Formula page

1. LATTICES

Reciprocal lattice $\boldsymbol{G}$ is defined by $\mathrm{e}^{i\boldsymbol{G}\cdot\boldsymbol{R}} = 1$ with $\boldsymbol{R}$ the lattice vector.

$\boldsymbol{a}_i$ is the primitive direct lattice vector $\boldsymbol{R} = \sum_i^d \boldsymbol{a}_i n_i$, d is the dimension, $n_i \in \mathcal{Z}$.

$\boldsymbol{b}_i$ is the primitive reciprocal lattice vector $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$, or

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

The primitive cell volume $V = |\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)|$.

Three dimensional Bravais Lattices:

2. DIFFRACTION

Bragg condition $|\boldsymbol{G}| = 2\,|\boldsymbol{k}|\sin(\phi/2)$, with $\boldsymbol{k} = \frac{2\pi}{\lambda}\hat{k}$ the incident wave and λ the wavelength. $\cos(\phi) = \hat{k}\cdot\hat{k}_{out}$

The structure factor $S_{\boldsymbol{G}} = \sum_i f_i \mathrm{e}^{i\boldsymbol{G}\cdot\boldsymbol{d}_i}$, with $\boldsymbol{d}_i$ the basis vectors, $f_i(\boldsymbol{G})$ the atomic form factor $f_i(\boldsymbol{G}) = -\frac{1}{e}\int_{\boldsymbol{r}} \rho_i(\boldsymbol{r})\mathrm{e}^{i\boldsymbol{G}\cdot\boldsymbol{r}}$. The intensity is $I \sim |S_{\boldsymbol{G}}|^2$.

3. COHESIVE ENERGY

Lennard Jones potential

$$u = 2\epsilon\left[A_{12}\left(\frac{\sigma}{r}\right)^{12} + A_6\left(\frac{\sigma}{r}\right)^{6}\right]$$
$$A_n = \sum_{\boldsymbol{R}\neq 0}\frac{1}{|\boldsymbol{R}|^n}$$

Coulomb energy $u = -\frac{e^2}{d}\alpha$, $\alpha = \sum_j \frac{(-1)^j}{|r_j/d|}$.

4. PHONONS

The Harmonic energy with potential $\phi(\boldsymbol{r})$

$$U^{Harmonic} = \frac{1}{2}\sum_{\boldsymbol{R}_1,\boldsymbol{R}_2}\sum_{\mu,\nu=x,y,z}[u_\mu(\boldsymbol{R}_1) - u_\mu(\boldsymbol{R}_2)]\frac{\partial^2\phi(\boldsymbol{r})}{\partial r_\mu \partial r_\nu}[u_\nu(\boldsymbol{R}_1) - u_\nu(\boldsymbol{R}_2)]$$

The equations of motions are $m\ddot{\boldsymbol{u}}(\boldsymbol{R}) = -\frac{\partial U}{\partial \boldsymbol{u}(\boldsymbol{R})}$, with periodic boundary conditions we seek solution of the form $\boldsymbol{u} = \boldsymbol{\epsilon}\ \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{R}-i\omega t}$, $\boldsymbol{\epsilon}$ the polarization vector.

In k space the dynamical matrix $\ddot{D}(\boldsymbol{k})\boldsymbol{\epsilon} = M\omega^2\boldsymbol{\epsilon}$. For oscillation in d dimensions of p atoms in a unit cell, there are d acoustic branches and $(p-1)d$ optical branches.

The vibrational energy and specific heat for each branch:

$$\frac{U}{V} = \sum_s \int_\omega g_s(\omega) f(\omega)\hbar\omega\, d\omega = \sum_s \int_{FBZ} \frac{d\boldsymbol{k}}{(2\pi)^3} f(\omega_s(\boldsymbol{k}))\hbar\omega_s(\boldsymbol{k})$$

$$c_V = \frac{1}{V}\frac{dU}{dT}$$

$$f(\omega) = \frac{1}{\mathrm{e}^{\beta\hbar\omega_s(\boldsymbol{k})} - 1}$$

$$g_s(\omega) = \frac{dn_s}{d\omega} \qquad \text{(density of states per unit volume for branch } s\text{)}$$

$$\Delta k = (2\pi)^d/V \qquad \text{(density in k-space)}$$

5. ELECTRONS

The Drude conductivity is $\sigma = ne^2\tau/m$, with n the number of electron per unit volume, and τ the mean free time. The equation of motion for the momentum in Drude theory is

$$\frac{d\boldsymbol{p}}{dt} = -e\left(\boldsymbol{E} + \frac{\boldsymbol{p}}{mc} \times \boldsymbol{H}\right) - \frac{\boldsymbol{p}}{\tau}$$

The cyclotron frequency is $\omega_c = \frac{eH}{mc}$, the plasma frequency is $\omega_p^2 = \frac{4\pi ne^2}{m}$ the current density is $\boldsymbol{j} = \frac{ne}{m}\boldsymbol{p}$, and the conductivity tensor σ is defined by $\boldsymbol{j} = \sigma\boldsymbol{E}$.

The occupation functions are

$$f(\epsilon) = \begin{cases} \frac{1}{\mathrm{e}^{\beta(\epsilon-\mu)}+1} & \text{Fermi-Dirac} \\ \frac{1}{\mathrm{e}^{\beta(\epsilon-\mu)}-1} & \text{Bose-Einstein} \end{cases}$$

Fermi surface $\epsilon(\boldsymbol{k}) = \epsilon_F$. Sommerfeld expansions are

$$\int_{-\infty}^{\infty} H(x)f(x)dx = \int_{-\infty}^{\mu} H(x)dx + \frac{\pi^2}{6}(k_BT)^2 H'(\mu) + \frac{7\pi^4}{360}(k_BT)^4 H'''(\mu) + \dots$$

$$\mu = \epsilon_F - \frac{\pi^2}{6}\frac{g'(\epsilon_F)}{g(\epsilon_F)}(k_BT)^2$$

$$u = u_0 + \frac{\pi^2}{6} g(\epsilon_F)(k_BT)^2$$

The specific heat of electron gas in low temperature is $c_v = \frac{\partial u}{\partial T} = \frac{\pi^2}{3}k_B^2 T g(\epsilon_F)$, where the density of states is $g(\epsilon) = \frac{\partial n(\epsilon)}{\partial \epsilon}$.

Bloch theorem $\psi(\boldsymbol{r} + \boldsymbol{R}) = \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{R}}\psi(\boldsymbol{r})$, electron velocity in energy $E_n(k)$: $\boldsymbol{v}_n(\boldsymbol{k}) = \frac{1}{\hbar}\nabla_{\boldsymbol{k}} E_n(\boldsymbol{k})$.

Effective mass tensor

$$\frac{1}{m^*_{i,j}} = \frac{1}{\hbar^2}\frac{\partial^2\epsilon(\boldsymbol{k})}{\partial k_i \partial k_j} \quad i,j = x,y,z$$

Therefore, $m^* \frac{d\boldsymbol{v}}{dt} = \hbar \frac{d\boldsymbol{k}}{dt}$

Electron $\boldsymbol{k}$ in a periodic potential

$$\epsilon^0_{\boldsymbol{k}-\boldsymbol{G}} c_{\boldsymbol{k}-\boldsymbol{G}} + \sum_{\boldsymbol{G}'} U_{\boldsymbol{G}'-\boldsymbol{G}} c_{\boldsymbol{k}-\boldsymbol{G}'} = \epsilon_{\boldsymbol{k}-\boldsymbol{G}} c_{\boldsymbol{k}-\boldsymbol{G}}$$

where $U_{\boldsymbol{G}} = \frac{1}{v_{p.u.c}} \int_{p.u.c} U(\boldsymbol{r}) \mathrm{e}^{-i\boldsymbol{G}\cdot\boldsymbol{r}} d\boldsymbol{r}$ are the Fourier components of the potential, $p.u.c$ = primitive unit cell. the $c_{\boldsymbol{k}-\boldsymbol{G}}$ are the Fourier components of the wave function and $\epsilon^0_{\boldsymbol{k}-\boldsymbol{G}} = \frac{\hbar^2}{2m}(\boldsymbol{k}-\boldsymbol{G})^2$ is the free electron energy.

For a weak potential, near a couple of degenerate states

$$\epsilon = \frac{1}{2}(\epsilon^0_{\boldsymbol{k}} + \epsilon^0_{\boldsymbol{k}-\boldsymbol{G}}) \pm \left[\left(\frac{\epsilon^0_{\boldsymbol{k}} - \epsilon^0_{\boldsymbol{k}-\boldsymbol{G}}}{2} \right)^2 + |U_{\boldsymbol{G}}|^2 \right]^{1/2}$$

Far from degenerate states

$$\epsilon_k = \epsilon^0_k + \sum_{\boldsymbol{G}} \frac{|U_{\boldsymbol{G}}|^2}{\epsilon^0_k - \epsilon^0_{k-\boldsymbol{G}}}$$

Tight Binding model

$$\epsilon(\boldsymbol{k}) = E_s - \sum_{\boldsymbol{R}} \gamma(\boldsymbol{R}) e^{i\boldsymbol{k}\cdot\boldsymbol{R}}$$

$$E_s = \int d\boldsymbol{r} \phi^*(\boldsymbol{r}) H \phi(\boldsymbol{r})$$

$$\gamma(\boldsymbol{R}) = -\int d\boldsymbol{r} \phi^*(\boldsymbol{r}) H \phi(\boldsymbol{r}-\boldsymbol{R})$$

6. CONSTANTS, INTEGRALS, MISC

Constants:

$$\begin{aligned} \hbar &= 1.054 \cdot 10^{-34} \text{ [J s]} \\ k_{\mathrm{B}} &= 1.38 \cdot 10^{-23} \text{ [J/K]} \\ N_{\mathrm{A}} &= 6.022 \cdot 10^{23} \text{ [1/mole]} \\ m_{\mathrm{e}} &= 9.11 \cdot 10^{-31} \text{ [kg]} \\ e &= 1.6 \cdot 10^{-19} \text{ [C]} \end{aligned}$$

Integrals:

$$
\begin{aligned}
\int_0^\infty \frac{x^4 \mathrm{e}^x}{(\mathrm{e}^x - 1)^2} dx &= \frac{4\pi^2}{15} \\
\int_0^1 \frac{x^4 \mathrm{e}^x}{(\mathrm{e}^x - 1)^2} dx &\approx 0.32 \\
\lim_{A \to 0} \int_0^A \frac{x^4 \mathrm{e}^x}{(\mathrm{e}^x - 1)^2} dx &= \frac{A^3}{3} \\
\int_0^\infty \frac{x^3 \mathrm{e}^x}{(\mathrm{e}^x - 1)^2} dx &= 6\zeta(3) \approx 7.2 \\
\int_0^\infty \frac{x^4 \mathrm{e}^x}{(\mathrm{e}^x + 1)^2} dx &= \frac{7\pi^4}{30} \\
\int_0^1 \frac{x^4 \mathrm{e}^x}{(\mathrm{e}^x + 1)^2} dx &\approx 0.042 \\
\lim_{A \to 0} \int_0^A \frac{x^4 \mathrm{e}^x}{(\mathrm{e}^x + 1)^2} dx &= \frac{A^5}{20}
\end{aligned}
$$

Ellipse equation and its area:

$$
\left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 = 1 \quad , \quad A = \pi a b
$$

Trigonometric identities:

$$
\begin{aligned}
&\sin(2\theta) = 2\sin(\theta)\cos(\theta) \\
&\cos(2\theta) = 2\cos^2(\theta) - 1
\end{aligned}
$$