


Semiconductor Physics Lectures

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Chapter 1

Periodic Structure of Crystalline Solids

1.1 Condensed matter

To introduce you to condensed matter, we will define some solid structures:

Definition 1.1.1: Solid structures

- Crystalline solids - metals
- Amorphous solids - glass
- Liquid crystals
- Quasi Crystals
- Polymers

1.2 Crystals

Definition 1.2.1: Crystal

A crystal is a lattice and a basis, which in essence is a **periodic arrangement of atoms**.

For now, let's define a lattice as follows:

Definition 1.2.2: Lattice (1)

A lattice is an infinite array of identical points, arranged such that each point sees the other points in an identical way.

We can define a basis in the following way:

Definition 1.2.3: Basis

A basis is a structural unit representation by lattice points. The units in which it can be defined are i.e.:

- Atoms
- Molecules
- Group of atoms

Let's look at some lattices, depicted in figure 1.1. The parameter a is the lattice parameter.

As we can probably see, we can always define a some minimal set of vectors that describe the lattice. That means we can indeed go to each lattice point by taking a linear combination of these vectors. An example is given in figure 1.4. *More examples can be found in the slides.* More on lattice vectors in 1.3.

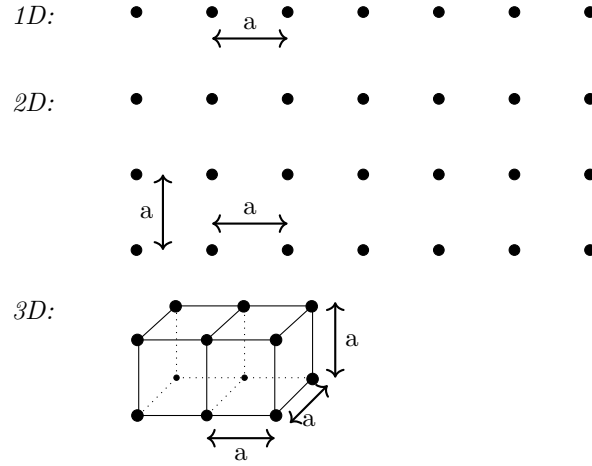


Figure 1.1: Lattices in different dimensions

Example 1.2.1 (Graphene)

To show what a lattice is and what it isn't this example is given, see also figure 1.2. As we know, graphene has a honeycomb lattice. That's why we call it a honeycomb crystal. But the lattice we can define is called a triangular lattice. Why?

By the definition of a lattice, we must have the same surrounding for every lattice point. This is not the case if we take one atom as basis. Therefore we take a set of two atoms to form the basis and define the lattice point as the center. This results in an equivalent surrounding for every basis structure.

Later on we will define a unit cell (section 1.4) and a conventional unit cell (section 1.6) for this lattice.

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1.3 Lattice vectors

As already touched upon at section 1.2, we can define a set of lattice vectors. To construct these we first define an origin O :

$$O = \vec{0} \quad (1.1)$$

Then we will define the lattice points in function of the PLV (*Primitive Lattice Vectors*).

$$\vec{a} = \text{PLV} \quad (1.2)$$

$$n_i \in \mathbb{Z} \quad (1.3)$$

$$A = [\vec{a}_1, \vec{a}_2, \vec{a}_3]^T \quad (1.4)$$

$$1D : \quad \vec{R} = n_1 \cdot \vec{a} \quad (1.5)$$

$$2D : \quad \vec{R} = [n_1, n_2] \cdot A \quad (1.6)$$

$$3D : \quad \vec{R} = [n_1, n_2, n_3] \cdot A \quad (1.7)$$

We can understand that a lattice must be defined unambiguous, therefore the definition of a lattice can be defined as:

Definition 1.3.1: Lattice (2)

A lattice is a set of points defined by Primitive Lattice Vectors (PLV).

Visually we can represent these vectors as can be seen in figure 1.3 and figure 1.4. We can also conclude that *PLVs* are not unique, one can also show that this is true for 3D. These are indeed *PLVs* because one can reach all lattice points.

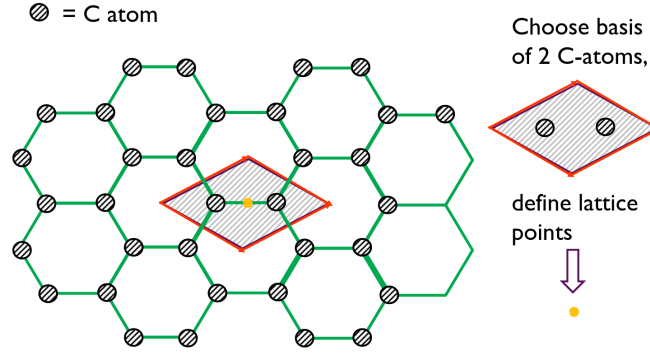


Figure 1.2: The graphene crystal



Figure 1.3: An example set of lattice vectors in 1D

1.4 Unit cell

Definition 1.4.1: Unit cell

A unit cell is a region of space such that when translated through the entire space by means of lattice vectors, reproduces the lattice without any overlaps or voids.

The definition of a unit cell is illustrated in figure 1.5

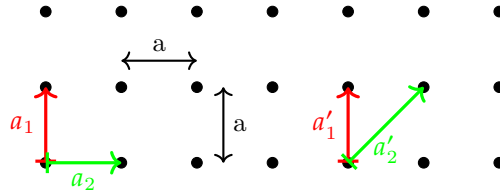


Figure 1.4: An example set of lattice vectors in 2D

1.5 Primitive unit cell

Definition 1.5.1: Primitive unit cell

A Primitive Unit Cell (PUC) is a unit cell that contains only one lattice parameter. By this is meant that when for example a cube is a primitive unit cell, each point counts as $\frac{1}{8}$, therefore the cube only has 1 lattice point.

We then see that:

- 1D: line spanned by *PLV* $\vec{a} \Rightarrow$ the line of the *PUC* = $\|\vec{a}\|$.

- 2D: area spanned by $PLV \vec{a}_1, \vec{a}_2 \Rightarrow$ the area of the $PUC = \|\vec{a}_1 \times \vec{a}_2\|$.
- 3D: volume spanned by $PLV \vec{a}_1, \vec{a}_2, \vec{a}_3 \Rightarrow$ the volume of the $PUC = \vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3$.

1.6 Conventional unit cell

Definition 1.6.1: Conventional unit cell

A conventional unit cell, a.k.a. a convenient unit cell, is a unit cell that contains more than 1 lattice point but has perpendicular axes.

1.7 Weigner-Seitz unit cell

Definition 1.7.1: Weigner-Seitz unit cell

A Weigner-Seitz unit cell is a primitive unit cell that has a region of space around a lattice point such that any point around that lattice point is closer to that lattice point as any other lattice point.

This concept is further elaborated below. The corresponding figure for a 2D example is seen in figure ??.

1. Take any lattice point (green in this case).
2. Look for the nearest lattice point and draw a line between them (in gray).
3. Draw the bisecting, perpendicular on this first line (in blue).
4. Do this for all other nearby lattice points (in cyan).



Figure 1.5: Several 1D unit cells

Chapter 2

Periodic Structure of Crystals

2.1 Bravais lattices

Definition 2.1.1: Bravais lattices

There are 14 different lattice types, these are called Bravais lattices. These lattices can be subdivided into 7 different lattice systems, these lattice systems are:

1. Triclinic
2. Monoclinic
3. Orthohombric
4. Tetragonal
5. Cubic
6. Triagonal
7. Hexagonal

The Cubic structure will mostly be studied during this course.

2.2 Cubic lattice systems

Cubic lattice systems come in three flavours, we will define them here. The different systems can be found in figure 2.1.

Definition 2.2.1: Simple cubic lattice

A simple cubic lattice is a conventional unit cell and therefore also a *PUC*. This lattice has a straightforward basis, as can be seen in figure 2.2.

The basis chosen is $\{\vec{a}_1, \vec{a}_2, \vec{a}_3\}$. As we can see (figure 2.2), the basis isn't body centered. Because the body centered atom is a different one as the other 'side' atoms, the smallest possible unit cell (or *PUC*) is the full cube. Whereas if the middle atom is the same, the basis is chosen in the middle, this is the **body centered cubic lattice**.

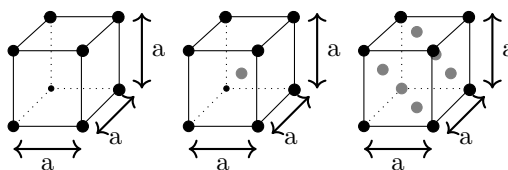


Figure 2.1: The three different cubic lattice systems

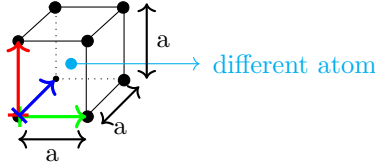


Figure 2.2: The basis for a simple cubic lattice

Definition 2.2.2: Body centered cubic lattice

A Body centered cubic lattice has 1 atom as primitive unit cell, its basis is depicted in figure 2.3. As mentioned before, all atoms are the same and that is why the *PUC* is smaller.

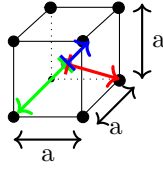


Figure 2.3: The three different cubic lattice systems

Definition 2.2.3: Face centered cubic lattice

If all atoms are the same and the extra atoms position themselves on the middle of every face, one gets the face centered cubic lattice. This is depicted in figure 2.4.

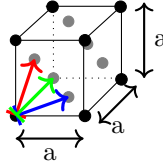


Figure 2.4: The three different cubic lattice systems

2.3 C/Si/Ge - lattice systems

As we know, the lattice systems for C, Si and Ge have a diamond lattice structure. This diamond structure takes the form of a fcc (face centered cubic) lattice. In figure 2.5, one can see the primitive unit cell. The basis vectors are:

$$\vec{a}_1 = \left(\frac{1}{2}, \frac{1}{2}, 0\right) \quad (2.1)$$

$$\vec{a}_2 = \left(0, \frac{1}{2}, \frac{1}{2}\right) \quad (2.2)$$

$$\vec{a}_3 = \left(\frac{1}{2}, 0, \frac{1}{2}\right) \quad (2.3)$$

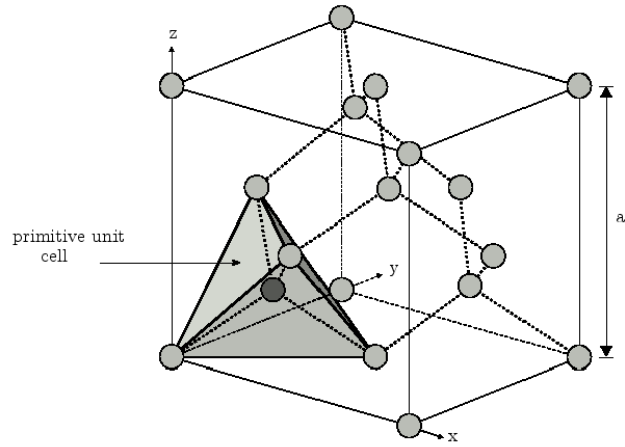


Figure 2.5: The diamond structure and its *PUC*

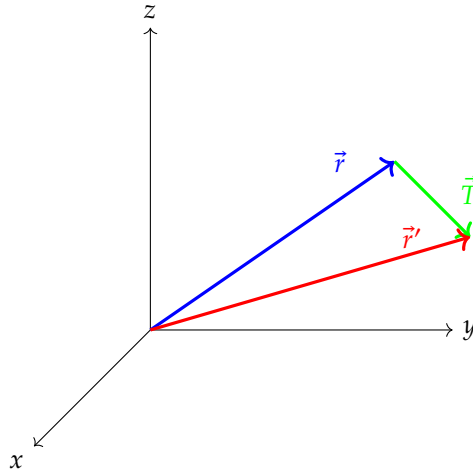


Figure 2.6: Translational symmetry

2.3.1 Translation symmetry

As a tiny intermezzo I'll introduce translation symmetry. This will be important later on for solving the Schrödinger equation.

$$\left\{ -\frac{\hbar}{2m} \nabla^2 + V(\vec{r}) \right\} \phi(\vec{r}) = E \phi(\vec{r}) \quad (2.4)$$

$$\longrightarrow V(\vec{r} + \vec{T}) = V(\vec{r}') = V(\vec{r}) \quad (2.5)$$

Because $V(\vec{r})$ is actually a periodic function in a crystal lattice, it becomes $V(\vec{r} + \vec{T})$. This \vec{T} is responsible for the translation in translational symmetry.

Definition 2.3.1: Translational symmetry

Translational symmetry is a symmetry operation for a crystal. This operation leaves the crystal invariant. Meaning that the addition of \vec{T} to \vec{r} returns the same value for $V(\vec{r})$. This is graphically represented in figure 2.6.

2.4 Lattice dimensions

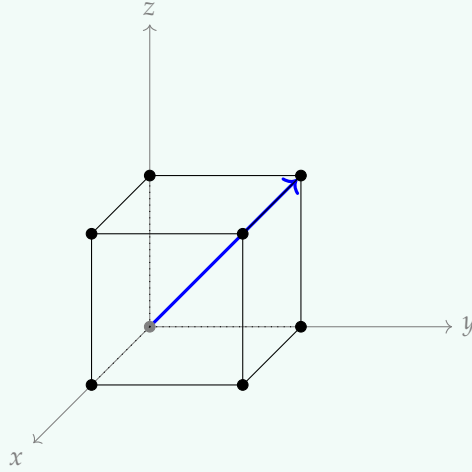
Definition 2.4.1: Lattice dimensions

Lattice dimensions are defined by the parameters $[u, v, w]$. These parameters are defined by a vector $\vec{r} = k(u\vec{a}_1 + v\vec{a}_2 + w\vec{a}_3)$.

$\vec{a}_1, \vec{a}_2, \vec{a}_3$ are unit cell vectors, k is a common factor in order that $u, v, w \in \mathbb{Z}_{\text{without common factor}}$. One thing to notice is that if $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are *PLVs*, $k \in \mathbb{Z}$. Else $k \in \mathbb{Q}$.

Example 2.4.1 (Lattice dimensions)

Take the following vector in the lattice:



Then the vector can be denoted as $[0, 1, 1]$.

Note:-

If one of u, v, w is negative, remove the $-$ and add a bar on top, i.e., $-x = \bar{x}$.

2.5 Lattice planes

Definition 2.5.1: Lattice planes

Lattice planes are defined by the parameters $[h, k, l]$

Chapter 3

Solids

3.1 Defining solids

Question 1: What is a solid?

Solid = nuclei + electrons

For describing solids we define following concepts:

Definition 3.1.1: Core electrons

- Tightly bound to nucleus
- Occupy lower shells
- Do not participate in bonding

Definition 3.1.2: Valence electrons

- Loosely bound to nucleus
- Occupy higher E-shells
- Responsible for bonding

To describe the Hamiltonian for solids for the Schödinger equation we use:

$$H = H_{electron} + H_{electron-electron} + H_{nucleus} + H_{nucleus-nucleus} + H_{electron-nucleus} \quad (3.1)$$

$$H = H_{electron} + H_{electron-electron} + H_{ion} + H_{ion-ion} + H_{electron-ion} \quad (3.2)$$

The following definitions for the H_i are used:

$$H_{electron} = \sum_{i=1}^N -\frac{\hbar^2}{2m_{electron}} \nabla_i^2 \quad (3.3)$$

$$H_{nucleus} = \sum_{i=1}^M -\frac{\hbar^2}{2 * M_i} \nabla_o^2 \quad (3.4)$$

$$H_{electron-electron} = \frac{1}{2} \sum_{i,j;i \neq j} \frac{e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_j|} \quad (3.5)$$

$$H_{nucleus-nucleus} = \frac{1}{2} \sum_{i,j;i \neq j} \frac{Z_i Z_j e^2}{4\pi\epsilon_0 |\vec{R}_i - \vec{R}_j|} \quad (3.6)$$

$$H_{electron-nucleus} = \sum_{i,j} -\frac{Z_j e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{R}_j|} \quad (3.7)$$

Note:-

In equation (1.5) and (1.11) we have $i \neq j$ in order that we do not double count i . Furthermore, in equation (1.8) we have Z_i which is an atomic number

To further describe the solid lattice, one has to describe ions. In essence, ions are just nuclei and core electrons together. In the following equations is $M' = M$ and the amount of valence electrons is N' .

Looking at the hamiltonians of the electron - ion interactions, these become:

$$H_{electron} = \sum_{i=1}^{N'} -\frac{\hbar^2}{2m_{electron}} \nabla_i^2 \quad (3.8)$$

$$H_{ion} = \sum_{i=1}^{M'} -\frac{\hbar^2}{2 * M_i} \nabla_o^2 \quad (3.9)$$

$$H_{electron-electron} = \frac{1}{2} \sum_{i,j;i \neq j} \frac{e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_j|} \quad (3.10)$$

$$H_{ion-ion} = \frac{1}{2} \sum_{i,j;i \neq j} V_{ion}(\vec{R}_i - \vec{R}_j) \quad (3.11)$$

$$H_{electron-ion} = \sum_{i,j} V_{electron-ion}(\vec{r}_i - \vec{R}_j) \quad (3.12)$$

We can see the equations for electron - ion interactions are very similar to electron nucleus interactions.

What we eventually want to solve is: $H\Phi = E\Phi$. We will therefore define following vectors:

$\vec{r} = (\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$ and $\vec{R} = (\vec{R}_1, \vec{R}_2, \dots, \vec{R}_M)$.

We can now define the probability density function as: $P(\vec{r}, \vec{R}) = |\Phi(\vec{r}, \vec{R})|^2$ Later on, we separate the degrees of freedom of valence electrons from the degrees of freedom of bound electrons, that's why we separated them here already.

3.2 Born-oppenheimer approximation

This definition comes down to saying electrons move much faster as ions thus ions are immobile.

$$H\Phi(\vec{r}, \vec{R}) = E\Phi(\vec{r}, \vec{R}) \quad (3.13)$$

Claim 3.2.1

$$\Phi(\vec{r}, \vec{R}) \approx \psi(\vec{r}, \vec{R})\phi(\vec{R})$$

$$H\Phi(\vec{r}, \vec{R}) = H\psi(\vec{r}, \vec{R})\phi(\vec{R}) \quad (3.14)$$

$$= (H_{electron} + H_{electron-electron} + H_{ion} + H_{ion-ion} + H_{electron-ion})\psi(\vec{r}, \vec{R})\phi(\vec{R}) \quad (3.15)$$

$$= (H_{electron} + H_{electron-electron} + H_{electron-ion})\psi(\vec{r}, \vec{R})\phi(\vec{R}) + (H_{ion} + H_{ion-ion})\psi(\vec{r}, \vec{R})\phi(\vec{R}) \quad (3.16)$$

$$= \phi(\vec{R})(H_{electron} + H_{electron-electron} + H_{electron-ion})\psi(\vec{r}, \vec{R}) + \psi(\vec{r}, \vec{R})(H_{ion} + H_{ion-ion})\phi(\vec{R}) \\ + (H_{ion} + H_{ion-ion})\psi(\vec{r}, \vec{R})\phi(\vec{R}) - \psi(\vec{r}, \vec{R})(H_{ion} + H_{ion-ion})\phi(\vec{R}) \quad (3.17)$$

We can move $\phi(\vec{R})$ to the front because there is no differnetial operation acting on it in the hamiltonians. In step 3 we perform a '+ $\psi(\vec{r}, \vec{R})(H_{ion} + H_{ion-ion})\phi(\vec{R})$ ' and '- $\psi(\vec{r}, \vec{R})(H_{ion} + H_{ion-ion})\phi(\vec{R})$ ' operation.

Because $m_{electron} \approx M \cdot 10^{-4}$, $(H_{ion} + H_{ion-ion})\psi(\vec{r}, \vec{R})\phi(\vec{R}) - \psi(\vec{r}, \vec{R})(H_{ion} + H_{ion-ion})\phi(\vec{R}) \approx 0$. We can now simplify equation (1.5) = $E\psi(\vec{r}, \vec{R})\phi(\vec{R})$ further by dividing with $\psi(\vec{r}, \vec{R})\phi(\vec{R})$.

Equation (1.5) now becomes:

$$\frac{(H_{electron} + H_{electron-electron} + H_{electron-ion})\psi(\vec{r}, \vec{R})}{\psi(\vec{r}, \vec{R})} + \frac{(H_{ion} + H_{ion-ion})\phi(\vec{R})}{\phi(\vec{R})} = E \quad (3.18)$$

Note:-

We cannot divide the leftover function as the numerator still acts on it!

We can now define:

$$E_{el}(\vec{R}) = E - \frac{(H_{ion} + H_{ion-ion})\phi(\vec{R})}{\phi(\vec{R})} \quad (3.19)$$

As mentioned before already, this makes it possible to separate valence electronic part and the ionic part.

Definition 3.2.1: Formulation of the solid hamiltonians

$$\begin{cases} (H_{electron} + H_{electron-electron} + H_{electron-ion})\psi(\vec{r}, \vec{R}) = E_{el}\psi(\vec{r}, \vec{R}) \\ \frac{(H_{ion} + H_{ion-ion})\phi(\vec{R})}{\phi(\vec{R})}\psi(\vec{r}, \vec{R}) = (E - E_{el})\psi(\vec{r}, \vec{R}) \end{cases} \quad (3.20)$$

3.3 Static approximation (w.r.t. the lattic)

We know $\vec{R} = (\vec{R}_1, \vec{R}_2, \dots, \vec{R}_M) \Rightarrow \vec{R}_i^{(0)} + \delta\vec{R}_i(t)$ This delta is small and can be ignored.

$$H_{electron-ion} = \sum V_{electron-ion}(\vec{r}_i - \vec{R}_j) \quad (3.21)$$

$$= \sum (V_{electron-ion}(\vec{r}_i - \vec{R}_j^{(0)}) + \delta\vec{R}_j(t) \cdot \vec{\nabla}_j V_{electron-ion}(\vec{r}_i - \vec{R}_j^{(0)})) \quad (3.22)$$

Note:-

- $\delta\vec{R}_j(t) \cdot \vec{\nabla}_j V_{electron-ion}(\vec{r}_i - \vec{R}_j^{(0)})$ is the electron - phonon interaction.
- Why does it only depend on distance? In normal circumstances, most interactions are distance related but sometimes it is (in anisotropic materials) vector dependent, therefore the $||$ is left out here in $H_{electron-ion}$.

Now we simplify equation (1.20), in hope for writing the time dependent Schrödinger equation easier. Namely it becomes a single electron particle operator instead of a complex Hamiltonian.

- $H_{electron}$ stays the same
- $H_{electron-ion}$ stays the same
- $H_{electron-electron} = 1/2 \sum \frac{e^2}{4\pi\epsilon_0|\vec{r}_i - \vec{r}_j|} \approx \sum v_i(\vec{r}_i)$

Such that:

$$\sum_i \left\{ -\frac{\hbar^2}{2m_{electron}} \nabla_i^2 + \sum_j \left\{ V_{electron-ion}(\vec{r}_i - \vec{R}_j) + v_i(\vec{r}_i) \right\} \right\} \psi(\vec{r}, \vec{R}) = E_{el}\psi(\vec{r}, \vec{R}) \quad (3.23)$$

$$\Rightarrow \sum h_i(\vec{r}_i)\psi(\vec{r}) = E_{el}\psi(\vec{r}) \quad (3.24)$$

$$\longrightarrow \psi(\vec{r}) = \xi(\vec{r}_1) + \xi(\vec{r}_2) + \dots \quad (3.25)$$

$$\Rightarrow h_i(r_i)\xi(\vec{r}_i) = \epsilon_i\xi(\vec{r}_i) \quad (3.26)$$

3.4 Hartree approximation

Question 2: What does this approximation mean?

First of all, the Hartree approximation is an electron - electron interaction approximation. It means that electron number i sees all other electrons as a continuous charge distribution.

$$g_i(\vec{r}) = \sum_{k \neq i} -e |\xi_k(\vec{r})|^2 \quad (3.27)$$

$$\longrightarrow \nabla^2 \Phi_i(\vec{r}) = \frac{g_i(\vec{r})}{\epsilon} \quad (3.28)$$

We can calculate the Potential energy as follows:

$$v_i(\vec{r}) = -e\Phi \quad (3.29)$$

$$= \sum_{k \neq i} \int_V \frac{e^2 |\xi_k(\vec{r})|^2}{4\pi\epsilon_0 |\vec{r} - \vec{r}'|} d\vec{r}' \quad (3.30)$$

Note:-

Φ is electrostatic potential. Furthermore, \vec{r}_i means it **belongs** to electron i .

Now we can solve the one electron problem by:

$$h(\vec{r})\xi(\vec{r}) = \epsilon\xi(\vec{r}) \quad (3.31)$$

$$\Rightarrow h(\vec{r}) = -\frac{\hbar^2}{2m_e} \nabla^2 + v(\vec{r}) + \sum V_{electron-ion}(\vec{r} - \vec{R}) \quad (3.32)$$

Looking at the last part of h we see that in a lattice, \vec{R} is a lattice vector. Then for a solid, the lattice is infinite and therefore $V_{electron-ion}$ will be periodic. We will call $\sum V_{electron-ion}(\vec{r} - \vec{R})$ a periodic potential: $U(\vec{r}) = U(\vec{r} - \vec{R}_l')$

Corollary 3.4.1 Conclusion

As show above we can now write the Schrödinger equation as a simplified wave function:

$$\left(-\frac{\hbar^2}{2m_e} \nabla^2 + V(\vec{r}) \right) \xi(\vec{r}_i) = \epsilon\xi(\vec{r}_i) \quad (3.33)$$