac{d^{\ell+m}}{dz^{\ell+m}} (z^2 - 1)^\ell \end{aligned} \quad (1.1.20)$$

Result 1.1.21. The **angular solution** $Y_\ell^m(\theta, \phi)$ has eigenvalues with eigenstates given by

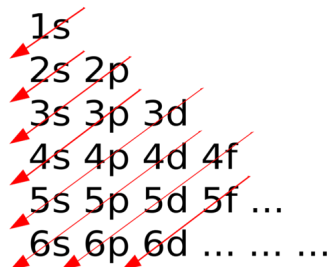
$$Y_\ell^m(\theta, \phi) = (-1)^m \sqrt{\frac{2(\ell+1)(\ell-m)!}{4\pi(\ell+m)!}} P_\ell^m(\cos\theta) e^{im\phi} \quad (1.1.21)$$

1.2 Electron Configurations

Theorem 1.2.1. The **Pauli exclusion principle** states that two or more identical particles cannot occupy the same state.

Theorem 1.2.2. **Hund's rules** state that electrons in a multi-electron atom fill shells according to the following rules.

1. Aligned Spins have lower energy. Maximize $S = \sum_i s_i$.
2. Minimized Electron Repulsions have lower energy. Maximize $L = \sum_i \ell_i$.
3. Shells fill according to the following pattern, $J = L - S$ when a shell is less than half full and $J = L + S$ when a shell is more than half full.



Definition 1.2.3. The **spectroscopic notation** for an electron configuration with total spin S , orbital angular momentum L and total angular momentum J is

$$^{2S+1}L_J \quad (1.2.3)$$

where L is replaced with letters S, P, D, F for $L = 0, 1, 2, 3$

1.2.4 Magnetism

Definition 1.2.5. **Diamagnetism** occurs when the total magnetic moment of an individual atom arranges opposite the direction of an applied field.

Definition 1.2.6. **Paramagnetism** occurs when the total magnetic moment of an individual atom arranges in the same direction of an applied field.

Definition 1.2.7. For a single atom with Hamiltonian H_0 and gyromagnetic factor $g \approx 2$ in an applied magnetic field \vec{B} such that $\vec{\nabla} \times \vec{A} = \vec{B}$ the Hamiltonian of a single atom is

$$H = H_0 + \underbrace{\mu_B \vec{B} (\vec{\ell} + g\vec{S})}_{\text{Paramagnetism}} + \underbrace{\frac{e^2}{2m} \vec{A}^2}_{\text{Diamagnetism}} \quad (1.2.7)$$

Proposition 1.2.8. For individual atoms, if $J = 0$ diamagnetism will occur otherwise if $J \neq 0$ paramagnetism will occur.

Definition 1.2.9. **Ferromagnetism** occurs when there is macroscopic permanent alignment of the magnetic moments of multiple atoms.

Definition 1.2.10. **Anti-ferromagnetism** occurs when there is macroscopic permanent anti-alignment of the magnetic moments of multiple atoms.

1.3 Diatomic Molecules

Definition 1.3.1. The Hamiltonian for H_2 is

$$H = \underbrace{\frac{-\hbar}{2m_A} \nabla_A^2 - \frac{\hbar}{2m_B} \nabla_B^2}_{\text{Nuclei Kinetic Energy}} - \underbrace{\frac{\hbar^2}{2m_e} \nabla_1^2 - \frac{\hbar^2}{2m_e} \nabla_2^2}_{\text{Electrons Kinetic Energy}} - \underbrace{\frac{Z_A e^2}{4\pi\epsilon_0 r_{1A}} - \frac{Z_B e^2}{4\pi\epsilon_0 r_{1B}} - \frac{Z_A e^2}{4\pi\epsilon_0 r_{2A}} - \frac{Z_A e^2}{4\pi\epsilon_0 r_{2B}}}_{\text{Nuclear-Electron Electrostatic Potential}} + \underbrace{\frac{e^2}{4\pi\epsilon_0 r_{12}}}_{\text{Nuclear-Nuclear Electrostatic Potential}} + \underbrace{\frac{Z_A Z_B e^2}{4\pi\epsilon_0 R_{AB}}}_{\text{Electron-Electron Electrostatic Potential}} \quad (1.3.1)$$

Corollary 1.3.2. The Hamiltonian for H_2 in Hartree units is

$$H = \frac{1}{2m_A} \nabla_A^2 - \frac{1}{2m_B} \nabla_B^2 - \frac{1}{2} \nabla_1^2 - \frac{1}{2} \nabla_2^2 - \frac{Z_A}{r_{1A}} - \frac{Z_B}{r_{1B}} - \frac{Z_A}{r_{2A}} - \frac{Z_B}{r_{2B}} + \frac{1}{r_{12}} + \frac{Z_A Z_B}{R_{AB}} \quad (1.3.2)$$

Proposition 1.3.3. The H_2 system cannot be solved due to the complexity of the electron-electron interaction.

1.3.4 Linear Combinations of Atomic Orbitals

Definition 1.3.5. The **linear combinations of atomic orbitals** approximation is a method for approximating diatomic molecules.

$$\psi \approx \frac{1}{\sqrt{2 \pm 2s}}(a(\vec{r}) \pm b(\vec{r})) \quad (1.3.5)$$

Definition 1.3.6. The **symmetric bond** written g (for gerade) is the even linear combination

$$\psi_+ = \frac{1}{\sqrt{2 + 2s}}(a(\vec{r}) + b(\vec{r})) \quad (1.3.6)$$

Definition 1.3.7. The **antisymmetric bond** written u (for ungerade) is the odd linear combination

$$\psi_- = \frac{1}{\sqrt{2 - 2s}}(a(\vec{r}) - b(\vec{r})) \quad (1.3.7)$$

Proposition 1.3.8. Symmetric bonds have an increased probability of electrons near both nuclei with strong binding. However, antisymmetric bonds have a decreased probability of electron near both nuclei with weak binding.

Definition 1.3.9. The **molecular orbital diagram** is a notation for linear combinations of atomic orbitals that represents the atom orbitals and the molecular orbitals.



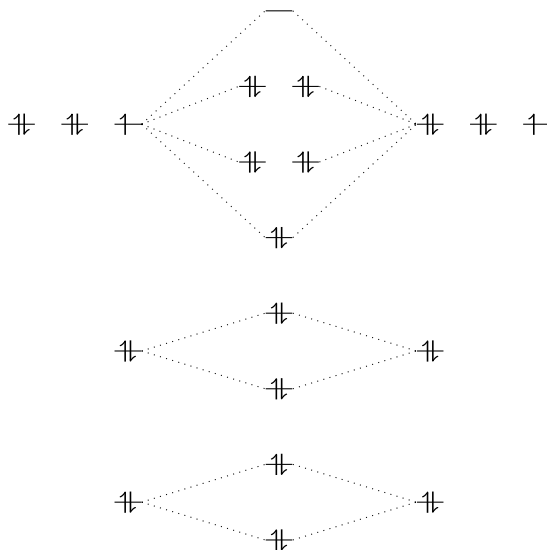
Definition 1.3.10. The **bond order** denoted B is defined as

$$B = \frac{[\# \text{ of bonding } e^-] - [\# \text{ of antibonding } e^-]}{2} \quad (1.3.10)$$

Corollary 1.3.11. A molecule will be stable if and only if $B > 0$.

Definition 1.3.12. For the s shell there are two bonding shells: the **s sigma bonding** shell is σ_g and the **s sigma antibonding** shell is σ_u^* . For the p shell there are 4 bonding shells: the **p sigma bonding** shell is σ_g , the **p sigma antibonding** shell is σ_u^* , the **p pi bonding** shell is π_u and the **p pi antibonding** shell is π_g^* .

Example. Consider diatomic Fluorine: F_2 . Fluorine has electron configuration $1s^2 2s^2 2p^5$, so the molecular orbital diagram is



This

Definition 1.3.13. The **spectroscopic notation** or **term symbols** for a molecular electron configuration with total spin S , orbital angular momentum L and total symmetry y is

$$^{2S+1}\Lambda_y \quad (1.3.13)$$

where Λ is replaced with symbols $\Sigma, \Pi, \Delta, \Phi$ for $L = 0, 1, 2, 3$ and $g \times g = g, u \times u = g, g \times u = u$.

Definition 1.3.14. The **Heitler-London Method** is a method of approximating molecular wavefunctions that uses LCAO but with the minor terms H^-H^+ terms dropped

$$\psi_{HL} = N(a(r_1)b(r_2) + b(r_1)a(r_2)) \quad (1.3.14)$$

Chapter 2

Crystal Structures

2.1 Lattice and Basis

Definition 2.1.1. A **crystal** is a periodic arrangement of atoms

Definition 2.1.2. A **lattice** is a set of points \mathbf{R} defined as integer sums of primitive lattice vectors.

Definition 2.1.3. The **primitive lattice vectors** of a lattice is a set of vectors that forms an integer basis for a lattice. Each primitive lattice vector must be integer linearly independent and the set of primitive lattices vectors must generate the set of lattice points.

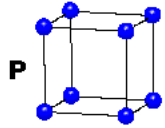
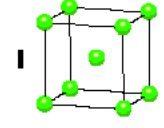
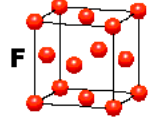
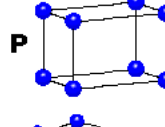
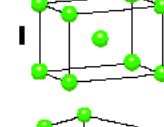
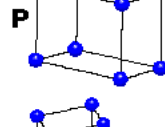

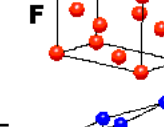
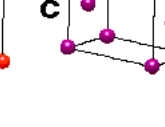
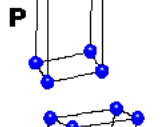
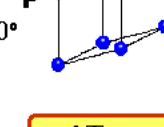
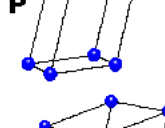
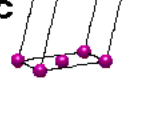
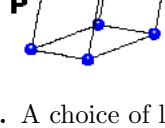
Definition 2.1.4. A set of vectors $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_n\}$ is **integer linearly independent** iff there does not exist non-zero integers $z_1, z_2, \dots, z_n \in \mathbb{Z}$ such that

$$z_1 \mathbf{v}_1 + z_2 \mathbf{v}_2 + \dots + z_n \mathbf{v}_n = \mathbf{0} \quad (2.1.4)$$

Definition 2.1.5. A set of vectors $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_n\}$ is **generating** iff for every lattice point \mathbf{r} there exists unique integers $z_1, z_2, \dots, z_n \in \mathbb{Z}$ such that

$$z_1 \mathbf{v}_1 + z_2 \mathbf{v}_2 + \dots + z_n \mathbf{v}_n = \mathbf{R} \quad (2.1.5)$$

Theorem 2.1.6. The set of all possible lattices is classified by the following 14 Bravais lattices:

<p>CUBIC $a = b = c$ $\alpha = \beta = \gamma = 90^\circ$</p>				
<p>TETRAGONAL $a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$</p>				
<p>ORTHORHOMBIC $a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$</p>				
<p>HEXAGONAL $a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$</p>		<p>TRIGONAL $a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$</p>		
<p>MONOCLINIC $a \neq b \neq c$ $\alpha = \gamma = 90^\circ$ $\beta \neq 120^\circ$</p>				
<p>TRICLINIC $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$</p>				

4 Types of Unit Cell
 P = Primitive
 I = Body-Centred
 F = Face-Centred
 C = Side-Centred
 +
7 Crystal Classes
 → **14 Bravais Lattices**

Proposition 2.1.7. A choice of lattice vectors is non unique.

Definition 2.1.8. A **basis** is a set of vectors that when repeated for every lattice points uniquely reproduces the entire lattice.

Theorem 2.1.9. Any crystal can be represented as a lattice and a basis.

Definition 2.1.10. A **unit cell** is a region of space which when repeated across a lattice completely reconstructs a crystal structure with no overlapping points.

Definition 2.1.11. A **primitive unit cell** is a unit cell with only one lattice point.

Definition 2.1.12. The **number of lattice points in a unit cell** is determined by location of the points in the unit cell. Corner points are 1/8, endpoints are 1/4, face point are 1/2, and points on in bulk of the cell are 1.

Definition 2.1.13. The **coordination number** is the number of neighbors for each point.

2.2 Reciprocal Space

Definition 2.2.1. The **reciprocal lattice** is the lattice of points \mathbf{G} such that $e^{i\mathbf{G}\cdot\mathbf{R}} = 1$ for all \mathbf{R} in the direct lattice.

Definition 2.2.2. The **reciprocal lattice vectors** are the set of vectors \mathbf{b}_i that generate the reciprocal lattice G .

$$\mathbf{b}_i = 2\pi \frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_i \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \quad , i, j, k = 1, 2, 3; 2, 3, 1; 3, 1, 2 \quad (2.2.2)$$

$$\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3, \quad h, k, l \in \mathbb{Z} \quad (2.2.3)$$

for a 2d lattice the reciprocal lattice vectors $\mathbf{b}_1 = (b_{1x}, b_{1y})$ and $\mathbf{b}_2 = (b_{2x}, b_{2y})$ are given by

$$b_{1x} = \frac{2\pi a_{2y}}{a_{1x}a_{2y} - a_{1y}a_{2x}}, \quad b_{1y} = \frac{-2\pi a_{2x}}{a_{1x}a_{2y} - a_{1y}a_{2x}} \quad (2.2.4)$$

$$b_{2x} = \frac{-2\pi a_{1y}}{a_{1x}a_{2y} - a_{1y}a_{2x}}, \quad b_{2y} = \frac{2\pi a_{1x}}{a_{1x}a_{2y} - a_{1y}a_{2x}} \quad (2.2.5)$$

$$(2.2.6)$$

Definition 2.2.7. The **miller indices** denoted (hkl) of a reciprocal lattice point \mathbf{G} are integers $h, k, l \in \mathbb{Z}$ such that

$$\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3 \quad (2.2.7)$$

Remark. The reciprocal lattice of fcc is bcc.

Definition 2.2.8. A **lattice plane** is a plane containing at least 3 non-colinear lattices points.

Definition 2.2.9. A **family of lattice planes** is an infinite set of equally spaced parallel lattice planes such that all lattice points are included in exactly one of the lattice planes.

Proposition 2.2.10. Every family of lattice planes is orthogonal to a reciprocal lattice vector \mathbf{a} and the spacing between lattice planes is

$$d = \frac{2\pi}{|\mathbf{a}_{\min}|} \quad (2.2.10)$$

where \mathbf{a}_{\min} is the smallest reciprocal lattice vector in direction \mathbf{a} .

Corollary 2.2.11. The distance between lattice planes in the family for a reciprocal lattice vector with miller indices (hkl) is

$$d = \frac{2\pi}{\sqrt{h^2\mathbf{b}_1 + k^2\mathbf{b}_2 + l^2\mathbf{b}_3}} \quad (2.2.11)$$

Corollary 2.2.12. For a cubic cell the distance between lattice planes in the family for a reciprocal lattice vector with miller indices (hkl) is

$$d = \frac{2\pi}{\sqrt{h^2 + k^2 + l^2}} \quad (2.2.12)$$

Proposition 2.2.13. MISSING PROP! Recall date: 2022-10-05. Using lecture notes from d2l. Prop about x,y,z intercepts and lattice planes.

Definition 2.2.14. Two miller indices are **equivalent** iff the corresponding families of lattice planes are homeomorphic by rotation.

Definition 2.2.15. The **multiplicity** of miller indices is the number of equivalent miller indices

Proposition 2.2.16. A set of lattice vectors is primitive if and only if the set of reciprocal lattice vectors is primitive.

2.3 X-Ray Scattering

Definition 2.3.1. The **electron density scattering model** predicts the intensity of scattered light for the wave vector \mathbf{k} of incoming light, the wave vector \mathbf{k}' of scattered light in reciprocal space, and the scattering potential $V(\mathbf{r})$ in direct space, the intensity of scattered light $\Gamma(\mathbf{k} - \mathbf{k}')$ is given by

$$\Gamma(\mathbf{k} - \mathbf{k}') = \frac{2\pi}{\hbar} |\langle \mathbf{k}' | V(\mathbf{r}) | \mathbf{k} \rangle|^2 \delta(E - E') \quad (2.3.1)$$

Result 2.3.2. Scattering amplitude from wave vector k of incoming light to wave vector k' of scattered light in reciprocal space is the Fourier transform of scattering potential $V(\mathbf{r})$.

$$\langle \mathbf{k}' | V(\mathbf{r}) | \mathbf{k} \rangle = \int e^{-i\mathbf{k}'\mathbf{r}} V(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}} d\mathbf{r} = \int e^{-i(\mathbf{k}' - \mathbf{k})\mathbf{r}} V(\mathbf{r}) d\mathbf{r} = \tilde{V}(\mathbf{k} - \mathbf{k}') \quad (2.3.2)$$

Definition 2.3.3. **Bragg's condition** for $n \in \mathbb{N}$, wavelength λ , lattice spacing d and scattering angle θ is satisfied when

$$n\lambda = 2d \sin \theta \quad (2.3.3)$$

Definition 2.3.4. The **X-ray scattering potential** $V(\mathbf{r})$ is proportional to the density of electrons and is given by

$$V(\mathbf{r}) = \sum_{\alpha} z_{\alpha} g_{\alpha}(\mathbf{r} - \mathbf{r}_{\alpha}) \quad (2.3.4)$$

Theorem 2.3.5. When **Bragg's condition** is satisfied the intensity $I_{\text{Scattering}}$ of scattered light is proportional to

$$I_{\text{Scattering}} \propto |\tilde{V}(\mathbf{k})|^2 \quad (2.3.5)$$

where $\tilde{V}(\mathbf{k})$ is the fourier transform of the scatter potential $V(\mathbf{r})$

Definition 2.3.6. The atomic form factor $f_{\alpha}(\mathbf{G})$ is defined as

$$f_{\alpha}(\mathbf{G}) = \int r e^{i\mathbf{G}\cdot\mathbf{r}} z_{\alpha} g_{\alpha}(\mathbf{r}) d^3\mathbf{r} \quad (2.3.6)$$

Result 2.3.7. The the fourier transform of the scatter potential of miller indices (h, k, l) where $[u_{\alpha}, v_{\alpha}, w_{\alpha}]$ are the positions of atoms is

$$\tilde{V}(\mathbf{k}) = \sum_{\alpha} e^{i\pi(hu_{\alpha} + kv_{\alpha} + lw_{\alpha})} f_{\alpha}(h, k, l) \quad (2.3.7)$$

Theorem 2.3.8. The the fourier transform of the scatter potential of miller indices (h, k, l) can be written in terms of the basis and lattice vectors

$$\tilde{V}(\mathbf{k}) = \sum_{\mathbf{R}} \sum_{\mathbf{x}} f_x(h, k, l) e^{i\mathbf{G}\cdot(\mathbf{R}+\mathbf{x})} = \sum_{\mathbf{R}} e^{i\mathbf{G}\cdot\mathbf{R}} \cdot \sum_{\mathbf{x}} f_x(h, k, l) e^{i\mathbf{G}\cdot\mathbf{x}} \quad (2.3.8)$$

where \mathbf{R} are the lattice vectors and \mathbf{x} are the basis vectors.

2.3.9 Experimental X-Ray Scattering

Definition 2.3.10. The **single crystal X-ray diffraction experiment** is an experiment where a single large crystal sample is rotated relative to a beam of X-rays and a detector.

Definition 2.3.11. The **powder X-ray diffraction experiment** is an experiment where X-rays are diffracted through a powdered sample of a crystal to generate diffraction rings on a detector screen.

Definition 2.3.12. **Debye-Scherrer rings** are the diffraction rings formed by X-ray diffraction through a powdered sample.

Definition 2.3.13. An **X-ray tube** is a device that uses excited electron states in copper to produce X-rays at $\lambda = 1.5407 \text{ \AA}$.

Theorem 2.3.14. To experimental determine the crystal structure of a powdered samples we measure the angle of the rings which is 2θ determined by Braggs condition:

$$d = \frac{\pi}{2 \sin \theta} \quad (2.3.14)$$

The ratio between the lattice plane spacing can be used to determine the crystal structure.

Chapter 3

Electrons in Crystals

3.1 Tight Binding Model

Definition 3.1.1. The **1D tight binding chain** is a simple model of a chain of atoms where we assume that electrons can only hop to the nearest neighbor atoms

$$H = \frac{P^2}{2m} + \sum_n V(\mathbf{X} - \boldsymbol{\alpha}_n) \quad (3.1.1)$$

$$\langle n|H|m\rangle = (E_{\text{atomic}} + V_0)\delta_{n,m} - t(\delta_{n,m+1} + \delta_{n,m-1}), \quad V_0 = |m\rangle \sum_{n \neq m} V_n |m\rangle \quad (3.1.2)$$

where $\boldsymbol{\alpha}_n$ are the positions of atoms and t is the binding constant. This model assumes that the total wavefunction is simply the sum of the individual wave functions for each atom

$$|\psi\rangle = \sum_n |n\rangle, \quad \langle n|m\rangle = \delta_{n,m} \quad (3.1.3)$$

Definition 3.1.4. A **dispersion relation** is the relation between energy and momentum in k-space. This is defined in terms of the momentum basis states $\Phi(\mathbf{k})$.

Theorem 3.1.5. The dispersion relation for the tight binding model is

$$\Phi_n(k) = e^{-ikna} \quad (3.1.5)$$

$$(E_{\text{atomic}} + V_0)e^{-ikna} - t(e^{-ik(n+1)a} + e^{-ik(n-1)a}) = Ee^{-ikna} \quad (3.1.6)$$

$$E = \varepsilon_0 - 2t \cos(ka), \quad \varepsilon_0 = E_{\text{atomic}} + V_0 \quad (3.1.7)$$

3.2 Nearly Free Electron Model