Notes of 141A
Solid State Physics

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目录

vibrations, phonon
conductivity
magnetism, spin
many-body physics, superconductivity

0 Review

0.1 Atoms

$$\hat{\mathbf{H}} = -\frac{1}{2}\nabla^2 - \frac{1}{r} \tag{0.1}$$

0.2 Bonding

–covalent
–ionic
–vdW
–metallic

0.2.1 Covalent

H_2

$$\hat{\mathbf{H}} = -\frac{1}{2}\nabla^2 - \frac{1}{r_A} - \frac{1}{r_B} \tag{0.2}$$

$$\hat{\mathbf{H}}\Psi = E\Psi \tag{0.3}$$

use variational principle

$$\Phi = C_A\Psi_A + C_B\Psi_B \tag{0.4}$$

$$\begin{aligned}\langle H\rangle &= \langle\Phi|\,\hat{\mathbf{H}}\,|\Phi\rangle \\ &= \langle C_A\Psi_A + C_B\Psi_B|\,\hat{\mathbf{H}}\,|C_A\Psi_A + C_B\Psi_B\rangle \\ &= \cdots\end{aligned} \tag{0.5}$$

$$\begin{aligned}E &= \frac{\langle\Phi|\,\hat{\mathbf{H}}\,|\Phi\rangle}{\langle\Phi\rangle\,\Phi} \\ &= \cdots\end{aligned} \tag{0.6}$$

$$\frac{\partial\Phi}{\partial C_A} = 0 \quad \frac{\partial\Phi}{\partial C_B} = 0 \tag{0.7}$$

$$\begin{pmatrix} H_{AA}-E & H_{AB}-ES \\ H_{AB}-ES & H_{BB}-E \end{pmatrix}\begin{pmatrix} C_A \\ C_B \end{pmatrix} = 0 \tag{0.8}$$

0.2.2 vdW Bonds

dipole interaction

$$\mathbf{E}_{dipole} \propto \frac{1}{r^3} \tag{0.9}$$

$$\mathbf{P}_{induced} \propto \mathbf{E} \tag{0.10}$$

thus

$$U_{dipole} \propto \mathbf{E}\cdot\mathbf{P} \propto -\frac{1}{r^6} \tag{0.11}$$

repulsive $\propto \frac{1}{r^1 2}$
L-J potential ...

0.2.3 Ionic Bonding

electropositive atom – low ionization potential (电离能)
electronegative atom – large electron affinity (电子亲和性)
E.g. NaCl
Na – $E_I = 5.1eV$, Cl – $E_A = 3.6eV$
Charge transfer – $-7.9eV$
total $5.1 - 3.6 - 7.9$

$$U_{ij} = \pm\frac{e^2}{4\pi\epsilon + 0 r_{ij}} + \frac{B}{r_{ij}^2} \tag{0.12}$$

0.2.4 Metallic Bonding

Cu, Ag, Au – extended covalent bonds
ion cohesion

1 Crystal Structure

"diamond" crystal
FCC lattice – Cu

1.1 definition

Bravais Lattice

1. infinite set of points so that everything looks the same no matter where you stand
2. set of points defined by $\mathbf{r}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$

primitive cell: smallest periodic space filling volume

E.g. CuO_2 layers
1 dot / unit cell
Wigner Seitz unit cell

symmetry of crystals: mapping that returns original lattice
– translational
– rotational
– inversion
– reflection

bravais 14 lattice
array of descrete points generated by translational operations

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2... \tag{1.1}$$

where $\mathbf{a}_i$ lattice translation vectors

1. triclinic - 2 三方
2. monoclinic - 2
3. orthorhumbic - 4
4. tetragonal - 2
5. cubic - 3

   simple cubic 简单立方

   face-centered cubic / FCC / 面心立方

   – Cu, Ag, Au, Ni, Al (soft metals); NaCl; Diamond, Si, Ge

   body-centered cubic / BCC / 体心立方

   – Fe, V, Ta, Nb, W, Mo, Cr (brittle except Ta)

6. trigonal - 1

7. hexagonal - 1

Index Crystal Planes: Miller Indices
crystals of inert atoms
L-J potential

$$U(r) = ... \tag{1.2}$$

first term: phenomenological repulsive potential to account for Pauli exclusion
second term: attractive potential due to spontaneous induced dipole.

Ionic crystals

$$U_{tot} = N(z\lambda\, \mathrm{e}^{-\frac{q}{\rho}} - \frac{\alpha q^2}{R}) \tag{1.3}$$

z – coordination number of the lattice
$\alpha = \sum_j \frac{(\pm)}{p_{ij}}$ – Madelung Cons.

2 Wave Diffraction and Reciprocal Lattice

Periodicity is important – band gap, diffraction

2.1 reciprocal lattice

for 1D lattice, $\{\mathbf{T}\} = \{ja\hat{\mathbf{x}}\}$.
Suppose $n(x)$ is the elec density
thus $n(x) = n(x+T)$
...

$$n(x) = \sum_j n_j \, \mathrm{e}^{\mathrm{i}g_j x} \tag{2.1}$$

where $g_j = \dfrac{2\pi}{\lambda_j}$
since $\lambda_j = \dfrac{a}{j}$

$$g_j = \frac{2\pi}{a} j \tag{2.2}$$

aka reciprocal lattice vectors.

$$\begin{aligned} &\int_0^a n(x) \, \mathrm{e}^{-g_j' x} \, \mathrm{d}x \\ &\qquad = n_j' a + \sum_{j \neq j'} \int_0^a n_j \, \mathrm{e}^{\frac{2\pi}{a}(j-j')x} \, \mathrm{d}x \qquad (2.3) \\ &\qquad = n_j' a \end{aligned}$$

$$n_j = \frac{1}{a} \int_0^a n(x) \, \mathrm{e}^{-g_j x} \, \mathrm{d}x \tag{2.4}$$

Generalize to 3D

$$n(\mathbf{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} \, \mathrm{e}^{\mathrm{i}\mathbf{G}\cdot\mathbf{r}} \tag{2.5}$$

$$\mathbf{G} = \nu_1 \mathbf{b}_1 + \nu_2 \mathbf{b}_2 + \nu_3 \mathbf{b}_3 \tag{2.6}$$

$$n(\mathbf{r}) = n(\mathbf{r} + \mathbf{T}) \tag{2.7}$$

$$\mathbf{T} = u_1 \mathbf{a}_1 + u_2 \mathbf{a}_2 + u_3 \mathbf{a}_3 \tag{2.8}$$

$$\mathbf{G} \cdot \mathbf{T} = 2\pi n \tag{2.9}$$

2.2 diffraction

Bragg Law ...
diffraction
picture ...

$$\mathbf{E}_T = \mathbf{E}_1 + \mathbf{E}_2 \tag{2.10}$$

$\mathbf{k} = \frac{2\pi}{\lambda}\hat{\mathbf{n}}$, $\mathbf{k}' = \frac{2\pi}{\lambda}\hat{\mathbf{n}'}$

$$\Delta r = \mathbf{r}\cdot\hat{\mathbf{n}} - \mathbf{r}\cdot\hat{\mathbf{n}'} \tag{2.11}$$

$$\Delta\phi = \mathbf{r}\cdot k\hat{\mathbf{n}} - \mathbf{r}\cdot k\hat{\mathbf{n}'} = \mathbf{r}\cdot(\mathbf{k}-\mathbf{k}') \tag{2.12}$$

$$\begin{aligned} I &= |\mathbf{E}_1 + \mathbf{E}_2|^2 \\ &= \left|\int \mathbf{E}\mathrm{d}^3\mathbf{r}\right|^2 \\ &\propto \left|\int n(\mathbf{r})\,\mathrm{e}^{\mathrm{i}\Delta\phi}\,\mathrm{d}^3\mathbf{r}\right|^2 \\ &\propto \left|\int n(\mathbf{r})\,\mathrm{e}^{\mathrm{i}\mathbf{r}\cdot(\mathbf{k}-\mathbf{k}')}\,\mathrm{d}^3\mathbf{r}\right|^2 \end{aligned} \tag{2.13}$$

the amplitude

$$\begin{aligned} F_{k'k} &= \int n(\mathbf{r})\,\mathrm{e}^{\mathrm{i}\mathbf{r}\cdot(\mathbf{k}-\mathbf{k}')}\,\mathrm{d}^3\mathbf{r} \\ &= \int \mathrm{e}^{-\mathrm{i}\mathbf{r}\cdot\mathbf{k}'}\,n(\mathbf{r})\,\mathrm{e}^{\mathrm{i}\mathbf{r}\cdot\mathbf{k}}\,\mathrm{d}^3\mathbf{r} \\ &= \langle k'|\,n(r)\,|k\rangle \end{aligned} \tag{2.14}$$

aka Born approx.

$$n(r) = \sum_G n_G\,\mathrm{e}^{\mathrm{i}\mathbf{G}\cdot\mathbf{r}} \tag{2.15}$$

$$\begin{aligned} F_{k'k} &= \sum_G n_G \int \mathrm{e}^{\mathrm{i}(\mathbf{G}-(\mathbf{k}-\mathbf{k}'))\cdot\mathbf{r}}\,\mathrm{d}^3\mathbf{r} \\ &= \sum_G n_G\delta(\mathbf{G}-(\mathbf{k}-\mathbf{k}')) \end{aligned} \tag{2.16}$$

Xray spot – $\mathbf{G} = \mathbf{k} - \mathbf{k}'$

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$$\mathbf{k}' - \mathbf{k} = \mathbf{G} \tag{2.17}$$

$$\mathbf{k} \cdot \left(\frac{1}{2}\mathbf{G}\right) = \left|\frac{1}{2}\mathbf{G}\right|^2 \tag{2.18}$$

4 Phonons I. Crystal Vibrations

Phonons: Quantized lattice vibrations

$$\omega = 2\sqrt{\frac{C}{m}}\left|\sin\frac{1}{2}ka\right| \tag{4.1}$$

– phonon dispersion relation
zeros: $\frac{1}{2}ka = n\pi \Rightarrow k = \frac{2\pi n}{a}$

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photo ..

$$u_s^k(t) = u_0 \, \mathrm{e}^{\mathrm{i}(ksa - \omega t)} \tag{4.2}$$

$$\omega(k) = 2\sqrt{\frac{c}{m}} \left| \sin \frac{1}{2} ka \right| \tag{4.3}$$

$$G = \frac{2\pi}{a} P, \quad P \in \mathbb{Z} \tag{4.4}$$

$$u_s^{k+G} = \tag{4.5}$$

ω vs k – $E = \hbar\omega$ vs $p = \hbar k$

limit

1. long wavelength limit

$\lambda \to \infty$, $k \to 0$

$$\omega(k) \to 2\sqrt{\frac{c}{m}} \left| \frac{1}{2} ka \right| \propto k \tag{4.6}$$

acoustic

$$v_p = \frac{\omega}{k} = \tag{4.7}$$

$$v_g = \frac{\mathrm{d}\omega}{\mathrm{d}k} = \tag{4.8}$$

2. short wl limit

$k \to \dfrac{\pi}{a}$

$$v_g = 0 \tag{4.9}$$

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Phonon scattering

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5 Phonons II. Thermal Properties

5.1 Phonon Heat Capacity

$$U(T) = \sum_{k,p} \langle n_{k,p} \rangle_T \, \hbar\omega_{k,p} \tag{5.1}$$

$$\begin{aligned} \langle n \rangle &= \frac{\sum_{\mathrm{n=0}}^{\infty} n \, \mathrm{e}^{-n\hbar\omega/\,\mathrm{k_B}\,T}}{\sum_{\mathrm{n=0}}^{\infty} \mathrm{e}^{-n\hbar\omega/\,\mathrm{k_B}\,T}} \quad \text{(Bose-Einstein Distr.)} \\ &= ... \\ &= \frac{1}{\mathrm{e}^{\hbar\omega/\,\mathrm{k_B}\,T} - 1} \end{aligned} \tag{5.2}$$

$$U(T) = \int_0^{\omega_{max}} \hbar\omega f(\omega) \tag{5.3}$$

High temp, Debye model, $T >> \theta_D$

$$C = 3Nk_B \tag{5.4}$$

Low temp, Einstein model, $T << \theta_D$

$$C(T) = ... = \frac{12\pi^4 N k_B}{5} \left(\frac{T}{\theta_D} \right)^3 \tag{5.5}$$

$\hbar\omega_{max} = k_B T$, $k_{max} = \dfrac{k_B T}{\hbar v}$

fraction of modes excited $= \left(\dfrac{k_{max}}{k_D} \right)^3$

$$\#\text{ of modes excited} = 3N\left(\frac{k_{max}}{k_D}\right)^3$$

$$\begin{aligned} U(T) &= (\#\text{ of modes excited})\langle E\rangle_{mode} \\ &= 3N\left(\frac{k_{max}}{k_D}\right)^3 k_B T \\ &= 3N\left(\frac{T}{\theta_D}\right)^3 k_B T \\ &= \end{aligned} \tag{5.6}$$

$$C(T) = ... \tag{5.7}$$

5.2 Anharmonic Crystal Interactions / Thermal Expansion

true potential of phonons are not hyperbolic but L-J-like

$$U = Cx^2 - gx^3 + ... \tag{5.8}$$

$$\langle x\rangle_T = \frac{\int_x x P_T(x)\mathrm{d}x}{\int_x P_T(x)\mathrm{d}x} \tag{5.9}$$

$$P_T(x) \propto \mathrm{e}^{-U(x)/k_B T} \tag{5.10}$$

$$\begin{aligned} \langle x\rangle_T &= \frac{\int_x x\,\mathrm{e}^{-U(x)/k_B T}\,\mathrm{d}x}{\int_x \mathrm{e}^{-U(x)/k_B T}\,\mathrm{d}x} \\ &= ... \\ &= \frac{3g}{4C^2} k_B T \end{aligned} \tag{5.11}$$

5.3 Thermal Conductivity

energy flux

$$j = \frac{\text{enrgy}}{\text{time}\cdot\text{area}} = \frac{P}{A} = -K\frac{\mathrm{d}T}{\mathrm{d}x} \tag{5.12}$$

K – thermal conductivity
similar to $j = \sigma E$

$$j = \rho v \tag{5.13}$$

10/2 ankit

5.4 Sommerfeld Model

3D

$$N = \frac{4}{3}\pi k^3 \left(\frac{L}{2\pi}\right)^3 = ... \tag{5.14}$$

$$D(\varepsilon) = ... \propto \varepsilon^{1/2} \tag{5.15}$$

2D

$$N = \pi k^2 \left(\frac{L}{2\pi}\right)^2 = ... \tag{5.16}$$

$$D(\varepsilon) = ... \propto 1 \tag{5.17}$$

$$1DN = 2k\left(\frac{L}{2\pi}\right) = ... \tag{5.18}$$

$$D(\varepsilon) = ... \propto \varepsilon^{-1/2} \tag{5.19}$$

5.5 Heat Capacity

$$U = \int_0^\infty \mathrm{d}\varepsilon D(\varepsilon) f(\varepsilon) \varepsilon \tag{5.20}$$

$$N = \int_0^\infty \mathrm{d}\varepsilon D(\varepsilon) f(\varepsilon) \tag{5.21}$$

In metals, $T << T_F$

Use Sommerfeld expansion

Consider integral of the form

$$\int_{-\infty}^\infty H(\varepsilon) f(\varepsilon) \mathrm{d}\varepsilon \tag{5.22}$$

$$K(\varepsilon) = \int_{-\infty}^\varepsilon H(\varepsilon') \mathrm{d}\varepsilon' \tag{5.23}$$

$$H = \frac{\mathrm{d}K}{\mathrm{d}\varepsilon} \tag{5.24}$$

$$\int_{-\infty}^\infty H(\varepsilon) f(\varepsilon) \mathrm{d}\varepsilon = \int_{-\infty}^\infty K(\varepsilon)(-\frac{\mathrm{d}f}{\mathrm{d}\varepsilon}) \mathrm{d}\varepsilon \tag{5.25}$$

$$K(\varepsilon) = K(\mu) + \sum_{n=1}^\infty \frac{1}{n!} \frac{\mathrm{d}^n K}{\mathrm{d}\varepsilon^n} (\varepsilon - \mu)^n \tag{5.26}$$

$$\int_{-\infty}^{\infty} H(\varepsilon)f(\varepsilon)\mathrm{d}\varepsilon = \int_{-\infty}^{\infty} K(\mu)(-\frac{\mathrm{d}f}{\mathrm{d}\varepsilon})\mathrm{d}\varepsilon + \sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\frac{1}{n!}\frac{\mathrm{d}^n K}{\mathrm{d}\varepsilon^n}(\varepsilon-\mu)^n\left(-\frac{\mathrm{d}f}{\mathrm{d}\varepsilon}\right)\mathrm{d}\varepsilon$$
$$= K(\mu) + ... \tag{5.27}$$
$$= \int_{-\infty}^{\mu} H(\varepsilon)\mathrm{d}\varepsilon + \frac{\pi^2}{6}(k_B T)^2 H(\mu) + \mathcal{O}((K_B T)^4)$$

thus

$$U = ... \tag{5.28}$$

$$N = ... \tag{5.29}$$

6 Free Electron Fermi Gas

6.1 Electrical Conductivity and Ohm's Law

$$\hbar\left(\frac{\mathrm{d}}{\mathrm{d}t} + \frac{1}{\tau}\right)\mathbf{k} = -e\mathbf{E} \tag{6.1}$$

6.2 Motion in Magnetic Fields

$\mathbf{B} = B\,\hat{\mathbf{k}}$, $\mathbf{v} = \dfrac{\hbar\mathbf{k}}{m}$

$$m\left(\frac{\mathrm{d}}{\mathrm{d}t} + \frac{1}{\tau}\right)\mathbf{v} = -e\left(\mathbf{E} + \frac{\mathbf{v}\times\mathbf{B}}{c}\right) \tag{6.2}$$

...

$$\begin{pmatrix} J_x \\ J_y \end{pmatrix} = \boldsymbol{\sigma}\begin{pmatrix} E_x \\ E_y \end{pmatrix} \tag{6.3}$$

$J_x = n(-e)v_x$

$$\boldsymbol{\sigma} = \frac{\sigma_{DC}}{1+\omega_0^2\tau^2}\begin{pmatrix} 1 & -\omega_0\tau \\ \omega_0\tau & 1 \end{pmatrix} \tag{6.4}$$

$\sigma_{DC} = \dfrac{ne^2\tau}{m}$

$$\boldsymbol{\rho} = \boldsymbol{\sigma}^{-1} = \frac{1}{\sigma_{DC}}\begin{pmatrix} 1 & \omega_0\tau \\ \omega_0\tau & 1 \end{pmatrix} \tag{6.5}$$

6.2.1 Hall Effect

6.3 AC Conductivity

$\mathbf{E} \sim \mathbf{E}_0\,\mathrm{e}^{I\omega t}$, $\omega >> 1/\tau$, $\omega_c = \dfrac{eB}{mc}$, $\mathbf{B} = B\,\hat{\mathbf{k}}$

$$m\left(\frac{\mathrm{d}}{\mathrm{d}t} + \frac{1}{\tau}\right)\mathbf{v} = -e\left(\mathbf{E} + \frac{\mathbf{v}\times\mathbf{B}}{c}\right) \tag{6.6}$$

assume $\mathbf{v} = \mathbf{v}_0\, \mathrm{e}^{\mathrm{i}\omega t}$

...

$$\begin{pmatrix} J_x \\ J_y \end{pmatrix} = \boldsymbol{\sigma} \begin{pmatrix} E_x \\ E_y \end{pmatrix} \tag{6.7}$$

$$\begin{aligned} \sigma_{xx} = \sigma_{yy} &= \frac{\omega_p^2 \tau (1 - \mathrm{i}\omega\tau)}{4\pi[(1 - \mathrm{i}\omega\tau)^2 + (\omega_c\tau)^2]} \\ \sigma_{xy} = -\sigma_{yx} &= \frac{\omega_p^2 \omega_c \tau^2}{4\pi[(1 - \mathrm{i}\omega\tau)^2 + (\omega_c\tau)^2]} \end{aligned} \tag{6.8}$$

$$\omega_p = \frac{4\pi n e^2}{m} \tag{6.9}$$

$$\boldsymbol{\sigma} = \frac{\omega_p^2}{4\pi\omega} \begin{pmatrix} \mathrm{i} & \omega_c/\omega \\ -\omega_c/\omega & \mathrm{i} \end{pmatrix} \tag{6.10}$$

6.4 Complex Dielectric Function

$$\begin{aligned} \boldsymbol{\nabla} \cdot \mathbf{D} &= 4\pi\rho_f \\ \boldsymbol{\nabla} \cdot \mathbf{B} &= 0 \\ \boldsymbol{\nabla} \times \mathbf{E} + \frac{1}{c}\frac{\partial \mathbf{H}}{\partial t} &= 0 \\ \boldsymbol{\nabla} \times \mathbf{H} - \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t} &= \frac{4\pi}{c}\mathbf{J}_f \end{aligned} \tag{6.11}$$

$$\boldsymbol{\nabla} \cdot \mathbf{J} = -\frac{\partial \rho}{\partial t} \tag{6.12}$$