

Solid State Physics Homework

Chapter3 No.1, Due on Apr 1st 2022, Friday

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Problem1 A&M Chapter12.2(a)

One can rewrite the energy

$$\varepsilon(\mathbf{k}) = \frac{\hbar^2}{2} \langle \mathbf{k} | \mathbf{M}^{-1} | \mathbf{k} \rangle \quad (1)$$

by taking the minimum energy to be zero and the corresponding wave vector at origin, which doesn't make changes. For calculating cyclotron effective mass, one can get

$$\sum_{a,b=x,y} \mathbf{M}^{-1}_{ab} k_a k_b + 2k_z \sum_{c=x,y} \mathbf{M}^{-1}_{cz} k_c = \frac{2\varepsilon}{\hbar^2} - \mathbf{M}^{-1}_{zz} k_z^2 \quad (2)$$

where ε and k_z should be constant. Make a translation transformation to reset the origin in the k_z plane, then one can simplify (2) as

$$\mathbf{M}^{-1}_{xx} k_x'^2 + \mathbf{M}^{-1}_{yy} k_y'^2 + 2\mathbf{M}^{-1}_{xy} k_x' k_y' = \frac{2\varepsilon}{\hbar^2} - C k_z^2 \quad (3)$$

Next, make a rotation transformation

$$A k_x''^2 + B k_y''^2 = \frac{2\varepsilon}{\hbar^2} - C k_z^2 \quad (4)$$

Therefore

$$A(\varepsilon, k_z) = \pi \frac{2\varepsilon/\hbar^2 - C k_z^2}{\sqrt{AB}}, \quad m^* = \frac{\hbar^2}{2\pi} \frac{\partial A(\varepsilon, k_z)}{\partial \varepsilon} = \frac{1}{\sqrt{AB}} \quad (5)$$

A, B can be simply written down by combining (3)(4). Using the linear algebra formula, one can prove

$$m^* = \frac{1}{\sqrt{AB}} = \left(\frac{|\mathbf{M}|}{\mathbf{M}_{zz}} \right)^{\frac{1}{2}} \quad (6)$$

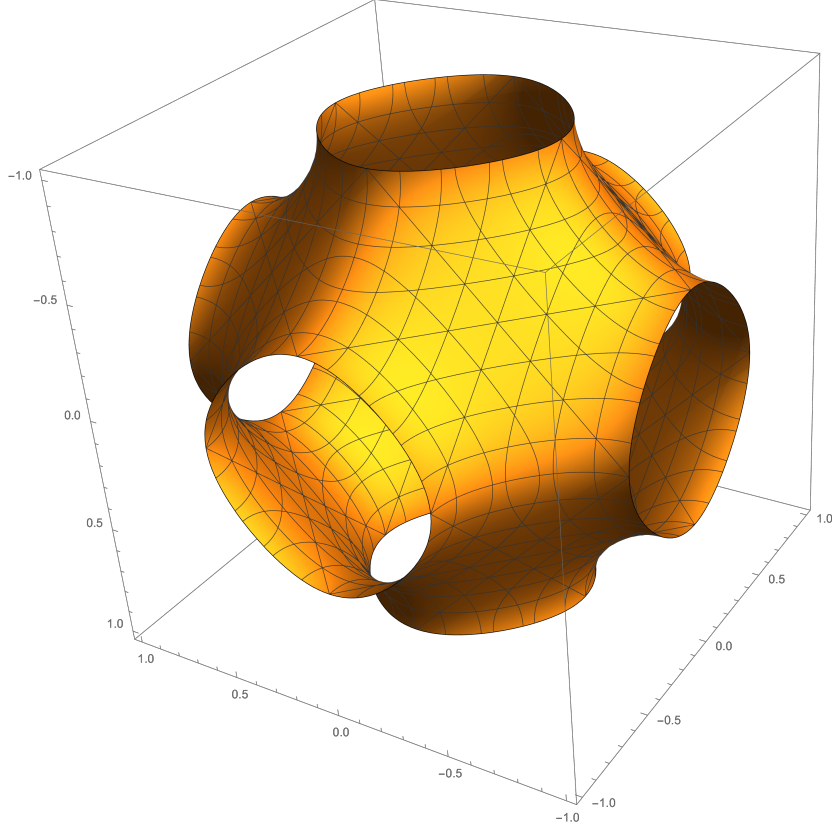
Problem2 Cyclotron effective mass

The tight-binding energy band of the simple cubic lattice is

$$\varepsilon(\mathbf{k}) = \varepsilon_s - J_0 - 2J_1(\cos k_x a + \cos k_y a + \cos k_z a) \quad (7)$$

For calculating cyclotron effective mass, the route in the k_z plane is determined by

$$\cos k_x a + \cos k_y a = \text{const} \quad (8)$$



Contour surface of energy in First Brillouin Zone: $\varepsilon = \varepsilon_s - J_0$. The unit coordinate is π/a

The area enclosed by the route(8) is $A(\varepsilon, k_z)$ (which is in the figure), and the effective mass is

$$m^* = \frac{\hbar^2}{2\pi} \frac{\partial A(\varepsilon, k_z)}{\partial \varepsilon} \quad (9)$$

Problem3 A&M Chapter14.1(b)

According to the definition of the reciprocal lattice vector, the pattern density in ΔA is

$$\sigma = \left(\frac{L}{2\pi}\right)^2 \quad (10)$$

Where L is the length of the cubic. So the number of energy states in the area is

$$N = 2\sigma\Delta A = 2\left(\frac{L}{2\pi}\right)^2 \frac{2\pi eH}{\hbar c} = \frac{2e}{\hbar c} H L^2 \quad (11)$$

Which is concisely equal to the degeneracy. Note the former factor 2 is for spin degeneracy.

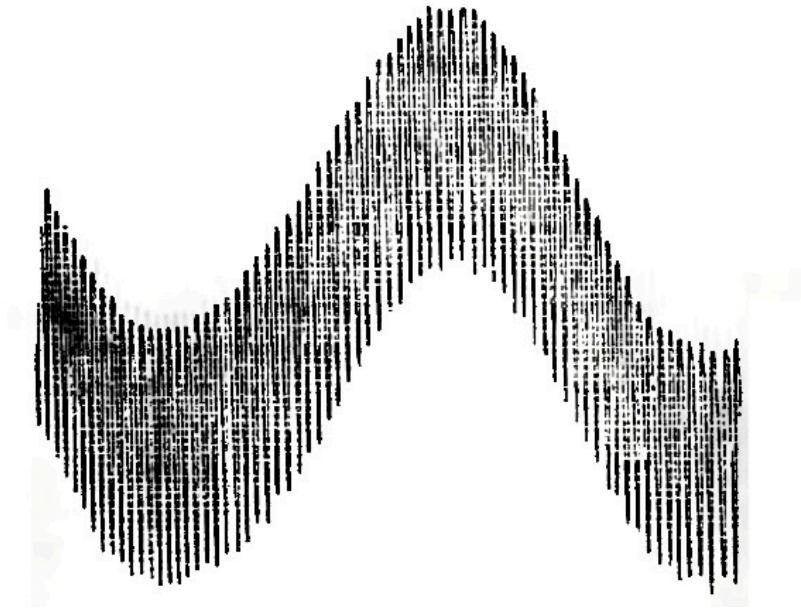
Problem4 A&M Chapter14.2

From the fundamental relation

$$\Delta\left(\frac{1}{H}\right) = \frac{2\pi e}{\hbar c} \frac{1}{A_e} \quad (12)$$

one can get the relation between the area of extremal orbits and its oscillation cycle

$$A_e \Delta T_A = \text{const} \quad (13)$$



De Haas-van Alphen oscillations in silver

For the oscillation cycle in the figure, one can find

$$0.5T_l \approx 30T_s \quad (14)$$

So the ratio of the area of two extremal orbits is

$$\frac{A_s}{A_l} \approx 60 \quad (15)$$

Solid State Physics Homework

Chapter3 No.8, Due on May 13th 2022, Friday

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Problem1 A&M Chapter13.2

According to (13.24) and (13.25), the conductivity tensor is a sum of contributions from each band

$$\sigma = \sum_n e^2 \int \frac{d\mathbf{k}}{4\pi^3} \tau_n(\varepsilon_n(\mathbf{k})) \mathbf{v}_n(\mathbf{k}) \mathbf{v}_n(\mathbf{k}) \left(-\frac{\partial f}{\partial \varepsilon} \right)_{\varepsilon=\varepsilon_n(\mathbf{k})} \quad (1)$$

one can simplify it by taking the anisotropy and irrelevant bands of crystals of cubic symmetry into consideration

$$\sigma_{\mu\nu} = e^2 \int \frac{d\mathbf{k}}{4\pi^3} \tau(\varepsilon_{\mathbf{k}}) \mathbf{v}_\mu(\mathbf{k}) \mathbf{v}_\nu(\mathbf{k}) \left(-\frac{\partial f}{\partial \varepsilon_{\mathbf{k}}} \right) \quad (2)$$

$$\sigma_{\mu\nu} = \sigma \delta_{\mu\nu} \quad (3)$$

i.e. the conductivity can be described as a vector. Divide the momentum space into equal energy areas

$$d\mathbf{k} = dS dk_\perp = dS \frac{d\varepsilon_{\mathbf{k}}}{|\nabla_{\mathbf{k}} \varepsilon_{\mathbf{k}}|} = \frac{dS}{\hbar |\mathbf{v}(\mathbf{k})|} d\varepsilon_{\mathbf{k}} \quad (4)$$

when $T = 0$, use the approximation

$$\left(-\frac{\partial f}{\partial \varepsilon_{\mathbf{k}}} \right) = \delta(\varepsilon_{\mathbf{k}} - \varepsilon_F) \quad (5)$$

then one can get the result below

$$\begin{aligned} \sigma_{\mu\nu} &= \frac{e^2}{4\pi^3 \hbar} \int \tau(\varepsilon_F) \frac{\mathbf{v}_\mu(\mathbf{k}) \mathbf{v}_\nu(\mathbf{k})}{|\mathbf{v}(\mathbf{k})|} dS_F, \\ \sigma &= \frac{1}{3} (\sigma_{xx} + \sigma_{yy} + \sigma_{zz}) \\ &= \frac{e^2}{12\pi^3 \hbar} \int \tau(\varepsilon_F) |\mathbf{v}(\mathbf{k})| dS_F \\ &= \frac{e^2}{12\pi^3 \hbar} \tau(\varepsilon_F) \bar{v} S_F \end{aligned} \quad (6)$$

which is same as (13.71) and (13.72). And it is easy to write down the result in free electron limit

$$\sigma = \frac{ne^2\tau(\varepsilon_F)}{m^*} \quad (7)$$

and it is precisely the Drude result, by replacing the electron mass with effective mass, and the relaxation-time is qualified by the Fermi surface.

Problem2 A&M Chapter13.5

For a metal subject simultaneously to a nonzero electric field and nonzero thermal gradient, the heat production per unit volume is given by

$$\frac{dq}{dt} = \frac{du}{dt} - \mu \frac{dn}{dt} = -\nabla \cdot \mathbf{j}^\epsilon + \mathbf{E} \cdot \mathbf{j} + \mu \nabla \cdot \mathbf{j}^n \quad (8)$$

where $\mathbf{j} = -e\mathbf{j}^n$ is the charge current density, \mathbf{j}^ϵ is the energy current density. substitute (13.40) into (8), one can get

$$\frac{dq}{dt} = -\nabla \cdot \mathbf{j}^q + \varepsilon \cdot \mathbf{j} \quad (9)$$

where $\varepsilon = \mathbf{E} + \frac{1}{e}\nabla\mu$ is the field associated with the electrochemical potential. And it is same as (13.83). Use (13.45) and the relations in A&M and take the symmetry into consideration, one can get

$$\mathbf{j} = L^{11}\varepsilon - L^{12}\nabla T, \quad \mathbf{j}^q = L^{21}\varepsilon - L^{22}\nabla T \quad (10)$$

$$\frac{1}{\rho} = L^{11}, \quad K = L^{22} - \frac{L^{21}L^{12}}{L^{11}}, \quad Q = \frac{L^{12}}{L^{11}} \quad (11)$$

substitute (10) and (11) into (9), one can get

$$\begin{aligned} \frac{dq}{dt} &= -\nabla \cdot \mathbf{j}^q + \varepsilon \cdot \mathbf{j} \\ &= \rho \mathbf{j}^2 + \nabla K \cdot \nabla T - T \nabla Q \cdot \mathbf{j} \\ &= \rho \mathbf{j}^2 + \frac{dK}{dT} (\nabla T)^2 - T \frac{dQ}{dT} \nabla T \cdot \mathbf{j} \end{aligned}$$

which is precisely (13.84).

For crude estimate in Problem3, Chapter1, the coefficient is(use (1.7))

$$A_c = \frac{ne\rho\tau}{m} \frac{d\varepsilon}{dT} = \frac{1}{e} \frac{d\varepsilon}{dT} = \frac{3k_B}{2e} \quad (12)$$

and for free quantum-mechanical electrons, the coefficient is(use (2.94))

$$Q = -\frac{\pi^2}{6} \frac{k_B^2 T}{e\varepsilon_F}, \quad A_q = \frac{\pi^2}{6} \frac{k_B^2 T}{e\varepsilon_F} \quad (13)$$

So the ratio is about

$$\frac{A_q}{A_c} = \frac{2\pi^2}{3} \frac{k_B T}{\epsilon_F} \quad (14)$$

At room temperature, and let $\epsilon_F = 5\text{eV}$, one can find the numerical value of this ratio to be on the order of 10^{-2} .

Problem3 A&M Chapter16.3

(a)

According to the Boltzmann equation and the relaxation-time approximation

$$e\hbar^{-1}(\mathbf{E} + \mathbf{v}(\mathbf{k}) \times \mathbf{B}) \cdot \nabla_{\mathbf{k}} g(\mathbf{k}) = \frac{g(\mathbf{k}) - g^0(\mathbf{k})}{\tau(\mathbf{k})} \quad (15)$$

because the energy band is $\varepsilon(\mathbf{k}) = \frac{\hbar^2 k^2}{2m^*}$, the distribution must be qualified by symmetry

$$g(\mathbf{k}) = g^0(\varepsilon) + \mathbf{a}(\varepsilon) \cdot \mathbf{k} \quad (16)$$

Substitute (16) and the energy band into (15), one can get

$$\hbar \left(\frac{\partial g^0}{\partial \varepsilon} \right) \mathbf{E} \cdot \mathbf{k} + (\mathbf{k} \times \mathbf{B}) \cdot \mathbf{a}(\varepsilon) = \frac{m^* \mathbf{a}(\varepsilon)}{e\tau(\mathbf{k})} \cdot \mathbf{k} \quad (17)$$

(b)

one can simplify (15)

$$\frac{e\hbar}{m^*} \tau(\mathbf{k}) \left(\frac{\partial g^0}{\partial \varepsilon} \right) \mathbf{E} = \frac{e\tau(\mathbf{k})}{m^*} \mathbf{a}(\varepsilon) \times \mathbf{B} + \mathbf{a}(\varepsilon) = \mathbf{T} \mathbf{a}(\varepsilon) \quad (18)$$

while \mathbf{T} is a tensor. So the conductivity is

$$\sigma = e^2 \int \frac{d\mathbf{k}}{4\pi^3} \tau(\varepsilon) \left(-\frac{\partial g^0}{\partial \varepsilon} \right) [\mathbf{v}_\mu \mathbf{v}_\nu] \mathbf{T}^{-1} \quad (19)$$

and it is simple to proof the result is equal to (13.69) and (13.70) at free electron band.

Problem4 A&M Chapter16.4

(a)

According to the Boltzmann equation and the impurity scattering approximation

$$e\hbar^{-1} \mathbf{E} \cdot \nabla_{\mathbf{k}} g(\mathbf{k}) = - \int \frac{d\mathbf{k}'}{(2\pi)^3} W_{\mathbf{k},\mathbf{k}'} [g(\mathbf{k}) - g(\mathbf{k}')] \quad (20)$$

and substitute the distribution form

$$g(\mathbf{k}) = f(\varepsilon) + \delta g(\mathbf{k}) \quad (21)$$

into (20), one can find

$$e \left(-\frac{\partial f}{\partial \varepsilon} \right) \mathbf{v}(\mathbf{k}) \cdot \mathbf{E} = \int \frac{d\mathbf{k}}{(2\pi)^3} W_{\mathbf{k},\mathbf{k}'} [\delta g(\mathbf{k}) - \delta g(\mathbf{k}')] \quad (22)$$

Define

$$\mathbf{v}(\mathbf{k}) = \int \frac{d\mathbf{k}}{(2\pi)^3} W_{\mathbf{k},\mathbf{k}'} [u(\mathbf{k}) - u(\mathbf{k}')] \quad (23)$$

$$g(\mathbf{k}) = e \left(-\frac{\partial f}{\partial \varepsilon} \right) u(\mathbf{k}) \cdot \mathbf{E} \quad (24)$$

then the conductivity should be

$$\sigma = e^2 \int \frac{d\mathbf{k}}{4\pi^3} \left(-\frac{\partial f}{\partial \varepsilon} \right) \mathbf{v}(\mathbf{k}) \mathbf{u}(\mathbf{k}) \quad (25)$$

which are same as (16.37) and (16.38).

(b)

it is easy to prove

$$\begin{aligned} \{\alpha, \gamma\} &= e^2 \int \frac{d\mathbf{k}}{4\pi^3} \left(-\frac{\partial f}{\partial \varepsilon} \right) \alpha(\mathbf{k}) \int \frac{d\mathbf{k}'}{(2\pi)^3} W_{\mathbf{k},\mathbf{k}'} [\gamma(\mathbf{k}) - \gamma(\mathbf{k}')] \\ &= e^2 \int \int \frac{d\mathbf{k}}{4\pi^3} \frac{d\mathbf{k}'}{(2\pi)^3} \left(-\frac{\partial f}{\partial \varepsilon} \right) W_{\mathbf{k},\mathbf{k}'} [\alpha(\mathbf{k})\gamma(\mathbf{k}) - \alpha(\mathbf{k})\gamma(\mathbf{k}')] \\ &= e^2 \int \int \frac{d\mathbf{k}}{4\pi^3} \frac{d\mathbf{k}'}{(2\pi)^3} \left(-\frac{\partial f}{\partial \varepsilon} \right) W_{\mathbf{k},\mathbf{k}'} [\alpha(\mathbf{k})\gamma(\mathbf{k}) - \alpha(\mathbf{k}')\gamma(\mathbf{k})] \\ &= \{\gamma, \alpha\} \end{aligned}$$

(c)

Obviously $\{\alpha, \alpha\} \geq 0$. Then

$$\begin{aligned} \{\alpha + \lambda\gamma, \alpha + \lambda\gamma\} &= \{\alpha, \alpha\} + 2\lambda\{\alpha, \gamma\} + \lambda^2\{\gamma, \gamma\} \\ &= \{\gamma, \gamma\} \left(\lambda + \frac{\{\alpha, \gamma\}}{\{\gamma, \gamma\}} \right)^2 + \{\alpha, \alpha\} - \frac{\{\alpha, \gamma\}^2}{\{\gamma, \gamma\}} \\ &\geq 0 \end{aligned}$$

let $\lambda = -\{\alpha, \gamma\}/\{\gamma, \gamma\}$, then one can get the result

$$\{\alpha, \alpha\} \geq \frac{\{\alpha, \gamma\}^2}{\{\gamma, \gamma\}} \quad (26)$$

(d)

Let $\alpha = u_x$ in (26), then

$$\begin{aligned}
\sigma_{xx} &= \{u_x, u_x\} \\
&\geq \frac{\{u_x, \gamma\}^2}{\{\gamma, \gamma\}} \\
&= \frac{(v_x, \gamma)^2}{\{\gamma, \gamma\}} \\
&= \frac{e^2 [\int \frac{d\mathbf{k}}{4\pi^3} \left(-\frac{\partial f}{\partial \varepsilon}\right) v_x(\mathbf{k}) \gamma(\mathbf{k})]^2}{\int \frac{d\mathbf{k}}{4\pi^3} \left(-\frac{\partial f}{\partial \varepsilon}\right) \gamma(\mathbf{k}) \int \frac{d\mathbf{k}'}{(2\pi)^3} W_{\mathbf{k}, \mathbf{k}'} [\gamma(\mathbf{k}) - \gamma(\mathbf{k}')] }
\end{aligned}$$

(e)

One can define

$$\sigma = \{u, u\}_W = \{u, u_1\}_{W1} = \{u, u_2\}_{W2} \quad (27)$$

$$\sigma_1 = \{u_1, u_1\}_{W1}, \quad \sigma_2 = \{u_2, u_2\}_{W2} \quad (28)$$

so

$$\sigma^2 = \{u, u_1\}_{W1} \{u, u_2\}_{W2} \leq \sqrt{\sigma_1 \sigma_2 \{u, u\}_{W1} \{u, u\}_{W2}} \leq \sqrt{\sigma_1 \sigma_2} \sigma / 2 \quad (29)$$

$$2\sigma = \{u, u_1\}_{W1} + \{u, u_2\}_{W2} \geq (\sigma_1 + \sigma_2) / 2 \quad (30)$$

using (29) and (30) one can derive

$$\frac{1}{\sigma} \geq \frac{1}{\sigma_1} + \frac{1}{\sigma_2} \quad (31)$$