Solid State Physics

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Contents

1 Blotzmann and Einstein Model

Why study condense matter physics?

- It is the world
- it is useful
- it is deep
- anti-reductionism
- It is a laboratory

1.1 Heat capacity(of solids)

Heat capacity

$$C = \frac{\partial Q}{\partial T} \tag{1}$$

In solid $C_p \approx C_v \approx C$ and the α is the thermal expansion coefficient , β is the isothermal compressibility

$$C_p - C_v = \frac{VT\alpha^2}{\beta} \tag{2}$$

And for monatomic gas the capacity is $C_v = 3k_B/2$, with k_B being Boltzmann's constant. For solid the capacity is $C = 3k_B$ Boltzmann constructed this model using a harmonic well formed by the interaction with its neighbors. Using equipartion THM every freedom has the energy $C/N = 1/2k_B$ It hold well at room temperature, but in low temperature,

1.2 Einstein's Calculation

Using quantum mechanics, $\omega = \sqrt{\frac{k}{m}}$

$$E_n = \hbar\omega(n + 1/2) \tag{3}$$

1 Dimension oscillator The partition function is defined as:

$$Z = \sum_i e^{-\beta E_i} \quad \beta = \frac{1}{k_B T} \tag{4}$$

The partition function $Z_{1D}$is then the sun over all state

$$Z_{1D} = \sum_{n=0}^{\infty} e^{-\beta E_n} = \sum e^{-\beta\hbar\omega(n+1/2)} \tag{5}$$

the probability of the system being in state n is:

$$P_n = \frac{e^{-\beta E_n}}{Z_{1D}} \tag{6}$$

Thus,the average energy is:

$$\langle E \rangle = \sum_{n=0}^{\infty} P_n E_n = -\frac{1}{Z_{1D}} \frac{\partial Z_{1D}}{\partial \beta} = \hbar\omega(n_B(\beta\hbar\omega) + 1/2) \tag{7}$$

where n_B is the Bose occupation factor

$$n_B(x) = \frac{1}{e^x - 1} \tag{8}$$

The heat capacity for a single oscillator

$$C = \frac{\partial \langle E \rangle}{\partial T} = k_B (\beta \hbar \omega)^2 \frac{e^{\beta \hbar \omega}}{(e^{\beta \hbar \omega} - 1)^2} \tag{9}$$

Note that the high-temperature limit of this expression gives $C = k_B$
Generalizing to the three-dimensional case,

$$E_{n_x,n_y,n_z} = \hbar\omega[(n_x + 1/2) + (n_y + 1/2) + (n_z + 1/2)] \tag{10}$$

and

$$Z_{3D} = \sum_{n_x,n_y,n_z \geqslant 0} e^{-\beta E m_{n_x,n_y,n_z}} = [Z_{1D}]^3 \tag{11}$$

resulting in $\langle E_{3D} \rangle = 3 \langle E_{1D} \rangle$,so correspondingly we obtain

$$C = 3k_B (\beta \hbar \omega)^2 \frac{e^{\beta \hbar \omega}}{(e^{\beta \hbar \omega} - 1)^2} \tag{12}$$

for diamond ω is high(most material ω is very low) the Einstein model fits very well

1.3 Debye's Calculation

Debye realized that oscillation of atoms is the same thing as sound, and sound is a wave, so it should be quantized the same way as Planck.

1.3.1 Periodic(Born-von Karman)Boundary Conditions

In one dimension, we consider a periodic condition that the two ends are connected together making the sample into a circle.So the wave e^{ikr} is required to have the same value for a position r as it has for r+L. Then restricts the possible values of k to be

$$k = \frac{2\pi n}{L} \tag{13}$$

In three dimensions, **K** can only take values in a sample of size L^3

$$\mathbf{k} = \frac{2\pi}{L}(n_1, n_2, n_3) \tag{14}$$

Sum over all possible **k** values we obtain

$$\sum_k \rightarrow \frac{L^3}{(2\pi)^3} \int \mathrm{d}\mathbf{k} \tag{15}$$

1.3.2 Debye's Calculation Following Planck

This is a test

2 Crystal Structure

2.1 Periodic Array of Atoms

The electrons have short wavelength components that respond dramatically to the regular periodic atomic other of the specimen. However light waves has longer wavelength than electrons and see an average over the order(Such as Noncrystalline materials), and not the less regular local order itself.

And the property is proved by x-ray diffraction, because x-ray have a wave-length comparable to the length of a building block of the structure.

2.1.1 Lattice Translation Vectors

An ideal crystal is constructed by the infinite repetition of identical groups of atom.

- **Basis**: A group is called the basis.
- **Lattice**:The set of mathematical points to which the basis is attached is called the lattice.

In three dimensions, **translation vectors** $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$,
The arrangement of atoms in the crystal looks the same when viewed from the point $\mathbf{r}$ as when viewed from every point **r'** translated by an integral multiple of the **a**'s:

$$\boxed{\mathbf{r}' = \mathbf{r} + u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3} \tag{16}$$

- **Primitive lattice**: The lattice is said to be primitive if any two point from which the atomic arrangement looks the same always satisfy 16 with a suitable choice of the integers u_i.
- **Primitive translation vectors $\mathbf{a}_\mathbf{i}$**

Primitive translation vectors define the crystal axes, which form three adjacent edges of the primitive parallelepiped.

2.1.2 Basis and the Crystal Structure

The **basis** of the crystal structure can be identified once the crystal axes have been chosen.
The number of atom in the basis may be one, or more than one. The position of the center of an atom j of the basis relative to the associated lattice point is

$$\boxed{\mathbf{r}_j = x_j\mathbf{a}_1 + y_j\mathbf{a}_2 + z_j\mathbf{a}_3} \tag{17}$$

2.1.3 Primitive Lattice Cell

The parallelepiped defined by primitive axes $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ is called a **primitive cell**.

- A primitive cell is a type of cell or unit cell
- A primitive cell is a minimum-volume cell

- There are many ways of choosing the primitive axes and primitive cell for a given lattice
- However the atoms in a primitive cell or primitive basis is always the same for a given crystal structure.
- There is always one lattice point per primitive cell.(each lattices point only share 1/8 in one cell.

The volume of a parallelepiped with axes $\mathbf{a_1}, \mathbf{a_2}, \mathbf{a_3}$ is

$$\boxed{V_c = |\mathbf{a_1} \cdot \mathbf{a_2} \times \mathbf{a_3}|} \tag{18}$$

No basis contains fewer atoms than a primitive basis contains.This is known to physicists as a **Wigner-Seitz cell**

2.2 Fundamental Types of Lattices

Crystal lattices can be carried or mapped into themselves by the lattice translations **T**

2.2.1 Two-Dimensional Lattice

Oblique lattice It is invariant only under rotation of π and 2π about any lattice point.But special lattices of the oblique type can be invariant under other rotation or mirror reflection by impose restrictive conditions on a_1,a_2

Bravais lattices Bravais lattice is the common phrase for a distinct lattice type. There are five Bravais lattices in two dimensions.

2.2.2 Three-Dimensional Lattice Types

The point symmetry groups in three dimensions require the 14 different lattice types. The general lattice is triclinic, and there are 13 special lattices.

There are three lattices in the cubic system: the simple cubic (sc) lattice, the body-centered cubic (bcc) lattice, and the face-centered cubic (fcc) lattice.

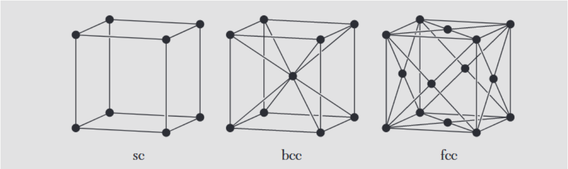

Figure 1: The cubic space lattices

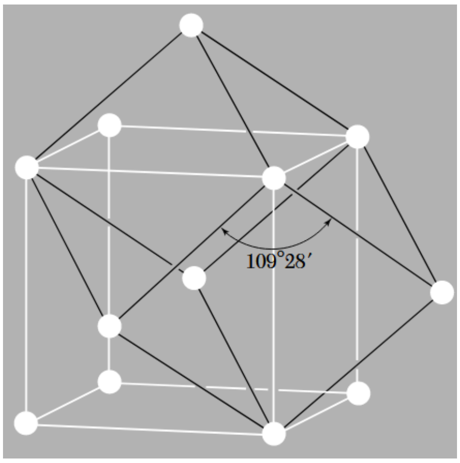

Figure 2: Body-centered cubic lattice, showing a primitive cell.

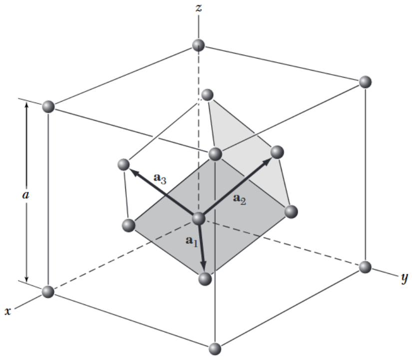

Figure 3: The rhombohedral primitive cell of the face-centered cubic crystal.

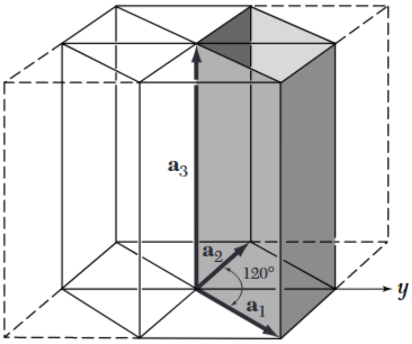

Figure 4: Relation of the primitive cell in the hexagonal system (heavy lines) to a prism of hexagonal symmetry.

2.2.3 Index System for Crystal Planes

The orientation of the plane by the indices determined by the following rules.

- Find the intercepts on the axes in terms of the lattice constants a_1, a_2, a_3
- Take the reciprocals of these numbers and then reduce to three integers having same ratio,usually the smallest three integers.

- The result, enclosed in parentheses (hkl), is called the **index** of the plane
- if a plane cuts the axis on the negative side of the origin, the corresponding index is negative, indicated by placing a minus sign above the index $(h\bar{k}l)$

The indices $[uvw]$ of a direction in a crystal are the set of the smallest integers that have the ratio of the components of a vector in the desired direction, referred to the axes.

2.3 Simple Crystal Structures

2.3.1 Sodium Chloride Structure

The lattice is face-centered cubic(fcc)

2.3.2 Cesium Chloride Structure

The cesium chloride structure is body-centered positions(bcp).

2.3.3 Hexagonal Close-Packed Structure (hcp)

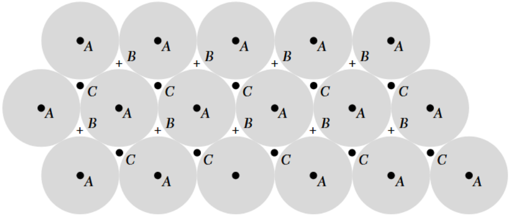

Figure 5: A close-packed layer of spheres is shown, with centers at points marked A

It can go in over A or over C. If it goes in over A, the sequence is ABABAB... and the structure is hexagonal close-packed. If the third layer goes in over C, the sequence is ABCABCABC... and the structure is face-centered cubic.

2.3.4 Diamond Structure

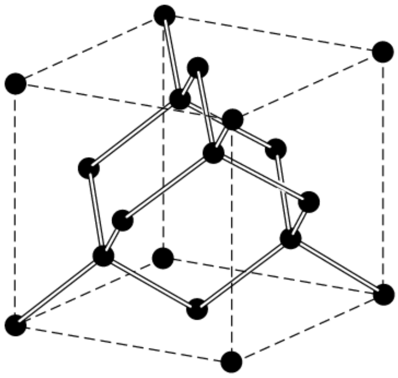

Figure 6: Crystal structure of diamond, showing the tetrahedral bond arrangement.

3 Wave Diffraction and the Reciprocal Lattice

3.1 Diffraction of Waves by Crystals

3.1.1 The Bragg law

$$2d\sin\theta = n\lambda \tag{19}$$

It can be statisfied only for wavelength $\lambda \leq 2d$

Only certain value of θ will the reflections from all periodic parallel planes add up in phase to give a strong reflected beam.

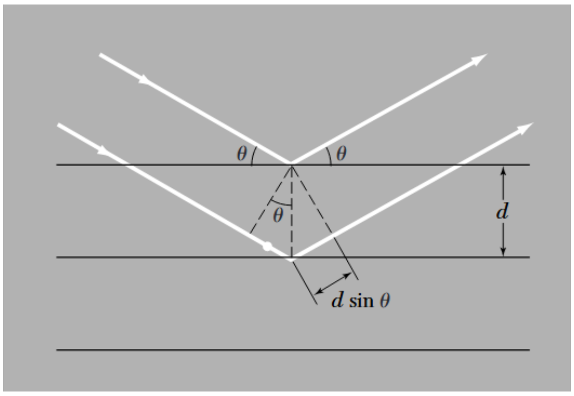

Figure 7: Bragg reflection

3.2 Scattered Wave Amplitude

spatial distribution of electrons within each cell.

3.2.1 Fourier Analysis

$\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ are the crystal axes, any local physical property of the crystal is invariant under **T**

Electron density $n(\mathbf{r})$ we can expand $n(x$ in a Fourier series:

$$n(x) = n_0 + \sum_{p>0}[C_p\cos(2\pi px/a) + S_p\sin(2\pi px/a)] \tag{20}$$

the $n(x$ has the period a:

$$\begin{aligned} n(x+a) &= n_0 + \sum[C_p\cos(2\pi px/a + 2\pi p) + S_p\sin(2\pi px/a) + 2\pi p] \quad (21)\\ &= n_0 + \sum[C_p\cos(2\pi px/a) + S_p\sin(2\pi px/a)] \quad (22)\end{aligned}$$

$2\pi p/a$ is the reciprocal lattice or Fourier space of the crystal. In a series form:

$$n(x) = \sum_p \exp\{i2\pi px/a\} \tag{23}$$

we require:

$$n^*_{-p} = n_p \tag{24}$$

Thus we have

$$n_p(\cos\varphi + i\sin\varphi) + n_{-p}(\cos\varphi - i\sin\varphi) = (n_p + n_{-p})\cos\varphi + i(n_p - n_{-p})\sin\varphi \tag{25}$$

which in turn is equal to the real function

$$2\mathrm{Re}\{n_p\}\cos\varphi - 2\mathrm{Im}\{n_p\}\sin\varphi \tag{26}$$

We can find a set of vectors **G** such that

$$n(\mathbf{r}) = sum_{\mathbf{G}} n_{\mathbf{G}} \exp(i\mathbf{G}\cdot\mathbf{r}) \tag{27}$$

is invariant under all crystal translations **T**,$n_{\mathbf{G}}$determines the x-ray scattering amplitude

3.2.2 Inversion of Fourier Series

$$n_p = a^{-1}\int_0^a \mathrm{d}x\ n(x)\exp(-i2\pi px/a) \tag{28}$$

$$n_p = a^{-1}\sum_{p'}\int_0^a \mathrm{d}x\exp(i2\pi(p'-p)x/a) \tag{29}$$

so the inversion

$$n_{\mathbf{G}} = V_c^{-1}\int_{cell}\mathrm{d}V n(\mathbf{r})\exp(-i\mathbf{G}\cdot\mathbf{r}) \tag{30}$$

V_c is the volume of a cell of the crystal

3.2.3 Reciprocal Lattice Vectors

To find the vector **G**, we construct the axis vectors $\mathbf{b}_1$,$\mathbf{b}_2$,$\mathbf{b}_3$ of the reciprocal latiice

$$\mathbf{b_1} = 2\pi\frac{\mathbf{a_2}\times\mathbf{a_3}}{\mathbf{a_1}\cdot\mathbf{a_2}\times\mathbf{a_3}} \tag{31}$$

$$\mathbf{b_2},\mathbf{b_3} = \cdots \tag{32}$$

If $\mathbf{a_1},\mathbf{a_2},\mathbf{a_3}$ are primitive vectors of the crystal lattice, then $\mathbf{b}_1$,$\mathbf{b}_2$,$\mathbf{b}_3$ are primitive vectors of the reciprocal lattice. Thus it has the property

$$\mathbf{b_i}\cdot\mathbf{a_j} = 2\pi\delta_{ij} \tag{33}$$

Points in the reciprocal lattice are mapped by the set of vectors

$$\mathbf{G} = v_1\mathbf{b_1} + v_2\mathbf{b_2} + v_3\mathbf{b_3} \tag{34}$$

G is a reciprocal lattice vector, Thus we have the desired invariance ,$n(\mathbf{r}+\mathbf{T}) = n(\mathbf{r}) = \sum n_{\mathbf{G}}\exp(i\mathbf{G}\cdot\mathbf{r})$

3.2.4 Diffraction Conditions

Theorem The set of reciprocal lattice vectors $\mathbf{G}$ determines the possible x-ray reflections.

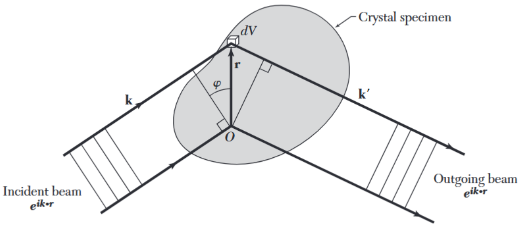

Figure 8: The difference in path length of the incident wave k

$$\mathbf{k} + \Delta\mathbf{k} = \mathbf{k}' \tag{35}$$

Here $\Delta\mathbf{k}$ is called the scattering vector, Scattering amplitude :

$$F = \int \mathrm{d}V\ n(\mathbf{r})\exp[i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}] = \int \mathrm{d}V\ n(\mathbf{r})\exp\{(-i\Delta\mathbf{k}\cdot\mathbf{r}\}) \tag{36}$$

So the lattice vector and the diffraciton condition:

$$\Delta\mathbf{k} = \mathbf{G} \tag{37}$$

$$2\mathbf{k}\cdot\mathbf{G} + G^2 = 0 \tag{38}$$

3.2.5 Laue Equations

From $\Delta\mathbf{k} = \mathbf{G}$ we get

$$\mathbf{a_1}\cdot\Delta\mathbf{k} = 2\pi v_1; \tag{39}$$

$$\mathbf{a_2}\cdot\Delta\mathbf{k} = 2\pi v_2; \tag{40}$$

$$\mathbf{a_3}\cdot\Delta\mathbf{k} = 2\pi v_3 \tag{41}$$