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Solutions

Solutions for Chap. 1

1.1:

Point lattice: Set of lattice vectors $\boldsymbol{R_n} = \sum_{i=1}^{d} n_i \boldsymbol{a}_i\,,\ n_i$ integer, $\boldsymbol{a}_i$ linear independent (d dimension of the system)

Reciprocal lattice: $\boldsymbol{G_m} = \sum_{j=1}^{d} m_j \boldsymbol{b}_j\,,\ m_j$ integer, $\boldsymbol{b}_j$ linear independent, and $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$

Wigner–Seitz cell: Contains all points which are closer to a given $\boldsymbol{R_n}$ Than to any other $\boldsymbol{R}_{n'} \neq \boldsymbol{R}_n$

(First) *Brillouin zone*: Wigner–Seitz cell of the reciprocal lattice

$d = 2$, *square lattice*: $\boldsymbol{a}_1 = a(1,0)\,, \quad \boldsymbol{a}_2 = a(0,1)$
$\rightarrow \boldsymbol{b}_1 = 2\pi/a(1,0)\,, \boldsymbol{b}_2 = 2\pi/a(0,1)$

$d = 3$, *simple cubic* (sc), *body centered cubic* (bcc), *face centered cubic* (fcc)

sc: $\boldsymbol{a}_1 = a(1,0,0)\,, \quad \boldsymbol{a}_2 = a(0,1,0)\,, \quad \boldsymbol{a}_3 = a(0,0,1)$
$\rightarrow \boldsymbol{b}_1 = 2\pi/a(1,0,0)\,, \quad \boldsymbol{b}_2 = 2\pi/a(0,1,0)\,, \quad \boldsymbol{b}_3 = 2\pi/a(0,0,1)$

bcc: $\boldsymbol{a}_1 = a/2(1,1,-1)\,, \quad \boldsymbol{a}_2 = a/2(1,-1,1)\,, \quad \boldsymbol{a}_3 = a/2(-1,1,1)$
$\rightarrow \boldsymbol{b}_1 = 2\pi/a(1,1,0)\,, \quad \boldsymbol{b}_2 = 2\pi/a(1,0,1)\,, \quad \boldsymbol{b}_3 = 2\pi/a(0,1,1)$

fcc: $\boldsymbol{a}_1 = a/2(0,1,1)\,, \quad \boldsymbol{a}_2 = a/2(1,0,1)\,, \quad \boldsymbol{a}_3 = a/2(1,1,0)$
$\rightarrow \boldsymbol{b}_1 = 2\pi/a(-1,1,1)\,, \boldsymbol{b}_2 = 2\pi/a(1,-1,1)\,, \boldsymbol{b}_3 = 2\pi/a(1,1,-1)$

1.2: Create Fibonacci sequence by replacing $LS \rightarrow L$ and $S \rightarrow L$ [21]:

LS
LSL
$LSLLS$
$LSLLSLSL$
$LSLLSLSLLSLLS$
$LSLLSLSLLSLLSLSLLSLSL$ not periodic

Replacing $LS \to L'$ and $L \to S'$ in the last line gives the configuration of the second but last line (self-similarity or fractality). For the Fourier transform see [35].

1.3: Given two vectors $\boldsymbol{a}_1, \boldsymbol{a}_2$, with $|\boldsymbol{a}_1| = a_1$, $|\boldsymbol{a}_2| = a_2$, and $\boldsymbol{a}_1 \cdot \boldsymbol{a}_2 = a_1 a_2 \cos\alpha$, spanning a plane. The following five cases can be distinguished:

$$\begin{aligned} a_1 = a_2, \quad & \alpha = \pi/2 \quad \textit{square} \\ & \alpha = \pi/3 \quad \textit{triangular} \text{ or } \textit{hexagonal} \\ & \alpha \neq \pi/2, \pi/3 \\ a_1 \neq a_2, \quad & \alpha = \pi/2 \quad \textit{rectangular} \\ & \alpha \neq \pi/2 \end{aligned}$$

1.4: $T_{\boldsymbol{R_n}}$ is the translation operator. It acts on a function according to

$$T_{\boldsymbol{R_n}} \phi(\boldsymbol{r}) = \phi(\boldsymbol{r} + \boldsymbol{R_n})$$

and commutes with the system Hamiltonian, $[T_{\boldsymbol{R_n}}, H] = 0$. Therefore, there exist simultaneous eigenfunctions of H and $T_{\boldsymbol{R_n}}$ with the property

$$T_{\boldsymbol{R_n}} \phi_{\boldsymbol{k}}(\boldsymbol{r}) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R_n}} \phi_{\boldsymbol{k}}(\boldsymbol{r})$$

i.e. the wave eigenfunctions in different Wigner–Seitz cells differ only by a phase factor with wave vector $\boldsymbol{k}$ from the first Brillouin zone.

1.5: Count nearest neighbors (n.n.) and spheres per cube:

$$\begin{aligned} \text{sc} \quad & 6 \text{ n.n.}, 1 \text{ sphere} \to \frac{4\pi}{3}\left(\frac{a}{2}\right)^3 \Big/ a^3 = \frac{\pi}{6} = 0.52, \\ \text{bcc} \quad & 8 \text{ n.n.}, 2 \text{ spheres} \to 2\frac{4\pi}{3}\left(\frac{\sqrt{3}a}{4}\right)^3 \Big/ a^3 = \frac{\sqrt{3}\pi}{8} = 0.68, \\ \text{fcc} \quad & 12 \text{ n.n.}, 4 \text{ spheres} \to 4\frac{4\pi}{3}\left(\frac{a}{2\sqrt{2}}\right)^3 \Big/ a^3 = \frac{\pi}{3\sqrt{2}} = 0.74, \\ \text{diamond} \quad & 4 \text{ n.n.}, 8 \text{ spheres} \to 8\frac{4\pi}{3}\left(\frac{\sqrt{3}a}{8}\right)^3 \Big/ a^3 = \frac{\sqrt{3}\pi}{16} = 0.34. \end{aligned}$$

1.6: A mass density $n(\boldsymbol{r}) = \delta(\boldsymbol{r} - \boldsymbol{r}_i)$ and using $\delta(\boldsymbol{r} - \boldsymbol{r}_i) = \sum_{\boldsymbol{q}} \exp(\mathrm{i}\boldsymbol{q} \cdot (\boldsymbol{r} - \boldsymbol{r}_i))/V$ gives for the scattering amplitude

$$F(\boldsymbol{k}, \boldsymbol{k}') = F(\boldsymbol{k} - \boldsymbol{k}') = \sum_{i,\boldsymbol{q}} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_i} \frac{1}{V} \int_V \mathrm{e}^{\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}'+\boldsymbol{q})\cdot\boldsymbol{r}} = \sum_{i,\boldsymbol{q}} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}_i} \delta_{\boldsymbol{q},\boldsymbol{k}-\boldsymbol{k}'}$$

and with $\boldsymbol{r}_i \to \boldsymbol{R_n} + \boldsymbol{\tau}$ for a crystalline solid

$$F(\boldsymbol{q}) = \sum_{\boldsymbol{\tau}} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\tau}} \sum_{\boldsymbol{n}} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R_n}},$$

where the last sum vanishes except for $\boldsymbol{q} = \boldsymbol{G}$ and $\sum_{\boldsymbol{n}} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R_n}} = N\delta_{\boldsymbol{q},\boldsymbol{G}}$. Thus the scattering amplitude, which equals the static structure factor (up to a factor N) has peaks for the reciprocal lattice vectors.

Consider the reciprocal lattice vector $\boldsymbol{G}_{hkl} = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3$ and the lattice plane with Miller indices (hkl) spanned by $\boldsymbol{a}_1/h' - \boldsymbol{a}_2/k'$ and $\boldsymbol{a}_3/l' - \boldsymbol{a}_2/k'$ with $(hkl) = p(h'k'l')$, $p =$ integer. The normal to the lattice plane is given by

$$\left(\frac{\boldsymbol{a}_1}{h'} - \frac{\boldsymbol{a}_2}{k'}\right) \times \left(\frac{\boldsymbol{a}_3}{l'} - \frac{\boldsymbol{a}_2}{k'}\right) = -\frac{1}{h'k'}\boldsymbol{a}_1 \times \boldsymbol{a}_2 - \frac{1}{k'l'}\boldsymbol{a}_2 \times \boldsymbol{a}_3 - \frac{1}{h'l'}\boldsymbol{a}_3 \times \boldsymbol{a}_1 \,.$$

Multiplication of this vector with $-2\pi h'k'l'/\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)$ gives $\boldsymbol{G}_{hkl}/p$, thus $\boldsymbol{G}_{hkl}$ is normal to the lattice planes (hkl). The distance of the considered plane from the origin of the vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$ is

$$d'_{hkl} = \frac{a_1}{h'}\frac{\boldsymbol{a}_1 \cdot \boldsymbol{G}_{hkl}}{a_1 G_{hkl}} = \frac{2\pi}{G_{hkl}}\frac{h}{h'} = \frac{2\pi}{G_{hkl}}p \,.$$

Thus, $2\pi/G_{hkl}$ is the distance between neighboring lattice planes.

Solutions for Chap. 2

2.1: The matrix representation of the commutator $[\widehat{H}, \hat{\rho}] = 0$ reads

$$\langle m|\widehat{H}\hat{\rho} - \hat{\rho}\widehat{H}|n\rangle = \sum_{n'} \left(H_{mn'}\rho_{n'n} - \rho_{mn'}H_{n'n}\right) = 0.$$

For eigenstates of $\widehat{H}$ one has $H_{mn'} = E_m\delta_{m,n'}$ and

$$\left(E_m - E_n\right)\rho_{mn} = 0,$$

which means for $E_m \neq E_n$ or $m \neq n$ for nondegenerate states that $\rho_{mn} = 0$. The same result is found by starting from the statistical operator of the canonical (or grand canonical) ensemble.

2.2: Denote the ground state by $|\Psi_0\rangle$ and show that $\left(\mathrm{Tr}\hat{\rho}\hat{A}\right)_{T=0} = \langle\Psi_0|\hat{A}|\Psi_0\rangle$. With $\hat{\rho} = \exp\left(-\beta\widehat{H}\right)/Z$ write

$$\mathrm{Tr}\left(\hat{\rho}\hat{A}\right) = \frac{1}{Z}\sum_{m,n}\langle\Psi_m|\mathrm{e}^{-\beta\widehat{H}}|\Psi_n\rangle\langle\Psi_n|\hat{A}|\Psi_m\rangle = \frac{1}{Z}\sum_m \mathrm{e}^{-\beta E_m}\langle\Psi_m|\hat{A}|\Psi_m\rangle.$$

$$\text{With} \quad Z = \mathrm{e}^{-\beta E_0}\sum_m \mathrm{e}^{-\beta(E_m - E_0)} \quad \text{we can write}$$

$$\mathrm{Tr}\left(\hat{\rho}\hat{A}\right) = \frac{\sum_m \mathrm{e}^{-\beta(E_m-E_0)}\langle\Psi_m|\hat{A}|\Psi_m\rangle}{\sum_m \mathrm{e}^{-\beta(E_m-E_0)}} \quad \begin{array}{c}\longrightarrow \\ T \to 0\end{array} \quad \langle\Psi_0|\hat{A}|\Psi_0\rangle$$

because with $E_m - E_0 > 0$ for all $m \neq 0$ all exponential factors vanish for $T \to 0$ except the one for the ground state $|\Psi_0\rangle$.

2.3: The thermal expectation value of the number operator is $\widehat{N} = \sum_\alpha \hat{n}_\alpha$ where $\hat{n}_\alpha$ is the operator counting the particles in an eigenstate of $\widehat{H}$. The grand canonical partition function can be written

$$Z_\mathrm{G} = \sum_{N=0}^{\infty}\sum_{\{n_\alpha\}_N} \mathrm{e}^{\beta\sum_\alpha(\mu - E_\alpha)n_\alpha} = \prod_\alpha \sum_{n_\alpha} \mathrm{e}^{\beta(\mu - E_\alpha)n_\alpha},$$

where $\{n_\alpha\}_N$ denotes those sets of particle numbers n_α whose sum is N. For fermions: n_α can be 0 or 1 and

$$Z_{\mathrm{G}} = \prod_{\alpha} \left(1 + \mathrm{e}^{\beta(\mu - E_\alpha)}\right),$$

while for bosons n_α can be any nonnegative integer and

$$Z_{\mathrm{G}} = \prod_{\alpha} \left(1 + \mathrm{e}^{\beta(\mu - E_\alpha)} + \dots\right) = \prod_{\alpha} \left(1 - \mathrm{e}^{\beta(\mu - E_\alpha)}\right)^{-1}.$$

Now make use of

$$\langle \widehat{N} \rangle = \frac{1}{\beta} \frac{\partial \ln Z_{\mathrm{G}}}{\partial \mu} = \frac{1}{\beta} \frac{1}{Z_{\mathrm{G}}} \frac{\partial Z_{\mathrm{G}}}{\partial \mu}$$

to obtain for fermions $\langle \widehat{N} \rangle = \sum_\alpha \langle \hat{n}_\alpha \rangle = \sum_\alpha \dfrac{1}{\exp\left(-\beta(\mu - E_\alpha)\right) + 1}$

and for bosons $\langle \widehat{N} \rangle = \sum_\alpha \langle \hat{n}_\alpha \rangle = \sum_\alpha \dfrac{1}{\exp\left(-\beta(\mu - E_\alpha)\right) - 1}.$

The function

$$f_\alpha^{\pm} = \frac{1}{\exp\left(-\beta(\mu - E_\alpha)\right) \pm 1}$$

is the Fermi–Dirac distribution (upper sign) and the Bose–Einstein distribution (lower sign). For large $k_{\mathrm{B}}T \gg \mu$ we have $\exp \beta\mu \simeq 1$ and $f_\alpha^{\pm} \to \exp\left(-\beta E_\alpha\right)$.

2.4: Ohm's law can be written $j_\lambda = \sigma_{\lambda\mu} E_\mu$, thus the observable to be measured is (a component of) the electrical current density

$$\hat{A} \to \hat{j}_\lambda = e \sum_{l=1}^{N} \hat{v}_{l,\lambda}$$

with the velocity operator $\hat{v}_{l,\lambda} = \hat{p}_{l,\lambda}/m$. It can be written also as

$$\hat{j}_\lambda(\boldsymbol{r}) = \frac{e}{2m} \sum_l \left(\hat{p}_{l,\lambda} \delta(\boldsymbol{r} - \boldsymbol{r}_l) + \delta(\boldsymbol{r} - \boldsymbol{r}_l) \hat{p}_{l,\lambda}\right).$$

The operator of the kinetic energy in the presence of an electro-magnetic field (here represented by the vector potential $\boldsymbol{A}(\boldsymbol{r}, t)$) is for the lth electron

$$\frac{1}{2m} \big(\hat{\boldsymbol{p}}_l - e\boldsymbol{A}(\boldsymbol{r}_l, t)\big)^2 = \frac{\boldsymbol{p}_l^2}{2m} - \frac{e}{2m} \big(\boldsymbol{p}_l \cdot \boldsymbol{A}(\boldsymbol{r}_l, t) + \boldsymbol{A}(\boldsymbol{r}_l, t) \cdot \boldsymbol{p}_l\big) + \mathcal{O}(\boldsymbol{A}^2).$$

Neglecting the last term on the *rhs*, we identify the perturbation as

$$\begin{aligned} V_{\mathrm{ext}}(t) &= -\sum_l \frac{e}{2m} \big(\boldsymbol{p}_l \cdot \boldsymbol{A}(\boldsymbol{r}_l, t) + \boldsymbol{A}(\boldsymbol{r}_l, t) \cdot \boldsymbol{p}_l\big) \quad \text{or} \\ &= -\int \mathrm{d}^3 r \underbrace{\frac{e}{2m} \sum_l \big(\boldsymbol{p}_l \delta(\boldsymbol{r} - \boldsymbol{r}_l) + \delta(\boldsymbol{r} - \boldsymbol{r}_l) \boldsymbol{p}_l\big)}_{\boldsymbol{j}(\boldsymbol{r})_l} \cdot \boldsymbol{A}(\boldsymbol{r}, t) \end{aligned}$$

and the observable $\widehat{B}$ as another component of the electric current density. The electric field component is given by

$$E_\mu = -\frac{\partial A_\mu}{\partial t} = -\mathrm{i}\omega A_\mu \quad \text{and we can write}$$

$$V_{\text{ext}}(t) = -\frac{\mathrm{i}}{\omega}\sum_{\mu}\int \mathrm{d}^3 r \hat{j}_\mu(\boldsymbol{r}) E_\mu(\boldsymbol{r}) \mathrm{e}^{\mathrm{i}\omega t}$$

which in the long-wave length limit, when the dependence of the vector potential on $\boldsymbol{r}$ can be neglected, gives

$$V_{\text{ext}}(t) = -\frac{\mathrm{i}}{\omega}\sum_{\mu}\int \mathrm{d}^3 r j_\mu(\boldsymbol{r}) E_\mu \mathrm{e}^{\mathrm{i}\omega t}$$

and we obtain the electric conductivity

$$\sigma_{\lambda\mu}(\omega) = \frac{\mathrm{i}}{\hbar\omega}\int_{-\infty}^{\infty} \mathrm{d}\tau\ \mathrm{e}^{\mathrm{i}\omega t}\theta(\tau)\langle[j_\lambda(\tau), j_\mu(0)]\rangle_0$$

as a correlation function for the components of the current density.

2.5: With $\Delta\rho(t) = \Delta\rho_1(t) + \Delta\rho_2(t) + \ldots$, where the index refers to different orders of V_{ext}, we can write the equations:

1. $[H_0, \Delta\rho_1] + [V_{\text{ext}}, \rho_0] = \mathrm{i}\hbar\dot{\rho}_1$ first order in V_{ext}.
2. $[H_0, \Delta\rho_2] + [V_{\text{ext}}, \rho_1] = \mathrm{i}\hbar\dot{\rho}_2$ second order V_{ext}.

The solution of (1)

$$\Delta\rho_1(t) = \frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{t} \mathrm{d}t' \mathrm{e}^{-\mathrm{i}H_0(t-t')/\hbar}[V_{\text{ext}}(t'), \rho_0]\mathrm{e}^{\mathrm{i}H_0(t-t')/\hbar}$$

is to be used in (2), which can be solved in the same way as (1), to yield

$$\Delta\rho_2(t) = \frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{t} \mathrm{d}t' \int_{-\infty}^{t'} \mathrm{d}t'' \mathrm{e}^{-\mathrm{i}H_0(t-t')/\hbar}\mathrm{e}^{\mathrm{i}H_0(t-t'')/\hbar}[\ldots,[\ldots,\ldots]]\mathrm{e}^{\mathrm{i}H_0(t-t')/\hbar}$$

where the double commutator

$$[\ldots,[\ldots,\ldots]] = \left[V_{\text{ext}}(t'), \mathrm{e}^{-\mathrm{i}H_0(t-t'')/\hbar}[V_{\text{ext}}(t''), \rho_0]\right]$$

indicates the structure of the second-order response function

$$\langle\Delta A_2\rangle_t = \ldots\left[\widehat{B}(\tau), [\widehat{B}(\tau'), \hat{A}(0)]\right].$$

It is a two-time correlation function.

2.6: Evaluate the principal value integral

$$\mathrm{Re}\chi(\omega) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{+\infty} \frac{\chi_0}{\omega' - \omega}\left(\delta(\omega_0 - \omega') - \delta(\omega_0 + \omega')\right)\mathrm{d}\omega',$$

which yields

$$\mathrm{Re}\chi(\omega) = \frac{\chi_0}{\pi}\left(\frac{1}{\omega_0 - \omega} + \frac{1}{\omega_0 + \omega}\right) = \frac{2\chi_0\omega_0}{\pi}\frac{1}{\omega_0^2 - \omega^2}.$$

Solutions for Chap. 3

3.1: The potential energy of the linear chain (Fig. 3.16) is

$$\mathcal{U} = \frac{f}{2}\left\{\sum_{n'} \underbrace{\left[u\begin{pmatrix} n' \\ 1 \end{pmatrix} - u\begin{pmatrix} n' \\ 2 \end{pmatrix}\right]^2}_{(1)} + \underbrace{\left[u\begin{pmatrix} n'+1 \\ 1 \end{pmatrix} - u\begin{pmatrix} n' \\ 2 \end{pmatrix}\right]^2}_{(2)}\right\},$$

here (1) is the contribution due to the relative displacements of M_1 and M_2 in the unit cell n and (2) that due to the relative displacement between M_1 in unit cell $n+1$ and M_2 in unit cell n.
Distinguish the force constants

$$n = m,\ \tau = \tau' :\ \phi\begin{pmatrix} n\ n \\ 1\ 1 \end{pmatrix} = \phi\begin{pmatrix} n\ n \\ 2\ 2 \end{pmatrix} = 2f$$

for the restoring force acting on $M_1(M_2)$ if the neighbor atoms are kept fixed,

$$n = m,\ \tau = 1,\ \tau' = 2 :\ \phi\begin{pmatrix} n\ n \\ 1\ 2 \end{pmatrix} = -f \quad \text{and}$$

$$n = m+1,\ \tau = 1,\ \tau' = 2 :\ \phi\begin{pmatrix} m+1\ m \\ 1\quad 2 \end{pmatrix} = -f.$$

Due to *actio = reactio* we have

$$\phi\begin{pmatrix} n\ n \\ 1\ 2 \end{pmatrix} = \phi\begin{pmatrix} n\ n \\ 2\ 1 \end{pmatrix} \quad \text{and with (3.13)}$$

$$\text{for } \tau = 1 :\ \phi\begin{pmatrix} n\ n \\ 1\ 1 \end{pmatrix} + \phi\begin{pmatrix} n\ n \\ 1\ 2 \end{pmatrix} + \phi\begin{pmatrix} n\ n-1 \\ 1\quad 2 \end{pmatrix} = 2f - f - f = 0$$

$$\text{for } \tau = 2 :\ \phi\begin{pmatrix} n\ n \\ 2\ 2 \end{pmatrix} + \phi\begin{pmatrix} n\ n \\ 2\ 1 \end{pmatrix} + \phi\begin{pmatrix} n\ n+1 \\ 2\quad 1 \end{pmatrix} = 2f - f - f = 0.$$

Translation invariance allows to shift the cell index.

Considering the equilibrium positions $x_{n1} = na$ for M_1 and $n_{n2} = na + r_0$ for M_2 along the chain, we find the elements of the dynamical matrix

$$D_{11}(q) = \frac{1}{M_1}\phi\begin{pmatrix} n\ n \\ 1\ 1 \end{pmatrix} = \frac{2f}{M_1}, \quad D_{22}(q) = \frac{2f}{M_2}$$

and

$$D_{12}(q) = \frac{1}{\sqrt{M_1 M_2}} \sum_n \phi\begin{pmatrix} n\ m \\ 1\ 2 \end{pmatrix} \mathrm{e}^{\mathrm{i}q(x_{n1} - x_{n2})}.$$

For $n = m,\ x_{n1} - x_{n2} = -r_0$ and for $n = m+1,\ x_{m+1,1} - x_{m,2} = a - r_0$, the force constant equals $-f$ and with $a = 2r_0$, we have

$$D_{12}(q) = \frac{-2f}{\sqrt{M_1 M_2}} \cos(qr_0) = D_{21}(q).$$

The eigensolutions of

$$\|D_{\alpha\beta}(q) - \omega^2(q)\delta_{\alpha,\beta}\| = \left\| \begin{array}{cc} \frac{2f}{M_1} - \omega^2 & \frac{-2f}{\sqrt{M_1 M_2}} \cos qr_0 \\ \frac{-2f}{\sqrt{M_1 M_2}} \cos qr_0 & \frac{2f}{M_2} - \omega^2 \end{array} \right\| = 0$$

are (with $M = M_1 + M_2$)

$$\omega_\pm^2(q) = \frac{f}{M_1 M_2}\left[M \pm \left\{M_1^2 + M_2^2 + 2M_1 M_2(1 - 2\sin^2 qr_0\right\}^{1/2}\right].$$

There are two solutions for each q. For $q = 0$, the squared frequencies are

$$\omega_+^2(0) = \frac{2fM}{M_1 M_2}, \quad \text{and} \quad \omega_-^2(0) = 0$$

and for $q \simeq 0$ with $1 - 2\sin^2 qr_0 = \cos qa \simeq 1 - q^2a^2/2$ (for $q \ll \pi/a$)

$$\omega^2(q) \simeq \frac{f}{M_1 M_2}\left[M \pm \left\{M^2 - M_1 M_2 q^2 a^2\right\}^{1/2}\right] \simeq \frac{f}{\mu}\left[1 \pm \left\{1 - \frac{\mu}{2M} q^2 a^2\right\}\right]$$

with the reduced mass $\mu = M_1 M_2/M$ and

$$\omega_+^2(q \ll \frac{\pi}{a}) \simeq \frac{2f}{\mu} \quad \text{independent of } q \quad \text{and}$$

$$\omega_-^2(q)(q \ll \frac{\pi}{a}) \simeq \frac{f}{2M} q^2 a^2 \;\rightarrow\; \omega_-(q \ll \frac{\pi}{a}) \simeq \sqrt{\frac{f}{2M}}\, aq.$$

For $q = \pi/a$ and $\cos qa = -1$ the solutions are

$$\omega_\pm^2\left(\frac{\pi}{a}\right)\left(M \pm \left\{M_1^2 + M_2^2 - 2M_1 M_2\right\}^{1/2}\right) \quad \text{or}$$

$$\omega_+\left(\frac{\pi}{a}\right) = \sqrt{\frac{2f}{M_2}}, \quad \omega_-\left(\frac{\pi}{a}\right) = \sqrt{\frac{2f}{M_1}}.$$

A plot of the two branches is shown in Fig. 10.1: the lower branch with the linear dependence around $q \simeq 0$ for the acoustic phonons and the flat upper branch for the optical phonons are separated by a gap which results from the different masses $M_1 \neq M_2$. For $M_1 = M_2 = M$ the gap closes and we have a chain with period a and the dispersion

$$\omega(q) = \sqrt{\frac{4f}{M}} \sin qa$$

extends to π/a (thin dashed line in Fig. 10.1), which is the limit of the Brillouin zone for the chain with lattice constant a.

Solving the eigenvector equations, we find

for $q = 0$: $\omega_-(0) = 0$ $\quad \boldsymbol{e}_-(0) \sim \left(\sqrt{M_1}, \sqrt{M_2}\right)$ $\quad$ move with same phase

$\omega_+(0) = \sqrt{\frac{2f}{\mu}}$ $\quad \boldsymbol{e}_+(0) \sim \left(\sqrt{M_2}, -\sqrt{M_1}\right)$ $\quad$ move with opposite phase

for $q = \frac{\pi}{a}$: $\omega_-(\frac{\pi}{a}) = \sqrt{\frac{2f}{M_1}}$ $\quad \boldsymbol{e}_-(\frac{\pi}{a}) \sim (1, 0)$ $\quad M_2$ in rest

$\omega_+(\frac{\pi}{a}) = \sqrt{\frac{2f}{M_2}}$ $\quad \boldsymbol{e}_+(\frac{\pi}{a}) \sim (0, 1)$ $\quad M_1$ in rest.

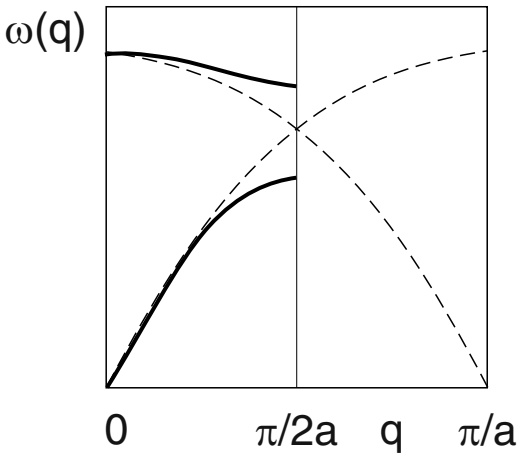

Fig. A.1. Dispersion for the linear chain with two different masses per unit cell (*solid lines*). The *dashed curves* show the result if the two masses are equal

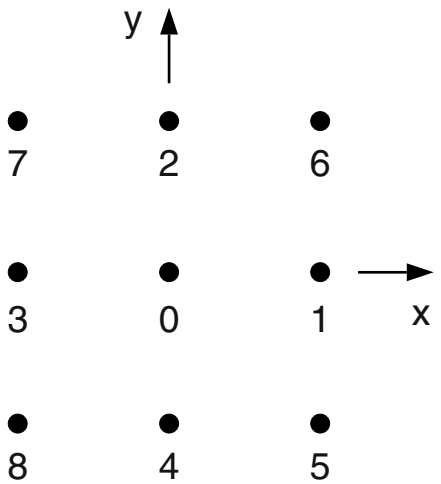

Fig. A.2. Sketch of the two-dimensional quadratic lattice with numbers to address the individual lattice point

3.2: For central forces the adiabatic potential depends on $r_{\boldsymbol{m},\boldsymbol{n}} = |\boldsymbol{R}^0_{\boldsymbol{m}} + \boldsymbol{u}_{\boldsymbol{m}} - \boldsymbol{R}^0_{\boldsymbol{n}} - \boldsymbol{u}_{\boldsymbol{n}}|$ and the force constants can be written

$$\phi\begin{pmatrix} \boldsymbol{m} & \boldsymbol{n} \\ i & j \end{pmatrix} = \frac{\partial^2 \mathcal{U}}{\partial r^2_{\boldsymbol{m},\boldsymbol{n}}} \frac{R^0_{\boldsymbol{k}i} R^0_{\boldsymbol{k}j}}{|\boldsymbol{R}^0_{\boldsymbol{k}}|^2} \quad \text{with} \quad \boldsymbol{k} = \boldsymbol{m} - \boldsymbol{n}.$$

Nearest neighbors to mass in the center (see Fig. 10.2) are

$$\boldsymbol{R}^0_1 = a\boldsymbol{e}_x\,,\ \boldsymbol{R}^0_2 = a\boldsymbol{e}_y\,,\ \boldsymbol{R}^0_3 = -a\boldsymbol{e}_x\,,\ \boldsymbol{R}^0_4 = -a\boldsymbol{e}_y$$

with force constants

$$\phi\begin{pmatrix}1&0\\x&x\end{pmatrix}=\phi\begin{pmatrix}2&0\\y&y\end{pmatrix}=\phi\begin{pmatrix}3&0\\x&x\end{pmatrix}=\phi\begin{pmatrix}4&0\\y&y\end{pmatrix}=\phi_1\,,\ \phi\begin{pmatrix}k&0\\x&y\end{pmatrix}=0\,0$$

next nearest neighbors are

$$\boldsymbol{R}_5^0=a\boldsymbol{e}_x-\boldsymbol{e}_y\,,\ \boldsymbol{R}_7^0=-a\boldsymbol{e}_x+a\boldsymbol{e}_y$$

with force constants

$$\phi\begin{pmatrix}5&0\\x&x\end{pmatrix}=\phi\begin{pmatrix}5&0\\y&y\end{pmatrix}=\phi\begin{pmatrix}7&0\\x&x\end{pmatrix}=\phi\begin{pmatrix}7&0\\y&y\end{pmatrix}=\frac{1}{2}\phi_2,$$

$$\phi\begin{pmatrix}5&0\\x&y\end{pmatrix}=\phi\begin{pmatrix}5&0\\y&x\end{pmatrix}=\phi\begin{pmatrix}7&0\\x&y\end{pmatrix}=\phi\begin{pmatrix}7&0\\y&x\end{pmatrix}=-\frac{1}{2}\phi_2$$

and

$$\boldsymbol{R}_6^0=a\boldsymbol{e}_x+a\boldsymbol{e}_y\quad\text{with}\quad\phi\begin{pmatrix}6&0\\x&x\end{pmatrix}=\phi\begin{pmatrix}6&0\\y&y\end{pmatrix}=\phi\begin{pmatrix}6&0\\x&y\end{pmatrix}=\frac{1}{2}\phi_2$$

and

$$\boldsymbol{R}_8^0=-a\boldsymbol{e}_x-a\boldsymbol{e}_y\quad\text{with}\quad\phi\begin{pmatrix}8&0\\x&x\end{pmatrix}=\phi\begin{pmatrix}8&0\\y&y\end{pmatrix}=\phi\begin{pmatrix}8&0\\x&y\end{pmatrix}=\frac{1}{2}\phi_2.$$

The force constant

$$\phi\begin{pmatrix}0&0\\i&j\end{pmatrix}\quad\text{follows from}\quad\sum_k\phi\begin{pmatrix}k&0\\i&j\end{pmatrix}=0$$

$$\rightarrow\quad\phi\begin{pmatrix}0&0\\i&j\end{pmatrix}=-\sum_{k=1}^{8}\phi\begin{pmatrix}k&0\\i&j\end{pmatrix}=-2(\phi_1+\phi_2)\delta_{i,j}.$$

The elements of the dynamical matrix are

$$\begin{aligned}D_{xx}(\boldsymbol{q})&=\frac{1}{M}\sum_k\phi\begin{pmatrix}k&0\\x&x\end{pmatrix}\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_k^0}\\&=-\frac{2}{M}\left(\phi_1(1-\cos q_xa)+\phi_2(1-\cos q_xa\cos q_ya)\right),\\D_{yy}(\boldsymbol{q})&=-\frac{2}{M}\left(\phi_1(1-\cos q_ya)+\phi_2(1-\cos q_xa\cos q_ya)\right),\\D_{xy}(\boldsymbol{q})&=-\frac{2}{M}\phi_2\sin q_xa\sin q_ya.\end{aligned}$$

The secular problem is

$$\begin{Vmatrix}D_{xx}(\boldsymbol{q})-\omega^2&D_{xy}(\boldsymbol{q})\\D_{xy}(\boldsymbol{q})&D_{yy}(\boldsymbol{q})-M\omega^2\end{Vmatrix}=0.$$

For $\Gamma-X:\ 0\le q_x\le\pi/a\,,\ q_y=0\,,\ \sin q_ya=0\,,\ \cos q_ya=1$ we have two branches

$$\omega_1^2(q_x)=\frac{2}{M}(\phi_1+\phi_2)(1-\cos q_xa)\quad\text{and}\quad\omega_2^2(q_x)=\frac{2}{M}\phi_2(1-\cos q_xa)$$

with $\omega q_x\sim q_x$ for $q_x\ll\pi/a$ but different slopes.

For $\Gamma - M:\ \boldsymbol{q} = (a,q)/\sqrt{2}\,,\ 0 \le q \le \sqrt{2}\pi/a$ the secular problem yields

$$\left(M\omega^2 - \underbrace{2\phi_1\left(1-\cos\frac{qa}{\sqrt{2}}\right) - 2\phi_2\left(1-\cos^2\frac{qa}{\sqrt{2}}\right)}_{2a} \right)^2 - \underbrace{4\,\phi_2^2 \sin^4\frac{qa}{\sqrt{2}}}_{b^2} = 0$$

with the solutions

$$M\omega^2 = 2a \pm 2b:\ M\omega_1^2 = 2\phi_1\left(1-\cos\frac{qa}{\sqrt{2}}\right),$$
$$M\omega_2^2 = 2\phi_1\left(1-\cos\frac{qa}{\sqrt{2}}\right) + 2\phi_2\left(1-\cos\frac{2qa}{\sqrt{2}}\right).$$

Again we find two branches with $\omega(q) \sim q$ for $q \ll \pi/a$ and different slopes.
For $X - M:\ \boldsymbol{q} = (\pi/a, q)\,,\ 0 \le q \le \pi/a$ the off-diagonal terms of the dynamical matrix vanish and one has

$$\omega_1^2 = \frac{2}{M}\big(2\phi_1 + \phi_2(1+\cos qa)\big) \quad \text{and} \quad \omega_2^2 = \frac{2}{M}\big(\phi_1 + \phi_2 - (\phi_1 - \phi_2)\cos qa\big).$$

The two branches have always finite frequencies and connect those already obtained for the X and M point.

For each of these directions one eigenvector is longitudinal ($\parallel \boldsymbol{q}$) and one transverse ($\perp \boldsymbol{q}$).

3.3: Periodic boundaries account for the fact that the physics of a solid repeats over macroscopic distances, i.e., the Bloch phase factor equals one for a translation $\boldsymbol{R_N} = N_1\boldsymbol{a}_1 + N_2\boldsymbol{a}_2 + N_3\boldsymbol{a}_3$ over a macroscopic length ($N_i \gg 1,\ i = 1,2,3$):

$$\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R_N}} = 1 \quad \text{or} \quad \boldsymbol{k}\cdot\boldsymbol{R_N} = 2\pi \times \text{ integer}.$$

This implies (take a simple cubic lattice with $V = L_1L_2L_3\,,\ L_i = N_i a$ as example) that the components of the wave vector take the discrete values (particle in the box) $k_i = 2\pi n_i/L_i\,,\ i = 1,2,3$ and $0 \le n_i \le N_i - 1$. Thus $N = N_1N_2N_3$ is the number of $\boldsymbol{k}$ in the first Brillouin zone and each $\boldsymbol{k}$ takes a volume $(2\pi)^3/V$. This can be exploited when replacing a sum over $\boldsymbol{k}$ by an integral according to

$$\sum_{\boldsymbol{k}} \cdots = \frac{V}{(2\pi)^3}\int \ldots \mathrm{d}^3k.$$

Similar considerations hold for systems with reduced dimension.

3.4: For the commutator $[a_s(\boldsymbol{q}), a_{s'}^\dagger(\boldsymbol{q}')]$ evaluate

$$[\omega_s(\boldsymbol{q})\hat{Q}_s(\boldsymbol{q}) + \mathrm{i}\hat{P}_s(-\boldsymbol{q}), \omega_{s'}(\boldsymbol{q}')\hat{Q}_{s'}(-\boldsymbol{q}') - \mathrm{i}\hat{P}_{s'}(\boldsymbol{q}')] =$$
$$-\mathrm{i}\omega_s(\boldsymbol{q})\underbrace{[\hat{Q}_s(\boldsymbol{q}), \hat{P}_{s'}(\boldsymbol{q}')]}_{\mathrm{i}\hbar\delta_{s,s'}\delta_{\boldsymbol{q},\boldsymbol{q}'}} + \mathrm{i}\omega_{s'}(\boldsymbol{q}')\underbrace{[\hat{P}_s(-\boldsymbol{q}), \hat{Q}_{s'}(-\boldsymbol{q}')]}_{-\mathrm{i}\hbar\delta_{s,s'}\delta_{\boldsymbol{q},\boldsymbol{q}'}} = 2\hbar\omega_s(\boldsymbol{q})\delta_{s,s'}\delta_{\boldsymbol{q},\boldsymbol{q}'}$$

to find $[a_s(\boldsymbol{q}), a_{s'}^\dagger(\boldsymbol{q}')] = \delta_{s,s'}\delta_{\boldsymbol{q},\boldsymbol{q}'}$. The two other commutation relations follow in the same way (note that $\omega_s(\boldsymbol{q}) = \omega_s(-\boldsymbol{q})$).

3.5: In the Schrödinger picture, we have

$$[a_s(\boldsymbol{q}), H_0] = \hbar\omega_{s'}(\boldsymbol{q}')a_s(\boldsymbol{q}) \quad \text{or} \quad a_s(\boldsymbol{q})H_0 = \big(H_0 + \hbar\omega_{s'}(\boldsymbol{q}')\big)a_s(\boldsymbol{q}).$$

Thus, for any power function $f(H_0)$ we can write

$$a_s(\boldsymbol{q})f(H_0) = f(H_0 + \hbar\omega_s(\boldsymbol{q}))a_s(\boldsymbol{q})$$

and obtain

$$\begin{aligned} a_s(\boldsymbol{q},t)a^\dagger_{s'}(\boldsymbol{q}',0) &= \mathrm{e}^{\mathrm{i}H_0 t/\hbar}a_s(\boldsymbol{q},0)\mathrm{e}^{-\mathrm{i}H_0 t/\hbar}a^\dagger_{s'}(\boldsymbol{q},0) \\ &= \mathrm{e}^{-\mathrm{i}\omega_s(\boldsymbol{q})t}a_s(\boldsymbol{q},0)a^\dagger_{s'}(\boldsymbol{q},0). \end{aligned}$$

Using the commutation relation and taking the thermal expectation value gives

$$\langle a_s(\boldsymbol{q},t)a^\dagger_{s'}(\boldsymbol{q}',0)\rangle = \mathrm{e}^{-\mathrm{i}\omega_s(\boldsymbol{q})t}\big(n_s(\boldsymbol{q},T)+1\big)\delta_{s,s'}\delta_{\boldsymbol{q},\boldsymbol{q}'}.$$

Similarly we have

$$a^\dagger_s(\boldsymbol{q})H_0 = \big(H_0 - \hbar\omega_{s'}(\boldsymbol{q}')\big)a^\dagger_s(\boldsymbol{q})$$

and by following the same steps we find the second relation. For the third relation we have, after extracting the exponential with the time-dependence, the thermal expectation value of a product of two annihilation operators, which vanishes.

3.6: The displacement is a time-dependent operator in the Heisenberg picture. Start by writing (with $[\rho_0, H_0] = 0$)

$$\langle\big(\boldsymbol{q}\cdot\boldsymbol{u}_{\boldsymbol{n}}(t)\big)^2\rangle = \mathrm{Tr}\left(\rho_0\,\mathrm{e}^{\mathrm{i}H_0 t/\hbar}\big(\boldsymbol{q}\cdot\boldsymbol{u}_{\boldsymbol{n}}(0)\big)^2\mathrm{e}^{-\mathrm{i}H_0 t/\hbar}\right)$$

and obtain by cyclic permutation under the trace

$$\langle\big(\boldsymbol{q}\cdot\boldsymbol{u}_{\boldsymbol{n}}(t)\big)^2\rangle = \mathrm{Tr}\left(\big(\boldsymbol{q}\cdot\boldsymbol{u}_{\boldsymbol{n}}(0)\big)^2\right),$$

which is independent of t. Formulate the lattice displacement with (3.23) and (3.39)

$$\boldsymbol{u}_{\boldsymbol{n}} = \sum_{s,\boldsymbol{q}}\left(\frac{\hbar}{2NM\omega_s(\boldsymbol{q})}\right)^{1/2}\big(a^\dagger_s(-\boldsymbol{q}) + a_s(\boldsymbol{q})\big)\boldsymbol{e}_s(\boldsymbol{q})\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}^0_{\boldsymbol{n}}}$$

in terms of phonon operators and evaluate

$$\begin{aligned} \big(\boldsymbol{q}\cdot\boldsymbol{u}_{\boldsymbol{n}}\big)^2 = \frac{1}{NM}\sum_{\substack{s',\boldsymbol{q}'\\ s'',\boldsymbol{q}''}}&\big(a^\dagger_{s'}(-\boldsymbol{q}') + a_{s'}(\boldsymbol{q}')\big)\big(a^\dagger_{s''}(-\boldsymbol{q}'') + a_{s''}(\boldsymbol{q}'')\big) \\ &\times\left(\frac{\hbar^2}{4\omega_{s'}(\boldsymbol{q}')\omega_{s''}(\boldsymbol{q}'')}\right)^{1/2}\mathrm{e}^{\mathrm{i}(\boldsymbol{q}'+\boldsymbol{q}'')\cdot\boldsymbol{R}^0_{\boldsymbol{n}}}\big(\boldsymbol{q}\cdot\boldsymbol{e}_{s'}(\boldsymbol{q}')\big)\big(\boldsymbol{q}\cdot\boldsymbol{e}_{s''}(\boldsymbol{q}'')\big). \end{aligned}$$

After multiplying out the operator terms, the thermal expectation value of this expression follows with the formulas of problem 3.4 as

$$\langle\big(\boldsymbol{q}\cdot\boldsymbol{u}_{\boldsymbol{n}}\big)^2\rangle = \frac{1}{NM}\sum_{s',\boldsymbol{q}'}\big(2n_{s'}(\boldsymbol{q}',T)+1\big)\,\frac{\hbar}{2\omega_{s'}(\boldsymbol{q}')}\big(\boldsymbol{q}\cdot\boldsymbol{e}_{s'}(\boldsymbol{q}')\big)^2$$

For $T \to 0$ we have $n_s(\boldsymbol{q}, T) \to 0$ which leaves only the contribution of the zero-point motion

$$\langle (\boldsymbol{q} \cdot \boldsymbol{u_n})^2 \rangle = \frac{1}{NM} \sum_{s',\boldsymbol{q}'} \frac{\hbar}{2\omega_{s'}(\boldsymbol{q}')} (\boldsymbol{q} \cdot \boldsymbol{e}_{s'}(\boldsymbol{q}'))^2 .$$

For $T > 0$, employ the Debye model by writing $\omega_s(\boldsymbol{q}) = vq$ for all s and independent of the direction of $\boldsymbol{q}$. Summation over s' yields a factor 3. Writing $\left(\boldsymbol{q} \cdot \boldsymbol{e}_{s'}(\boldsymbol{q}')\right)^2 = q^2 \cos\vartheta^2$ where ϑ is the angle between $\boldsymbol{q}$ and $\boldsymbol{e}_{s'}(\boldsymbol{q}')$, the sum over $\boldsymbol{q}'$ can be carried out in spherical polar coordinates with the cut-off at $q_\mathrm{D} = \omega_\mathrm{D}/v$ (with the Debye frequency ω_D) giving

$$\langle (\boldsymbol{q} \cdot \boldsymbol{u_n})^2 \rangle = \frac{6q^2}{M\omega_\mathrm{D}^3} \int_0^{\omega_\mathrm{D}} \hbar\omega \left(\frac{1}{\exp(\hbar\omega/k_\mathrm{B}T) - 1} + \frac{1}{2} \right) \mathrm{d}\omega .$$

For high temperatures, $k_\mathrm{B}T \gg \hbar\omega$, the distribution function after expanding the exponential yields $k_\mathrm{B}T/\hbar\omega$ and by neglecting the term $1/2$ we find for the Debye–Waller factor

$$W = \frac{3q^2}{M\omega_\mathrm{D}^3} k_\mathrm{B}T \int_0^{\omega_\mathrm{D}} \mathrm{d}\omega = \frac{3q^2 k_\mathrm{B}T}{M\omega_\mathrm{D}^2}$$

which is always positive.

For low temperatures, $k_\mathrm{B}T \ll \hbar\omega$, the integral over ω reads after substituting $\hbar\omega/k_\mathrm{B}T = x$

$$\int_0^{\omega_\mathrm{D}} \ldots \mathrm{d}\omega = \frac{\hbar\omega_\mathrm{D}^2}{4} + \frac{(k_\mathrm{B}T)^2}{\hbar} \int_0^{x_\mathrm{D}} \frac{x \mathrm{d}x}{\mathrm{e}^x - 1}$$

For $T \to 0$ the upper limit goes to ∞ and the integral takes the value $\pi^2/6$ (see Appendix A.3). Thus, we may write

$$W = \frac{3q^2}{M\omega_\mathrm{D}^3} \left(\frac{\hbar\omega_\mathrm{D}^2}{4} + \frac{\pi^2}{6} \frac{(k_\mathrm{B}T)^2}{\hbar} \right) = \frac{3\hbar^2 q^2}{M k_\mathrm{B} \Theta_\mathrm{D}} \left(\frac{1}{4} + \frac{\pi^2}{6} \left(\frac{T}{\Theta_\mathrm{D}} \right)^2 \right)$$

with the Debye temperature Θ_D.

3.7: (a) The point group of a cubic lattice consists of 48 elements (24 rotations, each can be combined with the inversion). Under these operations, which can be represented by orthogonal 3×3 matrices $S_{\alpha i}$, the coordinates x, y, z are interchanged and (under inversion) change their sign. Likewise the components of the elastic tensor transform according to

$$c_{\alpha\beta\gamma\delta} = S_{\alpha i} S_{\beta j} S_{\gamma k} S_{\delta l} c_{ijkl} \quad \text{(double index summation)} .$$

The invariance of the elastic tensor under these transformations leaves only those components different from zero, for which pairs of indices are identical and of the nonvanishing components all those are identical which transform into each other by the symmetry operations. Thus, there are only three independent tensor components

$$\begin{aligned} c_{xxxx} = c_{yyyy} = c_{zzzz} &= c_{11} \\ c_{xyxy} = c_{xzxz} = c_{yxyx} = c_{zxzx} &= c_{12} \\ c_{xxyy} = c_{yyzz} = c_{zzxx} = c_{xxzz} = c_{zzyy} &= c_{44} \end{aligned}$$

which are written here in Voigt notation.

(b) Using $u_i(\boldsymbol{r},t) = u_i \exp\left(\mathrm{i}(\boldsymbol{q}\cdot\boldsymbol{r} - \omega t)\right)$ the wave equation for the elastic displacement field leads to a set of coupled homogeneous linear equations for the components u_i, which has solutions if

$$\|\rho\omega^2\delta_{il} - c_{ijkl}q_jq_k\| = 0\,.$$

For $\Gamma - X$ or $\boldsymbol{q} = (q,0,0)$ it reads

$$\begin{Vmatrix} \rho\omega^2 - c_{11}q^2 & 0 & 0 \\ 0 & \rho\omega^2 - c_{12}q^2 & 0 \\ 0 & 0 & \rho\omega^2 - c_{12}q^2 \end{Vmatrix} = 0$$

and has solutions

$$\begin{aligned} \omega_{\mathrm{L}} &= \sqrt{\frac{c_{11}}{\rho}}\,q\,,\ \boldsymbol{e}_{\mathrm{L}} = (1,0,0) \quad \text{longitudinal} \\ \omega_{\mathrm{T}} &= \sqrt{\frac{c_{12}}{\rho}}\,q\,,\ \boldsymbol{e}_{\mathrm{T}} = (0,1,0) \quad \text{transverse} \\ &\qquad\qquad = (0,0,1) \quad \text{transverse}\,. \end{aligned}$$

For $\Gamma - K$ or $\boldsymbol{q} = (q,q,0)/\sqrt{2}$, we have $c_{ijkl}q_jq_k = \big(c_{ixxl} + c_{iyyl} + c_{ixyl} + c_{iyxl}\big)q^2/2$ and the secular problem

$$\begin{Vmatrix} \rho\omega^2 - \frac{1}{2}(c_{11}+c_{12})q^2 & -\frac{1}{2}(c_{12}+c_{44})q^2 & 0 \\ -\frac{1}{2}(c_{12}+c_{44})q^2 & \rho\omega^2 - \frac{1}{2}(c_{11}+c_{12})q^2 & 0 \\ 0 & 0 & \rho\omega^2 - c_{12}q^2 \end{Vmatrix} = 0\,.$$

One solution is immediately found to be

$$\omega_{\mathrm{T}_1} = \sqrt{\frac{c_{12}}{\rho}}\,q\,,\ \boldsymbol{e}_{\mathrm{T}_1} = (0,0,1) \quad \text{transverse}\,.$$

The other two follow from

$$\begin{Vmatrix} \rho\omega^2 - A & -B \\ -B & \rho\omega^2 - A \end{Vmatrix} = (\rho\omega^2 - A)2^- B^2 = 0$$

with $A = (c_{11}+c_{12})q^3/2$ and $B = (c_{12}+c_{44})q^2/2$ and read

$$\begin{aligned} \omega_{\mathrm{T}_2} &= \sqrt{\frac{2c_{12}+c_{11}+c_{44}}{2\rho}}\,q\,,\ \boldsymbol{e}_{\mathrm{T}_2} = (1,-1,0)/\sqrt{2} \quad \text{transverse} \\ \omega_{\mathrm{L}} &= \sqrt{\frac{c_{11}-c_{44}}{2\rho}}\,q\,,\ \boldsymbol{e}_{\mathrm{L}} = (1,1,0)/\sqrt{2} \quad \text{longitudinal}\,. \end{aligned}$$

These results can be compared with the phonon dispersion (e.g., those given in Sect. 3.6 which are all for lattices with cubic symmetry). The slope of the acoustic branches for given ρ can be taken to determine the elastic constants.

3.8: The cubic anharmonicity $\Delta(a^\dagger + a)^3)$ is first written in normal order

$$(a^\dagger + a)^3 = a^{\dagger 3} + 3a^{\dagger 2}a + 3(a^\dagger + a) + 3a^\dagger a^2 + a^3$$

and then truncated by replacing $a^\dagger a \to \langle a^\dagger a\rangle = n(T)$ and omitting the terms $a^{\dagger 3}$ and a^3. Thus the Hamiltonian reduces to

$$H = \hbar\omega_0 a^\dagger a + \Delta(T)(a^\dagger + a) \quad \text{with} \quad \Delta(T) = 3\Delta\big(n(T)+1\big).$$

Calculate now the corrections to the oscillator ground state $|n\rangle$ with $n = 0$ due to the anharmonicity, which by making use of $\langle 0|a|1\rangle\langle 1|a^\dagger|0\rangle = 1$ reads in Brillouin–Wigner perturbation theory

$$\varepsilon = E_0 - \frac{\hbar\omega_0}{2} = \frac{\Delta^2(T)}{\varepsilon - \hbar\omega_0}.$$

The smaller solution of the quadratic equation in ε

$$E_0 = \frac{1}{2}\hbar\omega_0 - \frac{\Delta^2(T)}{\hbar\omega_0}$$

expresses a zero-point energy which decreases as $\Delta(T)$ increases due to thermal phonon excitation with the temperature. This is the behavior of a soft mode.

Solutions for Chap. 4

4.1: The electrostatic potential of a homogeneous positive charge density $+eN(\boldsymbol{r})$ with $n(\boldsymbol{r}) = N/V$ is

$$\phi(\boldsymbol{r}) = \int_V \frac{e\,n(\boldsymbol{r}')}{4\pi\varepsilon_0|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}^3r'\,.$$

Its interaction energy with the homogeneous electron density $-en(\boldsymbol{r})$ is

$$\mathcal{H}_{\mathrm{el-ion}} = -e\int_V n(\boldsymbol{r})\phi(\boldsymbol{r})\,\mathrm{d}^3r = -\left(\frac{N}{V}\right)^2\int \mathrm{d}^3r\int \mathrm{d}^3r'\frac{e^2}{4\pi\varepsilon_0|\boldsymbol{r}-\boldsymbol{r}'|}\,.$$

With (see Appendix)

$$\frac{e^2}{4\pi\varepsilon_0|\boldsymbol{r}-\boldsymbol{r}'|} = \sum_{\boldsymbol{q}} v_{\boldsymbol{q}}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\,,\ v_{\boldsymbol{q}} = \frac{e^2}{\varepsilon_0 V q^2} \quad \text{the double integral can be evaluated}$$

$$\int \mathrm{d}^3r\int \mathrm{d}^3r'\frac{e^2}{4\pi\varepsilon_0|\boldsymbol{r}-\boldsymbol{r}'|} = \sum_{\boldsymbol{q}} v_{\boldsymbol{q}}\underbrace{\int \mathrm{d}^3r\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}}_{V\delta_{\boldsymbol{q},0}}\underbrace{\int \mathrm{d}^3r\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}'}}_{V\delta_{\boldsymbol{q},0}} = \sum_{\boldsymbol{q}} v_{\boldsymbol{q}}V^2\delta_{\boldsymbol{q},0}$$

giving $\mathcal{H}_{\mathrm{el-ion}} = -N^2 v_0$. Similarly the interaction energy of the homogeneous electron and ions systems can be calculated which each give the same result up to a factor $-1/2$. Thus the sum of all these divergent interaction energies vanish for the jellium model.

4.2: The electron density n determines via the density of states $D(E)$ and the Fermi–Dirac distribution function the chemical potential $\mu(T)$. For a 3D electron system we may write $D(E) = 3n\sqrt{E}/2E_{\mathrm{F}}^{3/2}$ define a function $G(E)$ with

$$\int_{-\infty}^{E} D(E')\mathrm{d}E' = G(E) = n\left(\frac{E}{E_{\mathrm{F}}}\right)^{3/2}$$

to express the particle density as

$$n = G(E)f(E,\mu,T)\big|_0^\infty - \int_{-\infty}^{\infty} \mathrm{d}E G(E)\frac{\partial f(E,\mu,T)}{\partial E}\,.$$

The first term vanishes and the integral can be evaluated by using the fact, that the derivative of $f(E,\mu,T)$ is strongly peaked at $E=\mu$ (for $k_\mathrm{B}T \ll \mu$). Expand $G(E)$ in a power series around $E=\mu$

$$G(E) = \int_{-\infty}^{\mu} \mathrm{d}E' D(E') + \sum_{n=1}^{\infty} \frac{(E-\mu)^n}{n!}\frac{\mathrm{d}^n G(E)}{\mathrm{d}E^n}\Big|_{E=\mu}\,.$$

The integral gives $G(\mu)$. Because $\partial f/\partial E$ is an even function only the even powers of the expansion contribute and we find as the two leading terms

$$n = -G(\mu)\int_{-\infty}^{\infty}\mathrm{d}E\frac{\partial f}{\mathrm{d}E} - \frac{3n}{8E_\mathrm{F}^{3/2}}\frac{1}{\sqrt{\mu}}\int_{-\infty}^{\infty}\mathrm{d}E(E-\mu)^2\frac{\partial f}{\mathrm{d}E}\quad(*).$$

The first term gives $n(\mu/E_\mathrm{F})^{3/2}$. With

$$\frac{\partial f}{\mathrm{d}E} = -\beta\frac{\mathrm{e}^{\beta(E-\mu)}}{(\mathrm{e}^{\beta(E-\mu)}+1)^2}\,,\ \beta = k_\mathrm{B}T \quad \text{and substituting} \quad x = \beta(E-\mu)$$

$$\int_{-\infty}^{\infty}\mathrm{d}E(E-\mu)^2\frac{\partial f}{\mathrm{d}E} = -\frac{1}{\beta^3}\int_{-\infty}^{\infty}\mathrm{d}x\,x^2\frac{\mathrm{e}^x}{(\mathrm{e}^x+1)^2}\,.$$

The value of the integral is $\pi^2/6$. Thus $(*)$ reduces to the relation

$$1 \simeq \left(\frac{\mu}{E_\mathrm{F}}\right)^{3/2}\left(1+\left(\frac{k_\mathrm{B}T}{\mu}\right)^2\frac{\pi^2}{8}\right)$$

which can be solved to give

$$\mu(T) \simeq E_\mathrm{F}\left(1-\frac{\pi^2}{12}\left(\frac{k_\mathrm{B}T}{\mu}\right)^2\right)\,.$$

This result corresponds to the Sommerfeld expansion (see Appendix A.4).

4.3: For 2D, the number of states (per unit area) $D(k)\mathrm{d}k$ in a circular ring with radius k and thickness $\mathrm{d}k$ is

$$D(k)\mathrm{d}k = \frac{2}{(2\pi)^2}2\pi\,k\mathrm{d}k \quad \text{(the factor 2 counts the spins)}\,.$$

Use the dispersion relation for free electrons $E_k = \hbar^2k^2/2m$ to substitute k by E

$$D(E)\mathrm{d}E = D(k)\frac{\mathrm{d}k}{\mathrm{d}E}\mathrm{d}E = \frac{1}{\pi}\sqrt{\frac{2m}{\hbar^2}}\sqrt{E}\sqrt{\frac{2m}{\hbar^2}}\frac{1}{2\sqrt{E}}\mathrm{d}E$$

$$\text{or} \quad D(E) = \frac{m}{\pi\hbar^2} = const\,.$$

For 1D the corresponding number of states per unit length is

$$D(k)\mathrm{d}k = \frac{2}{2\pi}\,\mathrm{d}k \quad \text{and} \quad D(k)\frac{\mathrm{d}k}{\mathrm{d}E}\mathrm{d}E = \frac{1}{\pi}\sqrt{\frac{2m}{\hbar^2}}\frac{1}{2\sqrt{E}}\mathrm{d}E$$

$$\text{or} \quad D(E) = \sqrt{\frac{m}{2\pi^2\hbar^2}}\,\frac{1}{\sqrt{E}}\,.$$

For a zero-dimensional system the spectrum is discrete (with energies E_i) and the density of states is given by

$$D(E) = 2\sum_i \delta(E - E_i)\,.$$

4.4: The condition to fill n electrons into the lowest (spin-degenerate) Landau level follows from (4.43) or in simplified form from $E_\mathrm{F} = \hbar\omega_\mathrm{c}$ and reads

$$\frac{\hbar^2}{2m}(3\pi^2 n)^{2/3} = \frac{\hbar e B}{m} \quad \text{which can be solved to give} \quad B = \frac{\hbar}{2e}(3\pi^2 n)^{2/3}\,.$$

Note, that B is related to the number of elementary flux quanta. Take the value for $\hbar/e = 0.658\,10^{-15}\,\mathrm{Tm}^2$ to obtain for a metal $n = 10^{23}\,\mathrm{cm}^{-3}$ a magnetic field of $B \simeq 1.37\,10^5\,\mathrm{T}$ and for a doped semiconductor with $n = 10^{14}\,\mathrm{cm}^{-3}$ $B \simeq 0.137\,\mathrm{T}$. The latter is easily achieved in a laboratory.

4.5: The Zeeman energy for free electrons is $\pm\mu_\mathrm{B}B$. It shifts the density of states of up and down spins (Landau quantization is not considered here) against each other

$$D_\pm(E,B) = \frac{1}{2}D(E \pm \mu_\mathrm{B}B) \simeq \frac{1}{2}D(E) \pm \frac{1}{2}\mu_\mathrm{B}B\frac{\mathrm{d}D(E)}{\mathrm{d}E} \quad \text{which yields}$$

$$D_\pm(E,B) \simeq \frac{1}{2}\frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}\left(1 \pm \frac{\mu_\mathrm{B}B}{E}\right)\,.$$

The number of spin up and down electrons $N_\pm(E,B)$ is obtained by integrating the density of states multiplied with the Fermi–Dirac distribution function and multiplying with the volume V. The first term of $D_\pm(E,B)$ gives $N(\mu)/2$ independent of B. The second term is evaluated by employing the Sommerfeld expansion (see Appendix A.4) leading to

$$\cdots = \pm\frac{1}{2}\mu_\mathrm{B}B\Big\{\int_{-\infty}^{\mu}\frac{\mathrm{d}D(E)}{\mathrm{d}E}\mathrm{d}E + \frac{\pi^2}{6}(k_\mathrm{B}T)^2\frac{\mathrm{d}^2D(E)}{\mathrm{d}E^2}\Big|_{E=\mu}\Big\}\,.$$

The integral gives $D(\mu)$ and with $D(E) \sim \sqrt{E}$ the second term can be rewritten using $\mathrm{d}^2D(E)/\mathrm{d}E^2 = -D(E)/4E^2$ to obtain

$$N_\pm(E,B) \simeq \frac{1}{2}N(\mu) \pm \frac{V}{2}\mu_\mathrm{B}BD(\mu)\Big\{1 - \frac{\pi^2}{24}\left(\frac{k_\mathrm{B}T}{\mu}\right)^2\Big\}\,.$$

The magnetization follows as

$$M = \mu_\mathrm{B}(N_+ - N_-)/V = \mu_\mathrm{B}^2BD(\mu)\Big\{1 - \frac{\pi^2}{24}\left(\frac{k_\mathrm{B}T}{\mu}\right)^2\Big\}\,.$$

For $T = 0$ with $D(\mu \simeq E_\mathrm{F}) = 3n/2E_\mathrm{F}$ this is identical with (4.53).

4.6: The HF approximation is better for the electron system with the smaller density parameter r_s. According to Table 4.1 the r_s-values of doped semiconductors are smaller than those of metals. On the other hand the electron density (per cm^{-3}) is

higher in metals. Note, that r_s is given in the length scale (effective Bohr radius) of the material.

4.7: Second-order perturbation yields a contribution

$$E_2 = -\sum_m \frac{|\langle\Psi_m|H_\mathrm{int}|\Psi_0\rangle|^2}{E_m - E_0}\,.$$

(a) Applying the interaction operator to the Fermi sphere $|\Psi_0\rangle$ gives nonvanishing contributions only if the states with $\boldsymbol{p},\boldsymbol{q}$ are inside and those with $\boldsymbol{p}-\boldsymbol{k},\boldsymbol{q}+\boldsymbol{k}$ outside of the Fermi sphere. Consider therefore the corresponding excited states $|\Psi_m\rangle$. These states with $E_m - E_0 = \hbar^2\boldsymbol{k}\cdot(\boldsymbol{q}-\boldsymbol{p}+\boldsymbol{k})/m$ contribute to E_2. b) The electron taken from $\boldsymbol{p}$ to $\boldsymbol{p}-\boldsymbol{k}$ is put back to $\boldsymbol{p}$ in the direct process but to $\boldsymbol{q}$ in the exchange process. For the former evaluate

$$\langle\Psi_0|\sum_{\substack{\boldsymbol{p}'\boldsymbol{q}'\boldsymbol{k}'\\ \rho\rho'}} v_{\boldsymbol{k}'} c^\dagger_{\boldsymbol{p}'-\boldsymbol{k}'\rho} c^\dagger_{\boldsymbol{q}'+\boldsymbol{k}'\rho'} c_{\boldsymbol{q}'\rho'} c_{\boldsymbol{p}'\rho}|\Psi_m\rangle\langle\Psi_m|\sum_{\substack{\boldsymbol{p}\boldsymbol{q}\boldsymbol{k}\\ \sigma\sigma'}} v_{\boldsymbol{k}} c^\dagger_{\boldsymbol{p}-\boldsymbol{k}\sigma} c^\dagger_{\boldsymbol{q}+\boldsymbol{k}\sigma'} c_{\boldsymbol{q}\sigma'} c_{\boldsymbol{p}\sigma}|\Psi_0\rangle$$

For the direct process the intermediate states have to fulfill the conditions

$$\begin{aligned}\boldsymbol{p},\sigma &= \boldsymbol{p}'-\boldsymbol{k}',\rho \quad \boldsymbol{p}-\boldsymbol{k},\sigma = \boldsymbol{p}',\rho\\ \boldsymbol{q},\sigma' &= \boldsymbol{q}'+\boldsymbol{k}',\rho' \quad \boldsymbol{q}+\boldsymbol{k},\sigma' = \boldsymbol{q}',\rho'\end{aligned}$$

or

$$\sigma=\rho\,,\ \sigma'=\rho'\,,\ \boldsymbol{p}'=\boldsymbol{p}-\boldsymbol{k}\,,\ \boldsymbol{q}'=\boldsymbol{q}+\boldsymbol{k}\,,\ \boldsymbol{k}'=-\boldsymbol{k}\,.$$

It remains to determine

$$\langle\Psi_0|c^\dagger_{\boldsymbol{p}\sigma}c^\dagger_{\boldsymbol{q}\sigma'}c_{\boldsymbol{q}+\boldsymbol{k}\sigma'}c_{\boldsymbol{p}-\boldsymbol{k}\sigma}c^\dagger_{\boldsymbol{p}-\boldsymbol{k}\sigma}c^\dagger_{\boldsymbol{q}+\boldsymbol{k}\sigma'}c_{\boldsymbol{q}\sigma'}c_{\boldsymbol{p}\sigma}|\Psi_0\rangle = \ldots,$$

which can easily be rearranged as for $\boldsymbol{k}\neq 0$ all fermion operators anti-commute and one obtains

$$\begin{aligned}\ldots &= \langle\Psi_0|c^\dagger_{\boldsymbol{p}\sigma}c_{\boldsymbol{p}\sigma}c^\dagger_{\boldsymbol{q}\sigma'}c_{\boldsymbol{q}\sigma'}c_{\boldsymbol{q}+\boldsymbol{k}\sigma'}c^\dagger_{\boldsymbol{q}+\boldsymbol{k}\sigma'}c_{\boldsymbol{p}-\boldsymbol{k}\sigma}c^\dagger_{\boldsymbol{p}-\boldsymbol{k}\sigma}|\Psi_0\rangle\\ &= n_{\boldsymbol{p}\sigma}n_{\boldsymbol{q}\sigma'}(1-n_{\boldsymbol{q}+\boldsymbol{k}\sigma'})(1-n_{\boldsymbol{p}-\boldsymbol{k}\sigma}),\end{aligned}$$

where $n_{\boldsymbol{q}\sigma}=\theta(k_\mathrm{F}-q)$ is the Fermi–Dirac distribution function for $T=0\,\mathrm{K}$. Summing over spin indices (factor 4) gives for the direct process

$$E_2^\mathrm{dir} = -4\sum_{\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}} v_{\boldsymbol{k}}^2 \frac{m}{\hbar^2\boldsymbol{k}\cdot(\boldsymbol{q}-\boldsymbol{p}+\boldsymbol{k})} n_{\boldsymbol{p}\sigma}n_{\boldsymbol{q}\sigma'}(1-n_{\boldsymbol{q}+\boldsymbol{k}\sigma'})(1-n_{\boldsymbol{p}-\boldsymbol{k}\sigma})\,.$$

c) For small $\boldsymbol{k}$, i.e., excitation close to the Fermi surface

$$n_{\boldsymbol{p}+\boldsymbol{k}} \simeq n_{\boldsymbol{p}} + \boldsymbol{k}\cdot\nabla_{\boldsymbol{p}} n_{\boldsymbol{p}}|_{k_\mathrm{F}} = n_{\boldsymbol{p}} - \boldsymbol{k}\cdot\boldsymbol{e}_p\delta(k_\mathrm{F}-p) \quad \text{and}$$

$$n_{\boldsymbol{p}}(1-n_{\boldsymbol{p}+\boldsymbol{k}}) = n_{\boldsymbol{p}}\{1-n_{\boldsymbol{p}}+\boldsymbol{k}\cdot\boldsymbol{e}_p\delta(k_\mathrm{F}-p)\} = n_{\boldsymbol{p}}\boldsymbol{k}\cdot\boldsymbol{e}_p\delta(k_\mathrm{F}-p) \sim k\,.$$

Replace now the denominator for small $\boldsymbol{k}$ by $2kk_\mathrm{F}$ and perform the sum over $\boldsymbol{p}$ and $\boldsymbol{q}$ in polar coordinates. Finally the sum over $\boldsymbol{k}$ is to be performed over an expression which contains $1/k^4$ from $v_{\boldsymbol{k}}$, $1/k$ from the denominator, and k^2 from the numerator which together with k^2 from integration in k-space leads to $\int \mathrm{d}k/k = \ln k$.

4.8: (a) The meaning of $c^\dagger_\alpha(c_\alpha)$ of creating(annihilating) a fermion in the state α with the probability amplitude $\psi_\alpha(\boldsymbol{r})$ implies, that $\Psi^\dagger(\boldsymbol{r})(\Psi(\boldsymbol{r}))$ creates(annihilates) a fermion at $\boldsymbol{r}$. (b) Write

$$\{\Psi^\dagger(\boldsymbol{r}),\Psi(\boldsymbol{r}')\}=\sum_{\alpha,\alpha'}\psi^*_\alpha(\boldsymbol{r})\psi_{\alpha'}(\boldsymbol{r}')\underbrace{\{c^\dagger_\alpha,c_{\alpha'}\}}_{\delta_{\alpha,\alpha'}}=\sum_\alpha\psi^*_\alpha(\boldsymbol{r})\psi_{\alpha'}(\boldsymbol{r}')=\delta(\boldsymbol{r}-\boldsymbol{r}')$$

and similar for $\{\Psi(\boldsymbol{r},\Psi(\boldsymbol{r}')\}=\{\Psi^\dagger(\boldsymbol{r},\Psi^\dagger(\boldsymbol{r}')\}=0$. (c) For free electrons the density operator is

$$\begin{aligned}\hat n(\boldsymbol{r})=\Psi^\dagger(\boldsymbol{r})\Psi(\boldsymbol{r})&=\sum_{\boldsymbol{k}',\boldsymbol{k}}\mathrm{e}^{-\mathrm{i}(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}}\frac{1}{V}c^\dagger_{\boldsymbol{k}'}c_{\boldsymbol{k}}\quad\text{and with}\quad\boldsymbol{q}=\boldsymbol{k}'-\boldsymbol{k}\\&=\sum_{\boldsymbol{q}}\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\frac{1}{V}\sum_{\boldsymbol{k}}c^\dagger_{\boldsymbol{k}+\boldsymbol{q}}c_{\boldsymbol{k}}\quad\to\quad\hat n_{\boldsymbol{q}}=\frac{1}{V}\sum_{\boldsymbol{k}}c^\dagger_{\boldsymbol{k}+\boldsymbol{q}}c_{\boldsymbol{k}}\,,\end{aligned}$$

$\hat n_{\boldsymbol{0}}=\sum_{\boldsymbol{k}}c^\dagger_{\boldsymbol{k}}c_{\boldsymbol{k}}/V=\hat n$ is the operator of particle density (its eigenvalue being n) while $\sum_{\boldsymbol{q}}c^\dagger_{\boldsymbol{k}+\boldsymbol{q}}c_{\boldsymbol{k}}=\hat n_{\boldsymbol{q}}$ describes density fluctuations. d) The Coulomb interaction can be rewritten with

$$c^\dagger_{\boldsymbol{p}+\boldsymbol{k}\sigma}c^\dagger_{\boldsymbol{q}-\boldsymbol{k}\sigma'}c_{\boldsymbol{q}\sigma'}c_{\boldsymbol{p}\sigma}=-c^\dagger_{\boldsymbol{p}+\boldsymbol{k}\sigma}\left(\delta_{\sigma,\sigma'}\delta_{\boldsymbol{q}-\boldsymbol{k},\boldsymbol{p}}-c_{\boldsymbol{p}\sigma}c^\dagger_{\boldsymbol{q}-\boldsymbol{k}\sigma'}\right)c_{\boldsymbol{q}\sigma'}$$

by applying the fermion commutation rules and by using the number operators the Coulomb interaction becomes

$$\frac{1}{2}\sum_{\substack{\boldsymbol{k}\neq0,\boldsymbol{p},\boldsymbol{q}\\\sigma,\sigma'}}v_{\boldsymbol{k}}c^\dagger_{\boldsymbol{p}+\boldsymbol{k}\sigma}c^\dagger_{\boldsymbol{q}-\boldsymbol{k}\sigma'}c_{\boldsymbol{q}\sigma'}c_{\boldsymbol{p}\sigma}=\frac{1}{2}\sum_{\boldsymbol{k}\neq0}v_{\boldsymbol{k}}\left(\widehat N_{\boldsymbol{k}}\widehat N_{-\boldsymbol{k}}-N\right)\,.$$

4.9: Replace in the given expression

$$\langle[\widehat N_{\boldsymbol{q}}(\tau),\widehat N_{-\boldsymbol{q}}(0)]\rangle_{\text{exact}}\;\to\;\langle[\widehat N_{\boldsymbol{q}}(\tau),\widehat N_{-\boldsymbol{q}}(0)]\rangle_0\quad\text{and}\quad N_{\text{ext}}\;\to\;N_{\text{ext}}+\langle\widehat N_{\boldsymbol{q}}\rangle$$

with the induced number fluctuation $\langle\widehat N_{\boldsymbol{q}}\rangle$. From Sect. 4.5, take

$$\lim_{\Gamma\to0}\frac{e^2}{\varepsilon_0Vq^2}\frac{1}{\mathrm{i}\hbar}\int_0^\infty\mathrm{d}\tau\mathrm{e}^{\mathrm{i}\omega\tau-\Gamma\tau}\langle\left[\widehat N_{\boldsymbol{q}}(\tau),\widehat N_{-\boldsymbol{q}}(0)\right]\rangle_0=v_{\boldsymbol{q}}\pi_0(\boldsymbol{q},\omega)$$

to write

$$\langle\widehat N_{\boldsymbol{q}}\rangle=v_{\boldsymbol{q}}\pi_0(\boldsymbol{q},\omega)\left(\langle\widehat N_{\boldsymbol{q}}\rangle+N_{\text{ext}}\right)\quad\text{or}\quad\langle\widehat N_{\boldsymbol{q}}\rangle=\frac{N_{\text{ext}}v_{\boldsymbol{q}}\pi_0(\boldsymbol{q},\omega)}{1-v_{\boldsymbol{q}}\pi_0(\boldsymbol{q},\omega)}$$

and identify with

$$\frac{1}{\varepsilon(\boldsymbol{q},\omega)}=1+\frac{\langle\widehat N_{\boldsymbol{q}}\rangle}{N_{\text{ext}}}\;\Rightarrow\;\varepsilon^{\text{RPA}}(\boldsymbol{q},\omega)=1-v_{\boldsymbol{q}}\pi_0(\boldsymbol{q},\omega)\,.$$

4.10: Using relations given in Sect. 4.6, the *lhs* of the given equation can be written

$$\int_0^\infty\mathrm{d}\omega\omega\mathrm{Im}\frac{1}{\varepsilon(\boldsymbol{q},\omega)}=-v_{\boldsymbol{q}}\frac{1}{\hbar}\sum_m|\langle\Psi_0|\widehat N_{\boldsymbol{q}}|\Psi_m\rangle|^2\int_0^\infty\mathrm{d}\omega\omega\delta(\omega-\omega_{m0})\,.$$

After showing (by inserting a complete set of eigenstates $|\Psi_m\rangle$ of $H_{\rm jell}$) that

$$-\sum_m 2\hbar\omega_{m0}|\langle\Psi_0|\widehat{N}_{\boldsymbol{q}}|\Psi_m\rangle|^2 = \langle\Psi_0|[[H_{\rm jell},\widehat{N}_{\boldsymbol{q}}],\widehat{N}_{-\boldsymbol{q}}]|\Psi_0\rangle$$

and one has to evaluate the double commutator. This is done with $H_{\rm jell}$ written in terms of density fluctuations (see (4.107) and Problem 4.8). Realize first with $\widehat{N}_{\boldsymbol{k}}^\dagger = \widehat{N}_{-\boldsymbol{k}}$ and $[\widehat{N}_{\boldsymbol{k}},\widehat{N}_{\boldsymbol{k}'}] = 0$ that the interaction term commutes with $\widehat{N}_{\boldsymbol{q}}$. Evaluate

$$[H_{\rm jell},\widehat{N}_{\boldsymbol{q}}] = [\sum_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}}c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}},\widehat{N}_{\boldsymbol{q}}] = \sum_{\boldsymbol{k},\boldsymbol{q}'}\epsilon_{\boldsymbol{k}}[c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}},c_{\boldsymbol{q}'-\boldsymbol{q}}^\dagger c_{\boldsymbol{q}'}]$$

which by applying fermion commutation rules yields

$$[H_{\rm jell},\widehat{N}_{\boldsymbol{q}}] = \sum_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}}\left(c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}+\boldsymbol{q}} - c_{\boldsymbol{k}-\boldsymbol{q}}^\dagger c_{\boldsymbol{k}}\right) = \sum_{\boldsymbol{k}}\left(\epsilon_{\boldsymbol{k}}-\epsilon_{\boldsymbol{k}+\boldsymbol{q}}\right)c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}+\boldsymbol{q}}$$

and with $\epsilon_{\boldsymbol{k}} = \hbar^2k^2/2m$

$$[H_{\rm jell},\widehat{N}_{\boldsymbol{q}}] = -\frac{\hbar^2q^2}{2m}n_{\boldsymbol{q}} - \frac{\hbar^2}{m}\sum_{\boldsymbol{k}}\boldsymbol{k}\cdot\boldsymbol{q}\,c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}+\boldsymbol{q}}$$

The first term $\sim N_{\boldsymbol{q}}$ does not contribute to the double commutator which, therefore, reads

$$\left[[H_{\rm jell},\widehat{N}_{\boldsymbol{q}}],\widehat{N}_{-\boldsymbol{q}}\right] = -\frac{\hbar^2}{m}\sum_{\boldsymbol{k},\boldsymbol{k}'}\boldsymbol{k}\cdot\boldsymbol{q}[c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}+\boldsymbol{q}},c_{\boldsymbol{k}'+\boldsymbol{q}}^\dagger c_{\boldsymbol{k}'}]\,.$$

Evaluating the commutator with the rules for fermion operators leads to

$$\begin{aligned}\left[[H_{\rm jell},\widehat{N}_{\boldsymbol{q}}],\widehat{N}_{-\boldsymbol{q}}\right] &= -\frac{\hbar^2}{m}\sum_{\boldsymbol{k}}\boldsymbol{k}\cdot\boldsymbol{q}\left(c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}} - c_{\boldsymbol{k}+\boldsymbol{q}}^\dagger c_{\boldsymbol{k}+\boldsymbol{q}}\right) \quad \text{and with} \quad \boldsymbol{k}+\boldsymbol{q}\to\boldsymbol{k}\\ &= -\frac{\hbar^2}{m}\sum_{\boldsymbol{k}}c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}} = -\frac{\hbar^2}{m}q^2N\,.\end{aligned}$$

Consider the factors one has

$$\int_0^\infty {\rm d}\omega\omega{\rm Im}\frac{1}{\varepsilon(\boldsymbol{q},\omega)} = -\frac{\pi v_{\boldsymbol{q}}}{\hbar}\left(-\frac{1}{2\hbar}\right)\left(-\frac{\hbar^2}{m}q^2N\right) = -\frac{1}{2}\omega_{\rm p}^2\,.$$

4.11: Evaluate for $\omega = 0$

$$\varepsilon_1(\boldsymbol{q},0) = 1 - \frac{e^2}{\varepsilon_0 Vq^2}\sum_{\boldsymbol{k},\sigma}\frac{f_{\boldsymbol{k}+\boldsymbol{q}}-f_{\boldsymbol{k}}}{\epsilon_{\boldsymbol{k}+\boldsymbol{q}}-\epsilon_{\boldsymbol{k}}} \quad \text{by writing for} \quad \boldsymbol{q}\to 0\text{:}$$

$$f_{\boldsymbol{k}+\boldsymbol{q}} - f_{\boldsymbol{k}} \simeq \boldsymbol{q}\cdot\nabla_{\boldsymbol{k}}f_{\boldsymbol{k}} = \boldsymbol{q}\cdot\nabla_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}}\frac{{\rm d}f}{{\rm d}\epsilon} \simeq -\boldsymbol{q}\cdot\nabla_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}}\delta(\epsilon_{\boldsymbol{k}}-E_{\rm F})$$

$$\text{and} \quad \epsilon_{\boldsymbol{k}+\boldsymbol{q}}-\epsilon_{\boldsymbol{k}} \simeq \boldsymbol{q}\cdot\nabla_{\boldsymbol{k}}\epsilon_{\boldsymbol{k}}$$

Thus one has

$$\varepsilon_1(\boldsymbol{q}) \simeq 1 + \frac{e^2}{\varepsilon_0 V q^2} \sum_{\boldsymbol{k},\sigma} \delta(\epsilon_{\boldsymbol{k}} - E_\mathrm{F})$$
$$= 1 + \frac{e^2}{\varepsilon_0 V q^2} \frac{2V}{(2\pi)^3} 4\pi \int_0^\infty \mathrm{d}k\, k^2 \delta(\epsilon_{\boldsymbol{k}} - E_\mathrm{F})$$
$$= 1 + \frac{e^2}{\varepsilon_0 q^2} \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} E_\mathrm{F}^{1/2} \quad \text{and}$$
$$\varepsilon_1(\boldsymbol{q}) \simeq 1 + \frac{e^2}{\varepsilon_0 q^2} \frac{1}{2\pi^2} \frac{2m}{\hbar^2} k_\mathrm{F} = 1 + \frac{k_\mathrm{FT}^2}{q^2} \quad \text{with} \quad k_\mathrm{FT}^2 = \frac{3ne^2}{2\varepsilon_0 E_\mathrm{F}}\,.$$

The meaning of k_FT becomes evident when looking at the screened Coulomb interaction $v_{\boldsymbol{q}}/\varepsilon_1(\boldsymbol{q}, 0)$ whose Fourier transform is of the form $\exp(-k_\mathrm{FT} r)/r$: $1/k_\mathrm{FT}$ is the Thomas–Fermi screening length.

4.12: Use the pair–distribution function (1.11)

$$g(\boldsymbol{r}) = 1 + \frac{1}{N} \sum_{\boldsymbol{q}} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} (S(\boldsymbol{q}) - 1) \quad \text{and use} \quad \frac{N}{V} = \sum_{\boldsymbol{p},\sigma} n_{\boldsymbol{p}\sigma} \quad \text{and}$$
$$S(\boldsymbol{q}) = \frac{1}{N} \sum_{\boldsymbol{p},\sigma} n_{\boldsymbol{p}\sigma}(1 - n_{\boldsymbol{p}+\boldsymbol{q}\sigma}) \quad \text{to write}$$
$$g(\boldsymbol{r}) = 1 + \frac{1}{NV} \sum_{\boldsymbol{q}} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \left[\frac{V}{N} \sum_{\boldsymbol{p},\sigma} n_{\boldsymbol{p}\sigma}\,(1 - n_{\boldsymbol{q}+\boldsymbol{q},\sigma}) - 1\right]$$
$$= 1 - \frac{V^2}{N^2} \sum_{\boldsymbol{q},\boldsymbol{p},\sigma} n_{\boldsymbol{p}\sigma} n_{\boldsymbol{p}+\boldsymbol{q}\sigma} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\,.$$

The summation can be carried out by writing

$$\cdots = \sum_{\boldsymbol{p},\sigma} n_{\boldsymbol{p}} \mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}} \sum_{\boldsymbol{q}} n_{\boldsymbol{p}+\boldsymbol{q}} \mathrm{e}^{\mathrm{i}(\boldsymbol{p}+\boldsymbol{q})\cdot\boldsymbol{r}} = 2 \sum_{\boldsymbol{p}} n_{\boldsymbol{p}} \mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}} \sum_{\boldsymbol{q}'} n_{\boldsymbol{q}'} \mathrm{e}^{\mathrm{i}\boldsymbol{q}'\cdot\boldsymbol{r}}\,.$$

This double sum with the occupation factors was carried out already in Sect. 4.4 for $T = 0\,\mathrm{K}$ by integrating over the Fermi sphere and yields $g(r) = 1 - \rho^\mathrm{HF}/en$ (see Fig. 4.13).

Solutions for Chap. 5

5.1: Taking spin into account, the expectation value of H_N with the Slater determinant Ψ_N is written

$$\langle \Psi_N | H_N | \Psi_N \rangle = \sum_{\alpha=1}^{N} \int \mathrm{d}x \psi_\alpha^*(x) \left(\frac{p^2}{2m} + V(\boldsymbol{r})\right) \psi_\alpha(x)$$
$$+ \frac{1}{2} \sum_{\substack{\alpha,\beta=1 \\ \alpha\neq\beta}}^{N} \int\int \mathrm{d}x \mathrm{d}x' \psi_\alpha^*(x) \psi_\beta^*(x') v(\boldsymbol{r} - \boldsymbol{r}') \psi_\alpha(x) \psi_\beta(x')$$
$$- \frac{1}{2} \sum_{\substack{\alpha,\beta=1 \\ \alpha\neq\beta}}^{N} \int\int \mathrm{d}x \mathrm{d}x' \psi_\alpha^*(x) \psi_\beta^*(x') v(\boldsymbol{r} - \boldsymbol{r}') \psi_\beta(x) \psi_\alpha(x').$$

Carrying out the summation over spin variables, the first two terms become identical with (5.8), while the third term (which appears because the Slater determinant is an antisymmetrized product of N single-particle wave functions) contributes only if ψ_α and ψ_β are states with the same spin. The variational principle leads for the first two terms to the Hartree equations, which become modified by a contribution from the third term, the exchange term (5.11).

5.2: For free electrons with $\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})/\sqrt{V}$ the averaged exchange density reads

$$\bar{n}^{\mathrm{HF}}(\boldsymbol{r},\boldsymbol{r}') = -\frac{2}{N}\sum_{\substack{\boldsymbol{k},\boldsymbol{k}'\\ |\boldsymbol{k}|,|\boldsymbol{k}'|\le k_{\mathrm{F}}}} \frac{1}{V}\mathrm{e}^{\mathrm{i}\boldsymbol{k}'\cdot(\boldsymbol{r}-\boldsymbol{r}')}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}$$

and with the Fourier transform of $1/|\boldsymbol{r}-\boldsymbol{r}'|$ the exchange potential becomes

$$\begin{aligned} V_{\mathrm{x,Slater}}(\boldsymbol{r}) &= -\frac{2e^2}{\varepsilon_0 NV}\sum_{\substack{\boldsymbol{k},\boldsymbol{k}'\\ |\boldsymbol{k}|,|\boldsymbol{k}'|\le k_{\mathrm{F}}}}\sum_{\boldsymbol{q}}\frac{1}{q^2}\underbrace{\frac{1}{V}\int_V \mathrm{e}^{\mathrm{i}(\boldsymbol{k}'-\boldsymbol{k}+\boldsymbol{q})\cdot(\boldsymbol{r}-\boldsymbol{r}')}\mathrm{d}^3r'}_{\delta_{\boldsymbol{k}-\boldsymbol{k}',\boldsymbol{q}}} \\ &= -\frac{2e^2}{\varepsilon_0 NV}\sum_{\substack{\boldsymbol{k},\boldsymbol{k}'\\ |\boldsymbol{k}|,|\boldsymbol{k}'|\le k_{\mathrm{F}}}}\frac{1}{|\boldsymbol{k}-\boldsymbol{k}'|^2} = -\frac{3}{8\pi^2\varepsilon_0}e^2 k_{\mathrm{F}}\,. \end{aligned}$$

With the exchange energy $\epsilon_x(n) = -3e^2 k_{\mathrm{F}}/16\pi^2\varepsilon_0$ from Sect. 4.4 one finds

$$V_x^{\mathrm{LDA}}(\boldsymbol{r}) = \frac{4}{3}\epsilon_x^{\mathrm{LDA}}(n(\boldsymbol{r})) = \frac{2}{3}V_{\mathrm{x,Slater}}(\boldsymbol{r}).$$

5.3: The number of discrete $\boldsymbol{k} = (k_1, k_2, k_3)$ with $k_i = 2\pi n_i/L_i$, $i = 1,2,3$ with $0 \le n_i < N_i$ in a Brillouin zone is $N = N_1N_2N_3$, which is the number of unit cells in the crystal or periodicity volume. Thus, for each electron in the unit cell with given spin there is one state in the energy band, i.e. each band can accommodate $2N$ electrons.

5.4: A point at the Brillouin zone boundary is characterized by the relation $\boldsymbol{k}' = \boldsymbol{k} - \boldsymbol{G}$. The condition of degeneracy is $k^2 = k'^2$, thus $(\boldsymbol{k}-\boldsymbol{G})^2 = (\boldsymbol{k}')^2$ becomes $2\boldsymbol{k}\cdot\boldsymbol{G} = \boldsymbol{G}^2$, which is the condition for Bragg reflection.

5.5: The primitive reciprocal lattice vectors of the square lattice are $\boldsymbol{b}_1 = (1,0)2\pi/a$, and $\boldsymbol{b}_2 = (0,1)2\pi/a$. Write the free electron energies

$$E(\boldsymbol{k}) = \frac{\hbar^2}{2m}(\boldsymbol{k}+\boldsymbol{G})^2 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2\kappa^2$$

for the smallest $\boldsymbol{G}$ at the points Γ, M, and X and connect corresponding points by parabolas defined by $\boldsymbol{G}$.

If $\nu = 1,2,3$ is the number of electrons per atom then, for one atom per unit cell, $n_s = \nu/a^2$ is the areal electron density. The radius of the Fermi circle is given by $k_{\mathrm{F}} = \sqrt{2\pi n_s}$ and the Fermi energy by

$$E_{\mathrm{F}} = \frac{\hbar^2}{2m}k_{\mathrm{F}}^2 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2\frac{\nu}{2\pi}$$

or $\kappa_{\mathrm{F}}^2 = \nu/2\pi$ which is 0.159 for $\nu = 1$.

5.6: Proceed as in Problem 5.5 and see [121] for the free-electron bands along $\Gamma - L$.

5.7: In the almost free-electron picture, the energy bands of Al, Si, and GaAs derive from the free-electron bands of the *fcc* lattice (see Problem 5.6). Due to the different crystal structures (Bravais lattice for Al, diamond structure for Si, zinc blende structure for GaAs) the energy gaps are determined by different Fourier components of the pseudo-potential:

$$V_{\mathrm{psp}}(\boldsymbol{r}) = \sum_{\boldsymbol{n},\boldsymbol{\tau}} v_{\mathrm{psp}}^{(\boldsymbol{\tau})}(\boldsymbol{r} - \boldsymbol{R}_{\boldsymbol{n}}^0 - \boldsymbol{\tau}) \quad \rightarrow \quad V_{\mathrm{psp}}(\boldsymbol{G}) = \mathrm{e}^{-\mathrm{i}\boldsymbol{g}\cdot\boldsymbol{\tau}} v_{\mathrm{psp}}^{(\boldsymbol{\tau})}(\boldsymbol{G}).$$

For Al with $\boldsymbol{\tau} = 0$, the structure factor $S(\boldsymbol{G}) = \sum_{\boldsymbol{\tau}} \exp(-\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{\tau})$ equals 1 for all $\boldsymbol{G}$. For diamond and zinc blende with $\boldsymbol{\tau} = \pm\boldsymbol{\tau}'$ with $\boldsymbol{\tau}' = (1,1,1)a/8$ one has

$$\begin{aligned} V_{\mathrm{psp}}(\boldsymbol{G}) &= \mathrm{e}^{-\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{\tau}'} v^{(+)}(\boldsymbol{G}) + \mathrm{e}^{\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{\tau}'} v^{(-)}(\boldsymbol{G}) \\ &= \cos(\boldsymbol{G}\cdot\boldsymbol{\tau}') v_{\mathrm{S}}(\boldsymbol{G}) - \mathrm{i}\sin(\boldsymbol{G}\cdot\boldsymbol{\tau}') v_{\mathrm{A}}(\boldsymbol{G}), \end{aligned}$$

where

$$v_{\mathrm{S}}(\boldsymbol{G}) = v^{(+)}(\boldsymbol{G}) + v^{(-)}(\boldsymbol{G}) \quad \text{and} \quad v_{\mathrm{A}}(\boldsymbol{G}) = v^{(+)}(\boldsymbol{G}) - v^{(-)}(\boldsymbol{G}).$$

In Si the anti-symmetric potential $v_{\mathrm{A}}(\boldsymbol{G})$ vanishes. Thus, Fourier components at different reciprocal lattice vectors determine the energy bands as Al, Si, GaAs. Especially, for $\boldsymbol{G} = (2,0,0)2\pi/a$ we have $\cos(\boldsymbol{G}\cdot\boldsymbol{\tau}) = 0$ but $\sin(\boldsymbol{G}\cdot\boldsymbol{\tau}) = 1$ and the anti-symmetric potential present in GaAs removes the degeneracy of the level X_1 in Si (see Fig. 5.11).

5.8: The crystal field splitting is determined by the matrix formed by

$$K_{\nu'\nu} = \sum_{\boldsymbol{n}} \int \mathrm{d}^3 r \phi_{\nu'}^*(\boldsymbol{r}) v(\boldsymbol{r} - \boldsymbol{R}_{\boldsymbol{n}}^0) \phi_{\nu}(\boldsymbol{r})$$

with $\nu = xy, yz, zx, 3z^2 - r^2, x^2 - y^2$. The point group operations of the cubic lattice turn the coordinate triple x, y, z into any other permutation including sign changes of x, y, and z, while leaving $\sum_{\boldsymbol{n}} v(\boldsymbol{r} - \boldsymbol{R}_{\boldsymbol{n}}^0)$ invariant. Thus, the groups of orbitals d_{xy}, d_{yz}, d_{zx} and $d_{3z^3-r^2}, d_{x^2-y^2}$ form invariant sets under the cubic point group, which are classified by the irreducible representations $\Gamma_{25'}$ and Γ_{12}, respectively, and the matrix with the elements $K_{\nu'\nu}$ has block-diagonal form. Further inspection shows, that each of the diagonal blocks is itself diagonal for the given basis with identical diagonal matrix elements, thus, the crystal field splitting gives a threefold ($\Gamma_{25'}$) and a twofold (Γ_{12}) state as can be seen at the Γ point of the band structures depicted in Figs. 5.14 and 5.15. There is no difference between sc, bcc, and fcc crystal structure because they have the same point group.

5.9: The overlap matrix $S_{\nu'\nu}(\boldsymbol{k})$ is hermitian and can be diagonalized by a unitary transformation U: $USU^{-1} = S'$ with $S'_{\mu'\mu} = S'_{\mu}\delta_{\mu,\mu'}$. The diagonal elements S'_{μ} of the transformed overlap matrix represent the norms of the new basis states which are always positive. Thus the eigenvalue equation can be rewritten

$$\underbrace{UHU^{-1}}_{H'}\,\underbrace{UC}_{C'} = E\,\underbrace{USU^{-1}}_{S'}\,\underbrace{UC}_{C'}.$$

One can multiply this equation with the inverse square root of the diagonal matrix S' to arrive at the eigenvalue equation

$$S'^{-1/2}H'S'^{-1/2}S'^{1/2}C' = ES'^{1/2}C'$$

and with $\tilde{H} = S'^{-1/2}H'S'^{-1/2}, \tilde{C} = S'^{1/2}C'$ one has the standard eigenvalue problem with the secular equation

$$\left\| \tilde{H}_{\mu'\mu} - E\delta_{\mu',\mu} \right\| = 0$$

with $\tilde{H} = S'^{-1/2}UH'U^{-1}S'^{-1/2}$.

5.10: The nearest neighbors in the sc crystal structure are

$$\boldsymbol{R}_{\boldsymbol{n}}^0 : a(\pm 1, 0, 0),\ (0, \pm 1, 0),\ (0, 0 \pm 1)$$

leading to the dispersion

$$E_s(\boldsymbol{k}) = E_s + 2J_{ss}(a)(\cos(k_x a) + \cos(k_y a) + \cos(k_z a))$$

which for $\boldsymbol{k} = (k, 0, 0)$ becomes $E_s(\boldsymbol{k}) = E_s + 2J_{ss}(a)\cos(ka)$ and for $\boldsymbol{k} = (k, k, k)$, $E_s(\boldsymbol{k}) = E_s + 6J_{ss}(a)\cos(ka)$ with band widths $E(0) - E((\pi/a, 0, 0)) = 4J_{ss}(a)$ and $E(0) - E((\pi/a, \pi/a, \pi/a)) = 12J_{ss}(a)$, respectively.
For the bcc crystal structure one has

$$\boldsymbol{R}_{\boldsymbol{n}}^0 : \frac{a}{2}(\pm 1, \pm 1, \pm 1),\ (\mp 1, \pm 1, \pm 1),\ (\pm 1, \mp 1, \pm 1),\ (\pm 1, \pm 1, \mp 1)$$

leading to the dispersion

$$E_s(\boldsymbol{k}) = E_s + 2J_{ss}\left(\frac{a}{\sqrt{3}}\right)\left\{\cos\left(\frac{a}{2}(k_x + k_y + k_z)\right) + \cos\left(\frac{a}{2}(-k_x + k_y + k_z)\right)\right.$$
$$\left. + \cos\left(\frac{a}{2}(k_x - k_y + k_z)\right) + \cos\left(\frac{a}{2}(k_x + k_y - k_z)\right)\right\}$$

which for $\boldsymbol{k} = (k, 0, 0)$ becomes $E_s(\boldsymbol{k}) = E_s + 8J_{ss}(a/\sqrt{3})\cos(ka/2)$ and for $\boldsymbol{k} = (k, k, k)$, $E_s(\boldsymbol{k}) = E_s + 2J_{ss}(a/\sqrt{3})(\cos(3ka/2) + 3\cos(ka/2))$ with band widths $E(0) - E((2\pi/a, 0, 0)) = 16J_{ss}(a/\sqrt{3})$ and $E(0) - E((\pi/a, \pi/a, \pi/a)) = 8J_{ss}(a/\sqrt{3})$.

5.11: For a solution see P.R. Wallace, Phys. Rev. **71**, 622 (1947) and the article by S.E. Louis in [114].

5.12: Use the Peierls substitution $\epsilon(\boldsymbol{k}) \to H(\boldsymbol{p} - e\boldsymbol{A})^2$ with the vector potential $\boldsymbol{A} = (0, B(x\cos\theta + z\sin\theta, 0))$ corresponding to $\boldsymbol{B} = B(\sin\theta, 0, \cos\theta)$ to write

$$H = \frac{p_x^2}{2m_t} + \frac{1}{2m_t}\left(p_y - eB(x\cos\theta + z\sin\theta)\right)^2 + \frac{p_z^2}{2m_l}.$$

The equations of motion for the components of the momentum are (up to terms $\sim p_y$ which vanish later due to $\dot{p}_y = 0$)

$$\dot{p}_x = -\frac{\mathrm{i}}{\hbar}[p_x, H] = -\frac{e^2B^2}{m_t}(x\cos\theta + z\sin\theta)\cos\theta$$
$$\dot{p}_z = -\frac{\mathrm{i}}{\hbar}[p_z, H] = -\frac{e^2B^2}{m_t}(x\cos\theta + z\sin\theta)\sin\theta.$$

Take the derivatives of these equation with respect to t and replace $\dot{x} = p_x/m_t$, $\dot{z} = p_z/m_l$ to obtain

$$-\ddot{p}_x = \omega_t^2 \cos^2\theta p_x + \omega_t\omega_l \sin\theta\cos\theta p_z$$
$$-\ddot{p}_z = \omega_t^2 \sin\theta\cos\theta p_x + \omega_t\omega_l \sin^2\theta p_z$$

with $\omega_{l,t} = eB/m_{l,t}$. With $p_{x,z} \sim \exp(-\mathrm{i}\omega t)$ this becomes a set of homogeneous linear equations and the eigenfrequencies follow from

$$\begin{Vmatrix} \omega_t^2\cos^2\theta - \omega^2 & \omega_t\omega_l \sin\theta\cos\theta \\ \omega_t^2 \sin\theta\cos\theta & \omega_t\omega_l \sin^2\theta - \omega^2 \end{Vmatrix} = 0$$

with the nontrivial solution

$$\omega^2 = \omega_t^2\cos^2\theta + \omega_t\omega_l \sin^2\theta = e^2B^2\left(\frac{\cos^2\theta}{m_t^2} + \frac{\sin^2\theta}{m_l m_t}\right).$$

The expression in the bracket is the squared inverse cyclotron mass for the anisotropic energy surface if the magnetic field includes the angle θ with the z-axis. See [4].

5.13: For $\boldsymbol{k} = (k_x, k_y, 0)$ and $\nabla V \| (001)$ the interface spin–orbit (or Rashba)-term reads

$$H_{\mathrm{SO}}(\boldsymbol{k}) = \alpha|\nabla V|(k_y\sigma_x - k_x\sigma_y)$$

and with $k_\pm = k_x \pm \mathrm{i}k_y = k\exp(\pm\mathrm{i}\varphi)$ and $\sigma_\pm = (\sigma_x \pm \mathrm{i}\sigma_y)/2$

$$H_{\mathrm{SO}}(k,\varphi) = \mathrm{i}\alpha|\nabla V|(k_+\sigma_- - k_-\sigma_+) = \mathrm{i}\alpha'(\mathrm{e}^{\mathrm{i}\varphi}\sigma_- - \mathrm{e}^{-\mathrm{i}\varphi}\sigma_+).$$

The subband Hamiltonian with spin–orbit interaction becomes

$$H(k,\varphi) = \begin{pmatrix} \epsilon_k & \mathrm{i}\alpha'\mathrm{e}^{-\mathrm{i}\varphi} \\ -\mathrm{i}\alpha'\mathrm{e}^{-\mathrm{i}\varphi} & \epsilon_k \end{pmatrix}.$$

Its eigenvalues $\epsilon_\pm(k) = \epsilon_k \pm \alpha|\nabla V|k$ do not depend on φ and are two parabolas shifted against each other. Use the eigenvectors

$$|\boldsymbol{k},\pm\rangle = \frac{1}{\sqrt{2}}\left|\begin{matrix} 1 \\ \mp\mathrm{i}\mathrm{e}^{\mathrm{i}\varphi}\end{matrix}\right\rangle$$

to calculate the expectation value of the vector of Pauli spin matrices:

$$\langle \boldsymbol{k},\pm|\boldsymbol{\sigma}|\boldsymbol{k},\pm\rangle = \pm(\boldsymbol{e}_x\sin\varphi - \boldsymbol{e}_y\cos\varphi).$$

Thus, the spin is always oriented perpendicular to the wave vector $\boldsymbol{k} = (k_x, k_y, 0)$ and rotates with φ. Note, that the states on each parabola form a Kramers pair. See [153].

Solutions for Chap. 6

6.1: Choose the quantum numbers for the Bloch states

$$\alpha = n\boldsymbol{k}\sigma,\ \beta = \bar{n}\bar{\boldsymbol{k}}\bar{\sigma},\ \alpha' = n'\boldsymbol{k}'\sigma',\ \beta' = \bar{n}'\bar{\boldsymbol{k}}'\bar{\sigma}'.$$

After carrying out the summation over spin variables the matrix element reduces to

$$V_{\alpha\beta\beta'\alpha'} = \int \mathrm{d}^3r \int \mathrm{d}^3r' \psi^*_{n\boldsymbol{k}\sigma}(\boldsymbol{r})\psi^*_{\bar{n}\bar{\boldsymbol{k}}\bar{\sigma}}(\boldsymbol{r}')\frac{e^2}{\kappa|\boldsymbol{r}-\boldsymbol{r}'|}\psi_{\bar{n}'\bar{\boldsymbol{k}}'\sigma}(\boldsymbol{r})\psi_{n'\boldsymbol{k}'\bar{\sigma}}(\boldsymbol{r}').$$

Decompose the Bloch function into plane wave and lattice periodic parts, expand the products of periodic parts with the same argument in a Fourier series

$$u^*_{n\boldsymbol{k}\sigma}(\boldsymbol{r})u_{\bar{n}'\bar{\boldsymbol{k}}'\sigma}(\boldsymbol{r}) = \sum_{\boldsymbol{G}} B_{n\bar{n}\boldsymbol{k}\bar{\boldsymbol{k}}\sigma}(\boldsymbol{G})\mathrm{e}^{\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{r}},$$

and use the Fourier transform of the Coulomb interaction to perform the integration over the space variables to find

$$\begin{aligned} V_{\alpha\beta\beta'\alpha'} = &\sum_{\boldsymbol{G},\boldsymbol{G}',\boldsymbol{q}} B_{n\bar{n}'\boldsymbol{k}\bar{\boldsymbol{k}}'\sigma}(\boldsymbol{G})B_{\bar{n}n'\bar{\boldsymbol{k}}\boldsymbol{k}'\bar{\sigma}}(\boldsymbol{G}') \\ &\times\frac{e^2}{\varepsilon_0 V q^2}\int \mathrm{d}^3 r \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}-\bar{\boldsymbol{k}}'-\boldsymbol{q}-\boldsymbol{G})\cdot\boldsymbol{r}}\int \mathrm{d}^3 r' \mathrm{e}^{-\mathrm{i}(\bar{\boldsymbol{k}}-\boldsymbol{k}'+\boldsymbol{q}-\boldsymbol{G}')\cdot\boldsymbol{r}'}. \end{aligned}$$

For the single-band approximation set $n = \bar{n} = \bar{n}' = n'$ and with only leading terms in the Fourier series, $\boldsymbol{G} = \boldsymbol{G}' = 0$, write

$$B_{n\bar{n}'\boldsymbol{k}\bar{\boldsymbol{k}}'\sigma}(\boldsymbol{G}) \to B_{\boldsymbol{k}\boldsymbol{q}},\ B_{\bar{n}n'\bar{\boldsymbol{k}}\boldsymbol{k}'\bar{\sigma}}(\boldsymbol{G}') \to B_{\bar{\boldsymbol{k}}\boldsymbol{q}}$$

and obtain

$$V_{\alpha\beta\beta'\alpha'} = \sum_{\boldsymbol{q}} v(\boldsymbol{q})V^2 B_{\boldsymbol{k}\boldsymbol{q}}B_{\bar{\boldsymbol{k}}\boldsymbol{q}}\delta_{\bar{\boldsymbol{k}}',\boldsymbol{k}-\boldsymbol{q}}\delta_{\bar{\boldsymbol{k}},\boldsymbol{k}'-\boldsymbol{q}}.$$

6.2: To check normalization and orthogonality write

$$\begin{aligned} &\sum_s \int \mathrm{d}^3 r \phi^*_{n\sigma}(\boldsymbol{r}-\boldsymbol{R})\phi_{n'\sigma'}(\boldsymbol{r}-\boldsymbol{R}') \\ &\quad = \frac{1}{N}\delta_{\sigma,\sigma'}\sum_{\boldsymbol{k},\boldsymbol{k}'}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'}\underbrace{\int \mathrm{d}^3 r\, \psi^*_{n\boldsymbol{k}\sigma}(\boldsymbol{r})\psi_{n'\boldsymbol{k}'\sigma}(\boldsymbol{r})}_{\delta_{n,n'}\delta_{\boldsymbol{k},\boldsymbol{k}'}} \\ &\quad = \underbrace{\frac{1}{N}\sum_{\boldsymbol{k}}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')}}_{\delta_{\boldsymbol{R},\boldsymbol{R}'}}\delta_{n,n'} = \delta_{n,n'}\delta_{\boldsymbol{R},\boldsymbol{R}'} \end{aligned}$$

Thus localized functions, represented by Bloch functions, are orthogonal when centered on different sites. Insofar the Wannier representation differs from the LCAO. Introduce fermion operators for these localized Wannier states by

$$c_{n\boldsymbol{R}\sigma} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}c_{n\boldsymbol{k}\sigma}$$

and calculate the anti-commutator

$$\begin{aligned} \left\{c_{n\boldsymbol{R}\sigma}, c^\dagger_{n'\boldsymbol{R}'\sigma'}\right\} &= \frac{1}{N}\sum_{\boldsymbol{k},\boldsymbol{k}'}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'}\underbrace{\left\{c_{n\boldsymbol{k}\sigma}, c^\dagger_{n'\boldsymbol{k}'\sigma'}\right\}}_{\delta_{n,n'}\delta_{\boldsymbol{k},\boldsymbol{k}'}\delta_{\sigma,\sigma'}} \\ &= \delta_{n,n'}\delta_{\sigma,\sigma'}\frac{1}{N}\sum_{\boldsymbol{k}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')} = \delta_{n,n'}\delta_{\sigma,\sigma'}\delta_{\boldsymbol{R},\boldsymbol{R}'}. \end{aligned}$$

The other anti-commutators yield

$$\left\{c^\dagger_{n\boldsymbol{R}\sigma}, c^\dagger_{n'\boldsymbol{R}'\sigma'}\right\} = \left\{c_{n\boldsymbol{R}\sigma}, c_{n'\boldsymbol{R}'\sigma'}\right\}.$$

6.3: Use the representation (6.7) of the Bloch functions to write

$$V_{\alpha\beta\beta'\alpha'} = \frac{1}{N^2} \sum_{\boldsymbol{R}_1,\boldsymbol{R}_2,\boldsymbol{R}'_1,\boldsymbol{R}'_2} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_1}\mathrm{e}^{-\mathrm{i}\bar{\boldsymbol{k}}\cdot\boldsymbol{R}_2}\mathrm{e}^{\mathrm{i}\bar{\boldsymbol{k}}'\cdot\boldsymbol{R}'_1}\mathrm{e}^{\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'_2}$$
$$\times \int \mathrm{d}^3r \int \mathrm{d}^3r'\, \phi^*(\boldsymbol{r}-\boldsymbol{R}_1)\phi^*(\boldsymbol{r}'-\boldsymbol{R}_2)\frac{e^2}{\kappa|\boldsymbol{r}-\boldsymbol{r}'|}\phi(\boldsymbol{r}-\boldsymbol{R}'_1)\phi(\boldsymbol{r}'-\boldsymbol{R}'_2).$$

Use (6.8) with the exponentials and sums over the wave vectors to replace the fermion operators of Bloch states in the interaction term by those of Wannier states to find (6.10).

6.4: The commutator between $c^\dagger_\uparrow c_\downarrow$ and $c^\dagger_\downarrow c_\uparrow$

$$[c^\dagger_\uparrow c_\downarrow, c^\dagger_\downarrow c_\uparrow] = c^\dagger_\uparrow c_\downarrow c^\dagger_\downarrow c_\uparrow - c^\dagger_\downarrow c_\uparrow c^\dagger_\uparrow c_\downarrow$$

is evaluated by using the anti-commutator for fermion operators and writing

$$\begin{aligned} c^\dagger_\uparrow c_\downarrow c^\dagger_\downarrow c_\uparrow &= c^\dagger_\uparrow(1-c^\dagger_\downarrow c_\downarrow)c_\uparrow = c^\dagger_\uparrow c_\uparrow - c^\dagger_\uparrow c^\dagger_\downarrow c_\downarrow c_\uparrow \\ &= c^\dagger_\uparrow c_\uparrow - c^\dagger_\downarrow(1-c_\uparrow c^\dagger_\uparrow)c_\downarrow = c^\dagger_\uparrow c_\uparrow - c^\dagger_\downarrow c_\downarrow + c^\dagger_\downarrow c_\uparrow c^\dagger_\uparrow, \end{aligned}$$

where the last term cancels in the commutator. Thus we have

$$[c^\dagger_\uparrow c_\downarrow, c^\dagger_\downarrow c_\uparrow] = c^\dagger_\uparrow c_\uparrow - c^\dagger_\downarrow c_\downarrow.$$

The other commutation relations

$$[c^\dagger_\uparrow c_\downarrow, c^\dagger_\uparrow c_\uparrow - c^\dagger_\downarrow c_\downarrow] = -2c^\dagger_\uparrow c_\downarrow\,, \quad \text{and} \quad [c^\dagger_\downarrow c_\uparrow, c^\dagger_\uparrow c_\uparrow - c^\dagger_\downarrow c_\downarrow] = 2c^\dagger_\downarrow c_\uparrow$$

follow in a similar way. These three commutators are the same as those between $S^\pm$ and S^z and correspond to the operator algebra of the Cartesian components of the angular momentum S^x, S^y, and S^z.

6.5: Evaluate the commutator

$$\begin{aligned} [S^\beta_i S^\beta_k, S^x_j] &= S^\beta_k S^x_j S^\beta_i - S^x_j S^\beta_i S^\beta_k \\ &= -\mathrm{i}\varepsilon_{x\beta\gamma} S^\gamma_j S^\beta_k \delta_{i,j} - S^\beta_i \mathrm{i}\varepsilon_{x\beta\gamma} S^\gamma_j \delta_{j,k}, \end{aligned}$$

to write the commutator of S^x_j with the first term of the Heisenberg hamiltonian

$$\sum_{\substack{i,k\\ i\neq k}} J_{ik} \sum_\beta [S^\beta_i S^\beta_k, S^x_j] = \begin{cases} -\sum_{k\neq j}\sum_{\beta,\gamma} J_{jk}\mathrm{i}\varepsilon_{x\beta\gamma} S^\gamma_j S^\beta_k & \text{for} \quad i=j,\ k\neq j \\ -\sum_{i\neq j}\sum_{\beta,\gamma} J_{ij}\mathrm{i}\varepsilon_{x\beta\gamma} S^\beta_i S^\gamma_j & \text{for} \quad k=j,\ k\neq i \end{cases}$$
$$= -\mathrm{i}\sum_{i\neq j} J_{ij}\left(\boldsymbol{S}_i \times \boldsymbol{S}_j\right)_x$$

where for obtaining the last line use was made of $i \neq k$ and of the meaning of the Levi–Civita symbol. For the commutator with the second term of the Heisenberg hamiltonian evaluate

$$\sum_i [S^z_i, S^x_j] = \sum_{i,\beta} \mathrm{i}\varepsilon_{zx\beta} S^\beta_j \delta_{i,j} = \mathrm{i}S^y_j.$$

Putting together both contributions find

$$\frac{\mathrm{d}S_j^x}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}\left[\mathcal{H}_{\mathrm{spin}}, S_j^x\right] = -\frac{1}{\hbar}\left(\sum_i J_{ij}\big(\boldsymbol{S}_i \times \boldsymbol{S}_j\big)_x + g\mu_{\mathrm{B}}\big(\boldsymbol{H}_{\mathrm{ext}} \times \boldsymbol{S}_j\big)_x\right).$$

6.6: Evaluate the commutator

$$\begin{aligned}\left[\alpha_{\boldsymbol{k}}, \alpha_{\boldsymbol{k}'}^\dagger\right] &= \left[u_{\boldsymbol{k}} b_{1\boldsymbol{k}} - v_{\boldsymbol{k}} b_{2\boldsymbol{k}}^\dagger, u_{\boldsymbol{k}'} b_{1\boldsymbol{k}'}^\dagger - v_{\boldsymbol{k}'} b_{2\boldsymbol{k}'}\right] \\ &= u_{\boldsymbol{k}} u_{\boldsymbol{k}'} \underbrace{\left[b_{1\boldsymbol{k}}, b_{1\boldsymbol{k}'}^\dagger\right]}_{\delta_{\boldsymbol{k},\boldsymbol{k}'}} + v_{\boldsymbol{k}} v_{\boldsymbol{k}'} \underbrace{\left[b_{2\boldsymbol{k}}^\dagger, b_{2\boldsymbol{k}'}\right]}_{-\delta_{\boldsymbol{k},\boldsymbol{k}'}} = \left(u_{\boldsymbol{k}}^2 - v_{\boldsymbol{k}}^2\right)\delta_{\boldsymbol{k},\boldsymbol{k}'},\end{aligned}$$

which for $\left(u_{\boldsymbol{k}}^2 - v_{\boldsymbol{k}}^2\right) = 1$ is a boson commutation relation. In the same way, calculate

$$\begin{aligned}[\alpha_{\boldsymbol{k}}, \beta_{\boldsymbol{k}'}] &= \left[u_{\boldsymbol{k}} b_{1\boldsymbol{k}} - v_{\boldsymbol{k}} b_{2\boldsymbol{k}}^\dagger, u_{\boldsymbol{k}'} b_{2\boldsymbol{k}'} - v_{\boldsymbol{k}'} b_{1\boldsymbol{k}'}^\dagger\right] \\ &= -u_{\boldsymbol{k}} v_{\boldsymbol{k}'}\left[b_{1\boldsymbol{k}}, b_{1\boldsymbol{k}'}^\dagger\right] - v_{\boldsymbol{k}} u_{\boldsymbol{k}'}\left[b_{2\boldsymbol{k}}^\dagger, b_{2\boldsymbol{k}'}\right] = 0.\end{aligned}$$

The remaining commutation relations are obtained in a similar way.

6.7: Using the new boson operators for coupled magnon–phonon modes, the hamiltonian becomes

$$\begin{aligned}H_{\mathrm{p-m}} = \sum_{\boldsymbol{k}} \big\{ &\alpha_{\boldsymbol{k}}^\dagger \alpha_{\boldsymbol{k}} \left(\hbar\omega_{\boldsymbol{k}}^{\mathrm{p}} \cos^2\Theta_{\boldsymbol{k}} + \hbar\omega_{\boldsymbol{k}}^{\mathrm{m}} \sin^2\Theta_{\boldsymbol{k}} - 2c_{\boldsymbol{k}} \sin\Theta_{\boldsymbol{k}} \cos\Theta_{\boldsymbol{k}}\right) \\ &+ \beta_{\boldsymbol{k}}^\dagger \beta_{\boldsymbol{k}} \left(\hbar\omega_{\boldsymbol{k}}^{\mathrm{p}} \sin^2\Theta_{\boldsymbol{k}} + \hbar\omega_{\boldsymbol{k}}^{\mathrm{m}} \cos^2\Theta_{\boldsymbol{k}} + 2c_{\boldsymbol{k}} \sin\Theta_{\boldsymbol{k}} \cos\Theta_{\boldsymbol{k}}\right) \\ &+ \alpha_{\boldsymbol{k}}^\dagger \beta_{\boldsymbol{k}} \left[(\hbar\omega_{\boldsymbol{k}}^{\mathrm{p}} - \hbar\omega_{\boldsymbol{k}}^{\mathrm{m}}) \sin\Theta_{\boldsymbol{k}} \cos\Theta_{\boldsymbol{k}} + c_{\boldsymbol{k}} \left(\cos^2\Theta_{\boldsymbol{k}} - \sin^2\Theta_{\boldsymbol{k}}\right)\right] \\ &+ \alpha_{\boldsymbol{k}} \beta_{\boldsymbol{k}}^\dagger \left[(\hbar\omega_{\boldsymbol{k}}^{\mathrm{p}} - \hbar\omega_{\boldsymbol{k}}^{\mathrm{m}}) \sin\Theta_{\boldsymbol{k}} \cos\Theta_{\boldsymbol{k}} + c_{\boldsymbol{k}} \left(\cos^2\Theta_{\boldsymbol{k}} - \sin^2\Theta_{\boldsymbol{k}}\right)\right] \big\}.\end{aligned}$$

It can be diagonalized with

$$\left(\hbar\omega_{\boldsymbol{k}}^{\mathrm{p}} - \hbar\omega_{\boldsymbol{k}}^{\mathrm{m}}\right) \sin\Theta_{\boldsymbol{k}} \cos\Theta_{\boldsymbol{k}} + c_{\boldsymbol{k}}\left(\cos^2\Theta_{\boldsymbol{k}} - \sin^2\Theta_{\boldsymbol{k}}\right) = 0$$

or

$$\tan 2\Theta_{\boldsymbol{k}} = \frac{-2c_{\boldsymbol{k}}}{\hbar\omega_{\boldsymbol{k}}^{\mathrm{p}} - \hbar\omega_{\boldsymbol{k}}^{\mathrm{m}}}.$$

For $\omega_{\boldsymbol{k}}^{\mathrm{p}} = \omega_{\boldsymbol{k}}^{\mathrm{m}} = \omega_{\boldsymbol{k}}$ we have $\cos^2\Theta_{\boldsymbol{k}} = \sin^2\Theta_{\boldsymbol{k}} = 1/2$ and find for the eigenenergies of the coupled modes

$$\hbar\omega_{\boldsymbol{k}}^{\alpha} = \hbar\omega_{\boldsymbol{k}} - c_{\boldsymbol{k}} \quad \text{and} \quad \hbar\omega_{\boldsymbol{k}}^{\beta} = \hbar\omega_{\boldsymbol{k}} + c_{\boldsymbol{k}}$$

and for the corresponding boson operators

$$\alpha_{\boldsymbol{k}} = \frac{1}{\sqrt{2}}\left(a_{\boldsymbol{k}} - b_{\boldsymbol{k}}\right) \quad \text{and} \quad \beta_{\boldsymbol{k}} = \frac{1}{\sqrt{2}}\left(a_{\boldsymbol{k}} + b_{\boldsymbol{k}}\right).$$

6.8: With the inverted transformation relations (6.59) write the terms of (6.56):

$$
\begin{aligned}
b_{1\boldsymbol{k}}^\dagger b_{1\boldsymbol{k}} &= \alpha_{\boldsymbol{k}}^\dagger \alpha_{\boldsymbol{k}} u_{\boldsymbol{k}}^2 + \beta_{\boldsymbol{k}}^\dagger \beta_{\boldsymbol{k}} v_{\boldsymbol{k}}^2 + \left(\alpha_{\boldsymbol{k}}^\dagger \beta_{\boldsymbol{k}}^\dagger + \alpha_{\boldsymbol{k}} \beta_{\boldsymbol{k}}\right) u_{\boldsymbol{k}} v_{\boldsymbol{k}} \\
b_{2\boldsymbol{k}}^\dagger b_{2\boldsymbol{k}} &= \beta_{\boldsymbol{k}}^\dagger \beta_{\boldsymbol{k}} u_{\boldsymbol{k}}^2 + \alpha_{\boldsymbol{k}} \alpha_{\boldsymbol{k}}^\dagger v_{\boldsymbol{k}}^2 + \left(\beta_{\boldsymbol{k}}^\dagger \alpha_{\boldsymbol{k}}^\dagger + \beta_{\boldsymbol{k}} \alpha_{\boldsymbol{k}}\right) u_{\boldsymbol{k}} v_{\boldsymbol{k}} \\
b_{1\boldsymbol{k}}^\dagger b_{2\boldsymbol{k}}^\dagger &= \left(\alpha_{\boldsymbol{k}}^\dagger \alpha_{\boldsymbol{k}} + \beta_{\boldsymbol{k}} \beta_{\boldsymbol{k}}^\dagger\right) u_{\boldsymbol{k}} v_{\boldsymbol{k}} + \alpha_{\boldsymbol{k}}^\dagger \beta_{\boldsymbol{k}}^\dagger u_{\boldsymbol{k}}^2 + \beta_{\boldsymbol{k}} \alpha_{\boldsymbol{k}} v_{\boldsymbol{k}}^2 \\
b_{1\boldsymbol{k}} b_{2\boldsymbol{k}} &= \left(\alpha_{\boldsymbol{k}} \alpha_{\boldsymbol{k}}^\dagger + \beta_{\boldsymbol{k}}^\dagger \beta_{\boldsymbol{k}}\right) u_{\boldsymbol{k}} v_{\boldsymbol{k}} + \alpha_{\boldsymbol{k}} \beta_{\boldsymbol{k}} u_{\boldsymbol{k}}^2 + \beta_{\boldsymbol{k}}^\dagger \alpha_{\boldsymbol{k}}^\dagger v_{\boldsymbol{k}}^2
\end{aligned}
$$

to obtain

$$
\begin{aligned}
\mathcal{H}_{\text{spin}} \simeq E_{\text{a}} + 2J_{\text{a}} \nu S \sum_{\boldsymbol{k}} \Big\{ &\left(\alpha_{\boldsymbol{k}}^\dagger \alpha_{\boldsymbol{k}} + \beta_{\boldsymbol{k}}^\dagger \beta_{\boldsymbol{k}}\right)\left(u_{\boldsymbol{k}}^2 + v_{\boldsymbol{k}}^2 + 2\gamma_{\boldsymbol{k}} u_{\boldsymbol{k}} v_{\boldsymbol{k}}\right) \\
&+ \left(\alpha_{\boldsymbol{k}}^\dagger \beta_{\boldsymbol{k}}^\dagger + \alpha_{\boldsymbol{k}} \beta_{\boldsymbol{k}}\right)\left(2u_{\boldsymbol{k}} v_{\boldsymbol{k}} + \gamma_{\boldsymbol{k}}(u_{\boldsymbol{k}}^2 + v_{\boldsymbol{k}}^2)\right) + 2(\gamma_{\boldsymbol{k}} u_{\boldsymbol{k}} v_{\boldsymbol{k}} + v_{\boldsymbol{k}}^2) \Big\}.
\end{aligned}
$$

Add and subtract $u_{\boldsymbol{k}}^2$ under the sum to find with $u_{\boldsymbol{k}}^2 - v_{\boldsymbol{k}}^2 = 1$ the expression (6.60).

6.9: Extend (6.53) by the terms due to the anisotropy field H_{A} and the external field H_{ext}

$$
\mathcal{H}_{\text{spin}} = J_{\text{a}} \sum_{n.n.ij} \boldsymbol{S}_{1i} \cdot \boldsymbol{S}_{2j} - g\mu_{\text{B}} \sum_i \left(\left(H_{\text{A}} + H_{\text{ext}}\right) S_{1i}^z - \left(H_{\text{A}} - H_{\text{ext}}\right) S_{2i}^z\right)
$$

and replace the spin operators by boson operators on each sublattice using the Holstein–Primakoff transformation to obtain

$$
\begin{aligned}
\mathcal{H}_{\text{spin}} = &- 2J_{\text{a}} \nu N S^2 - 4g\mu_{\text{B}} H_{\text{A}} N S \\
&+ 2J_a \nu S \sum_{\boldsymbol{k}} \left\{ b_{1\boldsymbol{k}}^\dagger b_{1\boldsymbol{k}} + b_{2\boldsymbol{k}}^\dagger b_{2\boldsymbol{k}} + \gamma_{\boldsymbol{k}} \left(b_{1\boldsymbol{k}}^\dagger b_{2\boldsymbol{k}}^\dagger + b_{1\boldsymbol{k}} b_{2\boldsymbol{k}}\right) \right\} \\
&+ 2g\mu_{\text{B}} H_{\text{A}} \sum_{\boldsymbol{k}} \left(b_{1\boldsymbol{k}}^\dagger b_{1\boldsymbol{k}} + b_{2\boldsymbol{k}}^\dagger b_{2\boldsymbol{k}} \right) + g\mu_{\text{B}} H_{\text{ext}} \sum_{\boldsymbol{k}} \left(b_{1\boldsymbol{k}}^\dagger b_{1\boldsymbol{k}} - b_{2\boldsymbol{k}}^\dagger b_{2\boldsymbol{k}} \right).
\end{aligned}
$$

Eliminate the coupling between the sublattices using the Bogoliubov transformation (6.57) and write with the abbreviations

$$
\begin{aligned}
\mathcal{C} &= -2J_{\text{a}} \nu N S^2 - 4g\mu_{\text{B}} H_{\text{A}} N S\,,\ A = 2J_{\text{a}} \nu S\,,\ B = 2g\mu_{\text{B}} H_{\text{A}}\,,\ C = g\mu_{\text{B}} H_{\text{ext}} \\
\mathcal{H}_{\text{spin}} \simeq \mathcal{C} + \sum_{\boldsymbol{k}} \Big\{ &A\gamma_{\boldsymbol{k}} \left(2u_{\boldsymbol{k}} v_{\boldsymbol{k}} \left(\alpha_{\boldsymbol{k}}^\dagger \alpha_{\boldsymbol{k}} + \beta_{\boldsymbol{k}}^\dagger \beta_{\boldsymbol{k}} + 1\right) + (u_{\boldsymbol{k}}^2 + v_{\boldsymbol{k}}^2)\left(\alpha_{\boldsymbol{k}}^\dagger \beta_{\boldsymbol{k}}^\dagger + \alpha_{\boldsymbol{k}} \beta_{\boldsymbol{k}}\right) \right) \\
&+ (A + B) \left((u_{\boldsymbol{k}}^2 + v_{\boldsymbol{k}}^2)\left(\alpha_{\boldsymbol{k}}^\dagger \alpha_{\boldsymbol{k}} + \beta_{\boldsymbol{k}}^\dagger \beta_{\boldsymbol{k}}\right) + 2u_{\boldsymbol{k}} v_{\boldsymbol{k}} \left(\alpha_{\boldsymbol{k}}^\dagger \beta_{\boldsymbol{k}}^\dagger + \alpha_{\boldsymbol{k}} \beta_{\boldsymbol{k}}\right) + 2v_{\boldsymbol{k}}^2 \right) \\
&+ C\left(\alpha_{\boldsymbol{k}}^\dagger \alpha_{\boldsymbol{k}} - \beta_{\boldsymbol{k}}^\dagger \beta_{\boldsymbol{k}}\right) \Big\}.
\end{aligned}
$$

Diagonalize with $A\gamma_{\boldsymbol{k}}\left(u_{\boldsymbol{k}}^2 + v_{\boldsymbol{k}}^2\right) = -2(A + B) u_{\boldsymbol{k}} v_{\boldsymbol{k}}$. Square this relation and use $u_{\boldsymbol{k}}^2 - v_{\boldsymbol{k}}^2 = 1$ to get a biquadratic equation for $u_{\boldsymbol{k}}$. Take its solution to find

$$
u_{\boldsymbol{k}}^2 + v_{\boldsymbol{k}}^2 = \pm \left\{ \frac{(A + B)^2}{(A + B)^2 - A^2 \gamma_{\boldsymbol{k}}^2} \right\}^{1/2},\ u_{\boldsymbol{k}} v_{\boldsymbol{k}} = \mp \frac{1}{2} \left\{ \frac{A^2 \gamma_{\boldsymbol{k}}^2}{(A + B)^2 - A^2 \gamma_{\boldsymbol{k}}^2} \right\}^{1/2}.
$$

Identify the prefactor of the magnon number operators as the magnon energy

$$\hbar\omega_{\boldsymbol{k}} = \left\{(A+B)^2 - A^2\gamma_{\boldsymbol{k}}^2\right\}^{1/2}$$

which without anisotropy field ($B = 0$) reduces to the dispersion relation for the antiferromagnetic magnons which for small k is linear. With anisotropy field one finds a finite magnon energy for $\boldsymbol{k} = 0$ and a quadratic dispersion for small k as can be seen in Fig. 6.8.

6.10: Evaluate for low temperature ($T \ll T_{\mathrm{C}}$) the magnetization (per unit volume)

$$M(T) = g\mu_{\mathrm{B}}\left(NS - \sum_{\boldsymbol{k}}\langle b_{\boldsymbol{k}}^{\dagger} b_{\boldsymbol{k}}\rangle\right) \quad \text{or}$$

$$\begin{aligned} M(0) - M(T) &= g\mu_{\mathrm{B}} \sum_{\boldsymbol{k}} \frac{1}{\exp\left(\hbar\omega_{\boldsymbol{k}}/k_{\mathrm{B}}T\right) - 1} \\ &= g\mu_{\mathrm{B}} \frac{4\pi}{(2\pi)^3} \int_0^{\infty} \frac{k^2 \mathrm{d}k}{\exp\left(Dk^2/k_{\mathrm{B}}T\right) - 1} \end{aligned}$$

where the quadratic dispersion for small k is used. The integral (it is a Bose integral) can be solved as described in the Appendix (A.3) to yield Bloch's $T^{3/2}$ law:

$$M(0) - M(T) = \zeta(\frac{3}{2}) \frac{g\mu_{\mathrm{B}}}{M(0)} \left(\frac{k_{\mathrm{B}}}{4\pi D}\right)^{3/2} T^{3/2}.$$

See [166].

6.11: Calculate the expectation value in (6.106) for $T = 0$:

$$\begin{aligned} \langle \ldots \rangle_0 = \sum_m \big\{ &\langle \Psi_0 | M_+(\boldsymbol{q}, \tau) | \Psi_m \rangle \langle \Psi_m | M_-(-\boldsymbol{q}, 0) | \Psi_0 \rangle \\ &- \langle \Psi_0 | M_-(-\boldsymbol{q}, 0) | \Psi_m \rangle \langle \Psi_m | M_+(\boldsymbol{q}, \tau) | \Psi_0 \rangle \big\}. \end{aligned}$$

Replace the operators $M_{\pm}$ by the fermion operators and extract the exponentials with the time dependence. The energy difference $E_m - E_0$ of exact eigenstates becomes in HF approximation the energy difference of single-particle energies for particle–hole excitations with spin-flip across the Fermi energy. By manipulations as in Sect. 4.5 one arrives at the spin susceptibility (6.108).

To evaluate (6.108), use

$$\epsilon_{\boldsymbol{k}+\boldsymbol{q}\uparrow} - \epsilon_{\boldsymbol{k}\downarrow} = -\Delta + \frac{\hbar^2}{m}\boldsymbol{k}\cdot\boldsymbol{q} + \epsilon_{\boldsymbol{q}}\,, \;\; \epsilon_{\boldsymbol{k}\uparrow} - \epsilon_{\boldsymbol{k}-\boldsymbol{q}\downarrow} = -\Delta + \frac{\hbar^2}{m}\boldsymbol{k}\cdot\boldsymbol{q} - \epsilon_{\boldsymbol{q}}$$

with $\epsilon_q = \hbar^2 q^2/2m$ and perform the sum over $\boldsymbol{k}$ with the substitution $\boldsymbol{k}\cdot\boldsymbol{q} = kq\cos\theta\,,\ \cos\theta = x$. The first term can be written

$$\begin{aligned} A_{\downarrow} &= \sum_{|\boldsymbol{k}| \le k_{\mathrm{F}\downarrow}} \frac{1}{\hbar\omega + \epsilon_{\boldsymbol{k}+\boldsymbol{q}\uparrow} - \epsilon_{\boldsymbol{k}\downarrow}} \\ &= \frac{V}{(2\pi)^2} \int_0^{k_{\mathrm{F}\downarrow}} \mathrm{d}k\, k^2 \int_{-1}^{+1} \frac{1}{\hbar\omega - \Delta + \epsilon_q + \hbar^2 kqx/m} \mathrm{d}x. \end{aligned}$$

The integral over x can be solved according to

$$\int_{-1}^{+1} \frac{\mathrm{d}x}{a+bx} = \frac{1}{b}\int_{a-b}^{a+b} \frac{\mathrm{d}z}{z} = \frac{1}{b}\ln\left|\frac{1+b/a}{1-b/a}\right|.$$

Looking for collective excitations at small q one has $b/a \ll 1$ and can use the expansion

$$\frac{1}{b}\ln\left|\frac{1+b/a}{1-b/a}\right| \simeq \frac{2}{b}\left\{\frac{b}{a}+\frac{1}{3}\left(\frac{b}{a}\right)^3\right\} = \frac{2}{a}\left\{1+\frac{1}{3}\left(\frac{b}{a}\right)^2\right\}$$

to obtain

$$A_\downarrow = \frac{2V}{(2\pi)^2}\frac{1}{\hbar\omega-\Delta+\epsilon_q}\int_0^{k_\mathrm{F}^-}\mathrm{d}k\,k^2\left\{1+\frac{k^2}{3}\left(\frac{\hbar^2 q}{m}\right)^2\left(\frac{1}{\hbar\omega-\Delta+\epsilon_q}\right)^2\right\}.$$

After integration and corresponding evaluation of the second term $A_\uparrow$ one arrives at (6.108).

Solutions for Chap. 7

7.1: Evaluate the commutator $[c_{\bar{\boldsymbol{k}},\bar\sigma}, c^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma}c^\dagger_{\boldsymbol{k}'-\boldsymbol{q}\sigma'}c_{\boldsymbol{k}'\sigma'}c_{\boldsymbol{k}\sigma}]$ by successively interchanging $c_{\bar{\boldsymbol{k}},\bar\sigma}$ with the four operators appearing in the interaction term. Each step leads to a change in sign and in addition gives a Kronecker δ for exchange with the creation operators, thus

$$c_{\bar{\boldsymbol{k}},\bar\sigma}c^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma}c^\dagger_{\boldsymbol{k}'-\boldsymbol{q}\sigma'}c_{\boldsymbol{k}'\sigma'}c_{\boldsymbol{k}\sigma} = \delta_{\bar{\boldsymbol{k}},\boldsymbol{k}+\boldsymbol{q}}\delta_{\bar\sigma,\sigma}c^\dagger_{\boldsymbol{k}'-\boldsymbol{q}\sigma'}c_{\boldsymbol{k}'\sigma'}c_{\boldsymbol{k}\sigma} - \delta_{\bar{\boldsymbol{k}},\boldsymbol{k}'-\boldsymbol{q}}c^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma}c_{\boldsymbol{k}'\sigma'}c_{\boldsymbol{k}\sigma}.$$

Interchange the last two operators in the second term and replace σ by σ' and $\boldsymbol{k}$ by $\boldsymbol{k}'$. Replace in the first term $\boldsymbol{q}$ by $-\boldsymbol{q}$ and consider the properties of the interaction matrix element to find the expression for $[c_{\bar{\boldsymbol{k}}}, \mathcal{H}_\mathrm{int}]$ (7.20). The commutator $[c^\dagger_{\bar{\boldsymbol{k}}}, \mathcal{H}_\mathrm{int}]$ is evaluated by analogous steps.

7.2: The equation of motion of the full Green function $G(\boldsymbol{k}\sigma; t-t')$ (7.21) can be written with (7.23) as

$$\left(\mathrm{i}\hbar\frac{\partial}{\partial t}-\epsilon_{\boldsymbol{k}\sigma}\right)G(\boldsymbol{k}\sigma;t-t') = \delta(t-t') + \int \mathrm{d}t''\,\Sigma(\boldsymbol{k}\sigma;t-t'')G(\boldsymbol{k}\sigma;t''-t').$$

Replace the Green function and the self-energy by their Fourier transform with respect to the time arguments and identify the integrands to obtain

$$(\hbar\omega-\epsilon_{\boldsymbol{k}\sigma})\,G(\boldsymbol{k}\sigma;\omega) = 1+\Sigma(\boldsymbol{k}\sigma;\omega)G(\boldsymbol{k}\sigma;\omega).$$

After multiplication with the Green function of the noninteracting system

$$G^0(\boldsymbol{k}\sigma;\omega) = (\hbar\omega-\epsilon_{\boldsymbol{k}\sigma})^{-1}$$

one arrives at the Dyson equation

$$G(\boldsymbol{k}\sigma;\omega) = G^0(\boldsymbol{k}\sigma;\omega) + G^0(\boldsymbol{k}\sigma;\omega)\Sigma(\boldsymbol{k}\sigma;\omega)G(\boldsymbol{k}\sigma;\omega).$$

7.3: The commutator of $n_{i-\sigma}c_{i\sigma}$ with the single-particle part H_0 yields three terms due to interchange of creation and annihilation operators:

$$
\begin{aligned}
[n_{i-\sigma}c_{i\sigma}, H_0] &= \sum_{mj\sigma'} t_{mj} \left(c^\dagger_{i-\sigma} c_{i-\sigma} c_{i\sigma} c^\dagger_{m\sigma'} c_{j\sigma'} - c^\dagger_{m\sigma'} c_{j\sigma'} c^\dagger_{i-\sigma} c_{i-\sigma} c_{i\sigma} \right) \\
&= \sum_{mj\sigma'} t_{mj} \left(\delta_{im}\delta_{\sigma\sigma'} n_{i-\sigma} c_{j\sigma} - \delta_{im}\delta_{\sigma-\sigma'} c^\dagger_{i-\sigma} c_{i\sigma} c_{j-\sigma} \right. \\
&\quad \left. - \delta_{ij}\delta_{\sigma-\sigma'} c^\dagger_{m-\sigma} c_{i-\sigma} c_{i\sigma} \right) \\
&= \sum_m t_{im} \left(n_{i-\sigma} c_{m\sigma} + c^\dagger_{i-\sigma} c_{m-\sigma} c_{i\sigma} - c^\dagger_{m-\sigma} c_{i-\sigma} c_{i\sigma} \right),
\end{aligned}
$$

where the last line is obtained by proper choice of the summation indices and rearranging the operators. Similarly the commutator with the interaction term is evaluated

$$
\begin{aligned}
[n_{i-\sigma}c_{i\sigma}, H_1] &= \frac{1}{2} U \sum_{m\sigma'} \left(n_{i-\sigma} c_{i\sigma} n_{m\sigma'} n_{m-\sigma'} - n_{m\sigma'} n_{m-\sigma'} n_{i-\sigma} c_{i\sigma} \right) \\
&= \frac{1}{2} U \sum_{m\sigma'} n_{i-\sigma} \left(c_{i\sigma} c^\dagger_{m\sigma'} c_{m\sigma'} n_{m-\sigma'} - n_{m\sigma'} n_{m-\sigma'} c_{i\sigma} \right) \\
&= \frac{1}{2} U \sum_{m\sigma'} n_{i-\sigma} \left(\delta_{im}\delta_{\sigma\sigma'} c_{i\sigma} n_{i-\sigma} + \delta_{im}\delta_{\sigma-\sigma'} n_{i-\sigma} c_{i\sigma} \right),
\end{aligned}
$$

which using $n^2_{i-\sigma} = n_{i-\sigma}$ becomes (7.55).

7.4: Calculate the derivative of the self-energy (7.70) and obtain the spectral weight

$$
Z(E) = \left(1 - \frac{\partial \Sigma}{\partial E} \right)^{-1} = \frac{\left(E - \epsilon_0 - U(1 - \langle n_{-\sigma} \rangle) \right)^2}{\left(E - \epsilon_0 - U(1 - \langle n_{-\sigma} \rangle) \right)^2 + U^2 \langle n_{-\sigma} \rangle (1 - \langle n_{-\sigma} \rangle)}.
$$

For the lower Hubbard band with $E = \epsilon_0 + 2t \cos ka$ this becomes

$$
Z_{\text{lower}} = \frac{\left(2t \cos ka - U(1 - \langle n_{-\sigma} \rangle) \right)^2}{\left(2t \cos ka - U(1 - \langle n_{-\sigma} \rangle) \right)^2 + U^2 \langle n_{-\sigma} \rangle (1 - \langle n_{-\sigma} \rangle)}
$$

and reduces for $k = \pi/2a$ to $Z_{\text{lower}} = 1 - \langle n_{-\sigma} \rangle$. For the upper Hubbard band with $E = \epsilon_0 + U + 2t \cos ka$ the result is

$$
Z_{\text{upper}} = \frac{\left(2t \cos ka + U \langle n_{-\sigma} \rangle \right)^2}{\left(2t \cos ka + U \langle n_{-\sigma} \rangle \right)^2 + U^2 \langle n_{-\sigma} \rangle (1 - \langle n_{-\sigma} \rangle)}
$$

and $Z_{\text{upper}} = \langle n_{-\sigma} \rangle$ for $k = \pi/2a$. Note that the spectral weights for $k = \pi/2a$ are those of the atomic limit (see Fig. 7.3).

7.5: This problem is solved in some detail in [169, 206]. It leads to the so-called $t-J$ model, where t is the hopping integral and $J \sim t^2/U$ is the effective exchange matrix element.

7.6: Describing the delocalized electrons by fermion operators $c^\dagger_{\boldsymbol{k}\sigma}, c_{\boldsymbol{k}\sigma}$ in a band with dispersion $\epsilon_{\boldsymbol{k}}$ and the localized electrons with energy ϵ_d by fermion operators $d^\dagger_\sigma, d_\sigma$, the Hamiltonian is formulated as

$$
\begin{aligned}
H &= \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \sum_\sigma \epsilon_d d^\dagger_\sigma d_\sigma \\
&\quad + \sum_{\boldsymbol{k},\sigma} V_{\boldsymbol{k}\sigma} \left(d^\dagger_\sigma c_{\boldsymbol{k}\sigma} + c^\dagger_{\boldsymbol{k}\sigma} d_\sigma \right) + U n^d_\uparrow n^d_\downarrow .
\end{aligned}
$$

Here the third term describes the hybridization between the localized and delocalized electrons. This is the Anderson impurity model. It can be extended by considering instead of a single impurity a periodic configuration of sites i with d electrons. For this case the fermion operators for d electrons become $d^\dagger_{i\sigma}, d_{i\sigma}$ and summation over the sites i is to be considered. See P.W. Anderson: Phys. Rev. **124** 41 (1961) and [64] Sect. 6.2, [122, 195].

7.7: For the solution see [122, 195]. It uses a contour integration in the complex frequency plane taking into account the position of the poles for quasi-particles and holes.

7.8: Start from (4.136) for the real part of the dielectric function, which for $T = 0$ reads

$$\varepsilon_1(\boldsymbol{q},\omega) = 1 + v_{\boldsymbol{q}} \sum_{|\boldsymbol{k}|\le k_\mathrm{F}} \frac{2\epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}-\boldsymbol{q}}}{(\hbar\omega - \epsilon_{\boldsymbol{k}} + \epsilon_{\boldsymbol{k}-\boldsymbol{q}})(\hbar\omega - \epsilon_{\boldsymbol{k}+\boldsymbol{q}} + \epsilon_{\boldsymbol{k}})}.$$

Making use of the free electron dispersion $\epsilon_{\boldsymbol{k}} = \hbar^2 k^2/2m$ the numerator simplifies to $-\hbar^2 q^2/m$ while the denominator takes the form

$$(\hbar\omega - \epsilon_{\boldsymbol{k}} + \epsilon_{\boldsymbol{k}-\boldsymbol{q}})(\hbar\omega - \epsilon_{\boldsymbol{k}+\boldsymbol{q}} + \epsilon_{\boldsymbol{k}}) = \left(\hbar\omega - \frac{\hbar^2}{m}\boldsymbol{k}\cdot\boldsymbol{q}\right)^2 - \left(\frac{\hbar^2}{2m}q^2\right)^2$$

and the expression to be evaluated by integration is

$$\sum_{|\boldsymbol{k}|\le k_\mathrm{F}} \frac{1}{\left(\hbar\omega - \frac{\hbar^2}{m}\boldsymbol{k}\cdot\boldsymbol{q}\right)^2 - \left(\frac{\hbar^2}{2m}q^2\right)^2} = \left(\frac{2m}{\hbar^2}\right)^2 \sum_{|\boldsymbol{k}|\le k_\mathrm{F}} \frac{1}{(q_s^2 - 2\boldsymbol{k}\cdot\boldsymbol{q})^2 - q^4},$$

with $q_s^2 = 2m\hbar\omega/\hbar^2$.

For $d = 1$ the vectors become scalars and the sum can be written as the integral (using the substitution $x = 2kq$)

$$I(q,\omega) = \frac{L}{2\pi}\int_{-k_\mathrm{F}}^{k_\mathrm{F}} \frac{\mathrm{d}k}{q_s^4 - q^4 - 4q_s^2 kq + 4k^2q^2} = \frac{L}{2\pi}\int_{-x_\mathrm{F}}^{x_\mathrm{F}} \frac{\mathrm{d}k}{x^2 - 2q_s^2 x + q_s^4 - q^4}.$$

The integral can be found in integral tables giving

$$I(q,\omega) = \frac{L}{2\pi}\frac{1}{4q^3}\ln\left|\frac{(2k_\mathrm{F}q - 2q^2)^2 - 4q_s^4}{(2k_\mathrm{F}q + 2q^2)^2 - 4q_s^4}\right|.$$

For $\omega = 0$ (or $q_s = 0$) this integral diverges for $q \to k_\mathrm{F}$.

For $d = 3$, considering from the beginning the simpler case $\omega = 0$, the corresponding integral is

$$I(q) = \frac{L^3}{(2\pi)^3} 2\pi \int_0^{k_\mathrm{F}} \mathrm{d}k\, k \int_{-1}^{+1} \frac{\mathrm{d}\cos\vartheta}{4k^2q^2\cos^2\vartheta - q^4} = \frac{L^3}{8\pi^2 q^3}\int_0^{k_\mathrm{F}} \mathrm{d}k\, \ln\left|\frac{k-q}{k+q}\right|,$$

and yields by integration

$$I(q) = \frac{L^3}{8\pi^2 q^2}\left\{\left(\frac{k_\mathrm{F}}{q} - 1\right)\ln\left(\frac{k_\mathrm{F}}{q} - 1\right) - \left(\frac{k_\mathrm{F}}{q} + 1\right)\ln\left(\frac{k_\mathrm{F}}{q} + 1\right)\right\}.$$

For $q \to k_\mathrm{F}$ this integral remains finite.

Solutions for Chap. 8

8.1: The operator for linear electron–phonon interaction

$$\mathcal{H}_{\mathrm{el-ph}} = -\sum_{l,\boldsymbol{n},\boldsymbol{\tau}} \nabla_l v(\boldsymbol{r}_l - \boldsymbol{R}_{\boldsymbol{n}\boldsymbol{\tau}})\big|_{\boldsymbol{R}^0_{\boldsymbol{n}\boldsymbol{\tau}}} \cdot \boldsymbol{u}_{\boldsymbol{n}\boldsymbol{\tau}}$$

can be written in terms of phonon and electron operators using (3.22) together with (3.39) and by replacing with (4.76)

$$\sum_{l} \nabla_l v(\boldsymbol{r}_l - \boldsymbol{R}_{\boldsymbol{n}\boldsymbol{\tau}})\big|_{\boldsymbol{R}^0_{\boldsymbol{n}\boldsymbol{\tau}}} \to \sum_{n,\boldsymbol{k},n',\boldsymbol{k}'} \langle n\boldsymbol{k}|\nabla v|n'\boldsymbol{k}'\rangle c^\dagger_{n\boldsymbol{k}} c_{n'\boldsymbol{k}'}.$$

The sum over the lattice sites $\boldsymbol{n}$ effects only the gradient of the potential and has the form of a Bloch function

$$\sum_{\boldsymbol{n}} \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}^0_{\boldsymbol{n}}} \nabla v(\boldsymbol{r} - \boldsymbol{R}_{\boldsymbol{n}\boldsymbol{\tau}})\big|_{\boldsymbol{R}^0_{\boldsymbol{n}\boldsymbol{\tau}}} = \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \mathcal{U}_{\boldsymbol{q}\boldsymbol{\tau}}(\boldsymbol{r})$$

where $\mathcal{U}_{\boldsymbol{q}\boldsymbol{\tau}}(\boldsymbol{r})$ is a lattice periodic function. After decomposition of the electron Bloch functions in the matrix element into plane wave and lattice periodic part the product $u^*_{n\boldsymbol{k}}(\boldsymbol{r}) u_{n'\boldsymbol{k}'}(\boldsymbol{r}) \mathcal{U}_{\boldsymbol{q}\boldsymbol{\tau}}(\boldsymbol{r})$ can be expanded in a Fourier series. Thus the integration over the crystal volume can be carried out with

$$\int \mathrm{d}^3 r\, \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}'-\boldsymbol{q}-\boldsymbol{G})\cdot\boldsymbol{r}} \sim \delta_{\boldsymbol{k},\boldsymbol{k}'+\boldsymbol{q}+\boldsymbol{G}}$$

and yields the relation between the involved wave vectors.

8.2: Using (3.76) one has $\partial u_i/\partial x_i = \epsilon_{ii}$ and can write

$$\nabla \cdot \boldsymbol{u}(\boldsymbol{r}) = \sum_i \frac{\partial}{\partial x_i} u_i(\boldsymbol{r}) = \sum_i \epsilon_{ii} = \mathrm{Tr}\boldsymbol{\epsilon}.$$

For $\boldsymbol{u}(\boldsymbol{r}) \sim \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}$ follows $\nabla \cdot \boldsymbol{u} = \mathrm{i}\boldsymbol{q} \cdot \boldsymbol{u}$ which differs from zero only for longitudinal phonons.

8.3: For transverse phonons with $\boldsymbol{q} = \sum_\alpha q_\alpha \boldsymbol{e}_\alpha, \boldsymbol{u} = \sum_\beta u_\beta \boldsymbol{e}_\beta$ we have in general $\boldsymbol{q}\cdot\boldsymbol{u} = \sum_\alpha q_\alpha u_\alpha = -\mathrm{i}\mathrm{Tr}\boldsymbol{\epsilon} = 0$ but e.g. for the special case $\boldsymbol{q} = (q, 0, 0), \boldsymbol{u} = (0, u_2, u_3)$ the strain tensor components are

$$\epsilon_{11} = \epsilon_{22} = \epsilon_{33} = \epsilon_{23} = 0, \text{ but } \epsilon_{12} = \frac{\mathrm{i}}{2} q u_2,\ \epsilon_{13} = \frac{\mathrm{i}}{2} q u_3,$$

giving a nonvanishing contribution to the electron–phonon interaction.

8.4: Start with the classical expression for the interaction energy (8.23) with

$$\begin{aligned}\nabla \cdot \boldsymbol{P}(\boldsymbol{r}) &= -\frac{1}{4} e_{14} |\varepsilon_{ijk}| \left(q_i q_k u_j + q_i q_j u_k\right) \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \quad \text{double index summation} \\ &= -2 e_{14} \left(q_y q_z u_x + q_z q_x u_y + q_x q_y u_z\right) \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}.\end{aligned}$$

Using (8.24) for the charge density, expressing the displacement field by phonon operators, and integrating over the crystal volume converts $E_{\rm int}$ into the operator

$$\mathcal{H}^{\rm P}_{\rm el-ph} = -\frac{2ee_{14}}{\varepsilon_0\varepsilon_\infty}\sum_{s,\boldsymbol{q}}\sqrt{\frac{\hbar N}{2M\omega_s(\boldsymbol{q})}}\frac{q_xq_ye^s_z(\boldsymbol{q})+c.p.}{q^2} \times\left(a^\dagger_s(-\boldsymbol{q})+a_s(\boldsymbol{q})\right)\sum_{\boldsymbol{k}}c^\dagger_{\boldsymbol{k}+\boldsymbol{q}}c_{\boldsymbol{k}}.$$

8.5: To be calculated is the expression $\langle\tau\rangle$ (8.71) with the given dependencies of τ. The integrals are solved with the substitution $\epsilon/k_{\rm B}T = x$ and we may write

$$\int_0^\infty \epsilon^{3/2}{\rm e}^{-\epsilon/k_{\rm B}T}{\rm d}\epsilon = (k_{\rm B}T)^{5/2}\int_0^\infty x^{3/2}{\rm e}^{-x}{\rm d}x \sim T^{5/2}.$$

Similar for $\tau \sim T^{-1}\epsilon^{-1/2}$

$$\int_0^\infty \tau\epsilon^{3/2}{\rm e}^{-\epsilon/k_{\rm B}T}{\rm d}\epsilon = T^{-1}\,(k_{\rm B}T)^2\int_0^\infty x{\rm e}^{-x}{\rm d}x \sim T$$

and for $\tau \sim T^{-1}\epsilon^{1/2}$

$$\int_0^\infty \tau\epsilon^{3/2}{\rm e}^{-\epsilon/k_{\rm B}T}{\rm d}\epsilon = T^{-1}\,(k_{\rm B}T)^3\int_0^\infty x{\rm e}^{-x}{\rm d}x \sim T^2.$$

Thus for deformation potential coupling $\mu(T) \sim T^{-3/2}$ and for piezoelectric coupling $\mu(T) \sim T^{-1/2}$. This explains the different slopes of the corresponding graphs in Fig. 8.5. For more details see [4, 246].

8.6: For the solution see [4], Chap. 7. The calculation is essentially the same as for the Fröhlich coupling but with the $1/q$ dependence of the interaction potential replaced by a $\sqrt{q}$ dependence. The number of virtually excited phonons being proportional to the square of the effective mass of the electron turns out to be much smaller than 1. Replacing the electron by the much heavier ion would increase this number to a value much larger than 1 indicating that the perturbation calculation is not appropriate.

8.7: We have to evaluate the commutator

$$[\mathcal{H}_{\rm el-ph}, S] = \sum_{\substack{\boldsymbol{k},\boldsymbol{q}\\ \boldsymbol{k}',\boldsymbol{q}'}} \mathcal{V}_{\boldsymbol{q}}\mathcal{V}_{\boldsymbol{q}'}\left[c^\dagger_{\boldsymbol{k}+\boldsymbol{q}}c_{\boldsymbol{k}}\left(a^\dagger_{-\boldsymbol{q}}+a_{\boldsymbol{q}}\right), c^\dagger_{\boldsymbol{k}'+\boldsymbol{q}'}c_{\boldsymbol{k}'}\left(\alpha a^\dagger_{-\boldsymbol{q}'}+\beta a_{\boldsymbol{q}'}\right)\right]$$

and write

$$[\ldots,\ldots] = \left[a^\dagger_{-\boldsymbol{q}}+a_{\boldsymbol{q}}, \alpha a^\dagger_{-\boldsymbol{q}'}+\beta a_{\boldsymbol{q}'}\right]c^\dagger_{\boldsymbol{k}+\boldsymbol{q}}c_{\boldsymbol{k}}c^\dagger_{\boldsymbol{k}'+\boldsymbol{q}'}c_{\boldsymbol{k}'} + \left[c^\dagger_{\boldsymbol{k}+\boldsymbol{q}}c_{\boldsymbol{k}}, c^\dagger_{\boldsymbol{k}'+\boldsymbol{q}'}c_{\boldsymbol{k}'}\right]\left(\alpha a^\dagger_{-\boldsymbol{q}'}+\beta a_{\boldsymbol{q}'}\right)\left(a^\dagger_{-\boldsymbol{q}}+a_{\boldsymbol{q}}\right).$$

The electron part of the first term can be rearranged giving

$$c^\dagger_{\boldsymbol{k}+\boldsymbol{q}}c_{\boldsymbol{k}}c^\dagger_{\boldsymbol{k}'+\boldsymbol{q}'}c_{\boldsymbol{k}'} = c^\dagger_{\boldsymbol{k}+\boldsymbol{q}}c^\dagger_{\boldsymbol{k}'+\boldsymbol{q}'}c_{\boldsymbol{k}'}c_{\boldsymbol{k}} + \delta_{\boldsymbol{k},\boldsymbol{k}'-\boldsymbol{q}}\hat{n}_{\boldsymbol{k}'}$$

where the first term has the structure of an electron–electron interaction (this is the one we are looking for). The phonon part of the first term gives

$$\left[a^{\dagger}_{-\boldsymbol{q}} + a_{\boldsymbol{q}}, \alpha a^{\dagger}_{-\boldsymbol{q}'} + \beta a_{\boldsymbol{q}'}\right] = (-\alpha + \beta)\delta_{\boldsymbol{q},\boldsymbol{q}'}.$$

The second term, being bilinear in the phonon operators, is neglected as well as the term with the electron number operator to obtain the approximate form of the commutator $[\mathcal{H}_{\mathrm{el-ph}}, S]$.

8.8: Using (8.120) the ground state expectation value of $\bar{\mathcal{H}}$ relative to the ground state of the normal system is

$$E_0 = \langle \bar{\mathcal{H}} \rangle + \sum_{\boldsymbol{k}} |E(\boldsymbol{k})|$$

and can be written with

$$\langle \sigma_{kz} \rangle = \cos\theta_{\boldsymbol{k}}\,,\ \langle \sigma_{kx} \rangle = \sin\theta_{\boldsymbol{k}} \quad \text{and} \quad \frac{V_{\mathrm{eff}}}{4} \sum_{\boldsymbol{k}'} \sin\theta_{\boldsymbol{k}'} = E(\boldsymbol{k}) \tan\theta_{\boldsymbol{k}}$$

as

$$E_0 = -\sum_{\boldsymbol{k}} E(\boldsymbol{k}) \left(\cos\theta_{\boldsymbol{k}} + \frac{1}{2}\tan\theta_{\boldsymbol{k}} \sin\theta_{\boldsymbol{k}}\right) + \sum_{\boldsymbol{k}} |E(\boldsymbol{k})|.$$

With

$$E(\boldsymbol{k}) \tan\theta_{\boldsymbol{k}} \sin\theta_{\boldsymbol{k}} = \frac{2\Delta^2}{V_{\mathrm{eff}}} \quad \text{and} \quad \cos\theta_{\boldsymbol{k}} = \frac{E(\boldsymbol{k})}{(E^2(\boldsymbol{k}) + \Delta^2)^{1/2}}$$

and by replacing the sum over $\boldsymbol{k}$ by an energy integral over the shell with thickness $\hbar\omega_{\mathrm{D}}$ at the Fermi energy, one finds

$$E_0 = 2D(E_{\mathrm{F}}) \int_0^{\hbar\omega_{\mathrm{D}}} \mathrm{d}\epsilon \left\{\epsilon - \frac{\epsilon^2}{(\epsilon^2 + \Delta^2)^{1/2}}\right\} - \frac{\Delta^2}{V_{\mathrm{eff}}},$$

where $D(E_{\mathrm{F}})$ is the density of states at the Fermi energy. The integration can easily be performed and yields

$$E_0 = D(E_{\mathrm{F}})(\hbar\omega_{\mathrm{D}})^2 \left\{1 - \left[1 + \left(\frac{\Delta}{\hbar\omega_{\mathrm{D}}}\right)^2\right]^{1/2}\right\} \simeq -\left(D(E_{\mathrm{F}})\hbar\omega_{\mathrm{D}}\right)^2 V_{\mathrm{eff}}.$$

The last expression, obtained for $1 \gg D(E_{\mathrm{F}})V_{\mathrm{eff}}$, tells us that the superconducting state is stable as long as the effective interaction is positive.

Solutions for Chap. 9

9.1: Besides the poles of $G_0(E)$ the full Green function $G(E)$ has additional poles for $1 - G_0(E)U = 0$. In site representation U has block-diagonal form with a non-zero block $U^1 = U_{\{R_I\}}$ only in the diagonal for lattice sites around the impurity. With $G_0(E)$ written in the corresponding block form (with $G_{0,\{R_I\}}(E) = G_0^1(E)$ and corresponding matrices for the other blocks), the matrix multiplication can be performed to give

$$G_0(E)U = \begin{pmatrix} G_0^1(E) & G_0^2(E) \\ G_0^3(E) & G_0^4(E) \end{pmatrix} \begin{pmatrix} U & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} G_0^1(E)U^1 & 0 \\ G_0^3(E)U^1 & 0 \end{pmatrix}.$$

The determinant of $1 - G_0(E)U$ is the product of the determinants of its diagonal blocks or $\|1 - G_{0,\{R_I\}}(E)U_{\{R_I\}}\| = 0$.

9.2: The average of the individual resistances is

$$\langle r\rangle = \frac{1}{N}\sum_{i=1}^{N} r_i \quad \text{and therefore} \quad \langle R\rangle = \langle\sum_{i=1}^{N} r_i\rangle = \sum_{i=1}^{N}\langle r_i\rangle = N\langle r\rangle.$$

The variance of R is given by

$$\mathrm{Var}R = \langle\sum_{ij} r_i r_j\rangle - N^2\langle r\rangle^2 = \langle\sum_{i} r_i^2\rangle + \langle\sum_{i\neq j} r_i r_j\rangle - N^2\langle r\rangle^2$$

and with uncorrelated fluctuations of the r_i

$$\mathrm{Var}R = N\langle r^2\rangle + N(N-1)\langle r\rangle^2 - N^2\langle r\rangle^2 = N\left(\langle r^2\rangle - \langle r\rangle^2\right).$$

The relative variance given by

$$\frac{\mathrm{Var}R}{\langle R\rangle^2} = \frac{1}{N}\frac{\mathrm{Var}r}{\langle r\rangle^2} \quad \text{vanishes for } N\to\infty.$$

9.3: The transverse response reads

$$\chi(0,\omega) = e^2\sum_{i,f,i',f'}\langle i|\hat{v}|f\rangle\langle f'|\hat{v}|i'\rangle\frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}\tau\langle[c_i^\dagger(\tau)c_f(\tau), c_{f'}^\dagger c_{i'}]\rangle_0.$$

The time dependence of the operators gives a factor $\exp\left(\mathrm{i}(\epsilon_i-\epsilon_f)\tau/\hbar\right)$ and the integral over τ yields

$$\frac{\mathrm{i}}{\hbar}\int_0^\infty \mathrm{d}\tau \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\hbar\omega+\epsilon_i-\epsilon_f+\mathrm{i}\delta)\tau} = -\frac{1}{\hbar\omega+\epsilon_i-\epsilon_f+\mathrm{i}\delta},$$

where the small parameter δ is introduced to regularize the integral. To evaluate the remaining thermal expectation value first calculate the commutator

$$[c_i^\dagger c_f, c_{f'}^\dagger c_{i'}] = c_i^\dagger c_{i'}\delta_{f,f'} - c_{f'}^\dagger c_f\delta_{i,i'}.$$

With the thermal expectation value of $\langle c_i^\dagger c_{i'}\rangle_0 = f(\epsilon_i)\delta_{i,i'}$ the response function takes the form of (9.87)

$$\chi(0,\omega) = -e^2\sum_{i,f}\left|\langle i|\hat{v}|f\rangle\right|^2\frac{f(\epsilon_i)-f(\epsilon_f)}{\hbar\omega+\epsilon_i-\epsilon_f+\mathrm{i}\delta}.$$

9.4: Write (for finite ω) the δ function in the form

$$\delta(\hbar\omega+\epsilon_i-\epsilon_f) = \int \mathrm{d}E\,\delta(E-\epsilon_i)\delta(E+\hbar\omega-\epsilon_f)$$

so that with $\epsilon_i = E$ and $\epsilon_f = E+\hbar\omega$ the conductivity is expressed by

$$\sigma(0,\omega) = \pi e^2\int \mathrm{d}E\frac{f(E)-f(E+\hbar\omega)}{\omega}\sum_{i,f}\left|\langle i|\hat{v}|f\rangle\right|^2\delta(E-\epsilon_i)\delta(E+\hbar\omega-\epsilon_f).$$

The δ functions can be replaced with (2.77) and $E^+ = E+\mathrm{i}\delta$ by the imaginary part of the corresponding single-particle Green functions and give for the double sum

expression under the integral

$$\sum_{i,f} \ldots = \sum_{i,f} \langle i|\hat{v}|f\rangle\langle f|\hat{v}|i\rangle \mathrm{Im}G_{ii}(E^+)\mathrm{Im}G_{ff}(E^+ + \hbar\omega)$$
$$= \frac{1}{\pi^2} \sum_{i,f} \langle i|\hat{v}G(E^+ + \hbar\omega)|f\rangle\langle f|\hat{v}G(E^+)|i\rangle,$$

which for $\omega \to 0$ leads to $\mathrm{Tr}(\hat{v}\mathrm{Im}G(E^+)\hat{v}\mathrm{Im}G(E^+))$.

9.5: Write $\beta(g)$ in the form

$$\beta(g) = \frac{\mathrm{d}g}{\mathrm{d}L}\frac{L}{g}.$$

For $g \to \infty$ use $g(L) = \sigma L^{d-2}$ and σ independent of L to find

$$\frac{\mathrm{d}g}{\mathrm{d}L} = \sigma(d-2)L^{d-3} = (d-2)\frac{g}{L}$$

which means

$$\lim_{g\to\infty} \beta(g) = d - 2.$$

For $g \to 0$ use $g(L) \sim \exp(-L/\lambda)$ with $\mathrm{d}g/\mathrm{d}L = -g/\lambda$ and

$$\lim_{g\to 0} \beta(g) = -\frac{L}{\lambda}.$$

The sign of $\beta(g)$ is determined by $\mathrm{d}g/\mathrm{d}L$. For $d \leq 2$ and assuming a monotonous function it is always negative while for $d > 2$ there is a sign change.

Solutions for Chap. 10

10.1: For Bloch states $c\boldsymbol{k}, v\boldsymbol{k}'$ write

$$\frac{1}{m}\langle c\boldsymbol{k}|\boldsymbol{p}|v\boldsymbol{k}'\rangle = -\frac{\mathrm{i}}{\hbar}\langle c\boldsymbol{k}|\boldsymbol{r}H_0 - H_0\boldsymbol{r}|v\boldsymbol{k}'\rangle = \frac{\mathrm{i}}{\hbar}\left(E_c(\boldsymbol{k}) - E_v(\boldsymbol{k}')\right)\langle c\boldsymbol{k}|\boldsymbol{r}|v\boldsymbol{k}'\rangle$$

which for direct transitions at $\boldsymbol{k} = 0$ gives $e\boldsymbol{p}_{cv} = -\mathrm{i}E_\mathrm{g}\boldsymbol{d}_{cv}/\hbar$. Use $\boldsymbol{E}(t) = -\partial\boldsymbol{A}/\partial t$ and $\boldsymbol{A}(t)\ \exp(\mathrm{i}\omega t)$ with $\hbar\omega = E_c(\boldsymbol{k}) - E_v(\boldsymbol{k})$ to obtain

$$\frac{e}{m}\boldsymbol{p}_{cv}\cdot\boldsymbol{A} = \frac{\mathrm{i}}{\omega}\frac{e}{m}\boldsymbol{p}_{cv}\cdot\boldsymbol{E} = \frac{E_\mathrm{g}}{\hbar\omega}\boldsymbol{d}_{cv}\cdot\boldsymbol{E} \simeq \boldsymbol{d}_{cv}\cdot\boldsymbol{E}$$

with $\hbar\omega \simeq E_\mathrm{g}$ for near band gap excitations.

10.2: Express Bloch functions by Wannier functions (see Problem 6.2) to write

$$\langle n\boldsymbol{k}|\boldsymbol{p}|n'\boldsymbol{k}'\rangle = \frac{1}{N}\sum_{\boldsymbol{R},\boldsymbol{R}'} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'}\int \phi_n^*(\boldsymbol{r}-\boldsymbol{R})\boldsymbol{p}\phi_{n'}(\boldsymbol{r}-\boldsymbol{R}')\mathrm{d}^3r\,.$$

Replace $\boldsymbol{R}' = \boldsymbol{R} - \boldsymbol{R}''$ and change integration variable to $\boldsymbol{r}' = \boldsymbol{r} - \boldsymbol{R}$ to find

$$\langle n\boldsymbol{k}|\boldsymbol{p}|n'\boldsymbol{k}'\rangle = \frac{1}{N}\sum_{\boldsymbol{R}} \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}}\sum_{\boldsymbol{R}''} \mathrm{e}^{\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}''}\int \phi_n^*(\boldsymbol{r}')\boldsymbol{p}\phi_{n'}(\boldsymbol{r}'-\boldsymbol{R}'')\mathrm{d}^3r'\,.$$

The first sum gives $N\delta_{\boldsymbol{k},\boldsymbol{k}'}$.

10.3: The solution of the Schroedinger equation with a spherically symmetric potential is

$$\phi_{nlm}(\boldsymbol{r}) = R_{nl}(r)Y_{lm}(\theta,\varphi)\,.$$

The radial solution for the Coulomb problem is given by

$$R_{nl}(r) = N_n\rho^l \mathrm{e}(-\rho/2)F(l+1-\eta;2l+2;\rho)$$

with the hypergeometric function depending on the variables η (for the energy) and ρ (for the radial coordinate). For bound states one has $E_n = -R_{\mathrm{exc}}/n^2$ and $\rho = 2r/na_{\mathrm{B}}$. Only s-states with $l = 0$ have a nonvanishing amplitude at $r = 0$, thus $\phi_n(0) = N_nF(1-n;2;0)$ with $N_n = 1/na_{\mathrm{B}}$ and $|\phi_n(0)|^2 = (\pi a_{\mathrm{B}}^3 n^3)^{-1}$. For the continuum ($E = \hbar\omega - E_{\mathrm{g}} > 0$), $\eta = \mathrm{i}\gamma$, $\gamma = (R_{\mathrm{exc}}/(\hbar\omega - E_{\mathrm{g}}))^{1/2}$ and $N = \Gamma(1-\mathrm{i}\gamma)\exp(\pi\gamma/2)$ one obtains

$$|\phi(0)|^2 = \pi\gamma\frac{\exp(\pi\gamma)}{\sinh(\pi\gamma)}\,.$$

The absorption coefficient is the one of (10.23) for the uncorrelated electron-hole pairs multiplied by the enhancement factor $C(\omega)$.

10.4: Using (10.37) and (10.38) one can write

$$B^\dagger_{\nu\boldsymbol{Q}}|\Psi_0\rangle = |\Psi_{\nu\boldsymbol{Q}}\rangle = \sum_{\substack{c\boldsymbol{k}_h, c\boldsymbol{k}_e \\ \boldsymbol{k}_e - \boldsymbol{k}_h = \boldsymbol{Q}}} \Phi_{\nu\boldsymbol{Q}}(\boldsymbol{k}) c^\dagger_{c\boldsymbol{k}_e} c_{v\boldsymbol{k}_h}|\Psi_0\rangle\,.$$

Thus, in application to the ground state $|\Psi_0\rangle$, the exciton operator is a linear combination of products $c^\dagger_{c\boldsymbol{k}_e}c_{v\boldsymbol{k}_h}$. Let us assume a two-band model, i.e. the excitons are formed from states with fixed c, v, and consider for simplicity the exciton with $\boldsymbol{Q} = 0$ which implies $\boldsymbol{k}_e = \boldsymbol{k}_h = \boldsymbol{k}$. Then, the commutator $[B^\dagger_{\nu,0}, B_{\nu',0}]$ is determined by the commutators

$$\begin{aligned}
[c^\dagger_{v\boldsymbol{k}}c_{c\boldsymbol{k}}, c^\dagger_{c\boldsymbol{k}'}c_{v\boldsymbol{k}'}] &= c^\dagger_{v\boldsymbol{k}}c_{c\boldsymbol{k}}c^\dagger_{c\boldsymbol{k}'}c_{v\boldsymbol{k}'} - c^\dagger_{c\boldsymbol{k}'}c_{v\boldsymbol{k}'}c^\dagger_{v\boldsymbol{k}}c_{c\boldsymbol{k}} \\
&= c^\dagger_{v\boldsymbol{k}}c_{v\boldsymbol{k}'}\delta_{\boldsymbol{k},\boldsymbol{k}'} - c^\dagger_{c\boldsymbol{k}'}c_{c\boldsymbol{k}}\delta_{\boldsymbol{k},\boldsymbol{k}'} \\
&= \delta_{\boldsymbol{k},\boldsymbol{k}'}\left(c^\dagger_{v\boldsymbol{k}}c_{v\boldsymbol{k}} - c^\dagger_{c\boldsymbol{k}}c_{c\boldsymbol{k}}\right) = (1 - n_e(\boldsymbol{k}) - n_h(\boldsymbol{k}))\,\delta_{\boldsymbol{k},\boldsymbol{k}'}\,.
\end{aligned}$$

Without the electron and hole occupation this relation would lead to $[B_{\nu,0}, B^\dagger_{\nu',0}] = \delta_{\nu,\nu'}$, classifying excitons as bosons. This relation is valid, however, only if we consider a single exciton. The electron and hole occupations remind of the fact, that excitons are composed of fermions.

10.5: The zero of (10.42) close to the exciton resonance at $\omega_{\nu 0}$ determines the frequency of the corresponding longitudinal exciton:

$$\varepsilon_1(\omega_{\mathrm{L}}) \simeq 1 + \frac{4e^2}{\varepsilon_0 m}\frac{f_{\nu 0}}{\omega^2_{\nu 0}} - \omega^2_{\mathrm{L}} = 0\,,$$

which for $\omega_{\mathrm{L}} \simeq \omega_{\nu 0}$ and $\Delta_{\mathrm{LT}} = \hbar(\omega_{\mathrm{L}} - \omega_{\nu 0})$ allows to express the LT-splitting in terms of the exciton oscillator strength:

$$\Delta_{\mathrm{LT}} = \frac{2e^2\hbar^2}{\varepsilon_0 m}\frac{f_{\nu 0}}{E_{\nu 0}} \quad \text{with} \quad E_{\nu 0} = \hbar\omega_{\nu 0}\,.$$

On the other hand the first term of the exchange interaction $V_{\rm exch}$ in (10.62) gives a contribution only for longitudinal excitons (with $\boldsymbol{Q}\|\boldsymbol{P}_{cv}$) which can be calculated as a perturbation correction to the transverse exciton energy $E_{\nu 0}$ with the exciton envelope function $\phi_{\nu 0}(\boldsymbol{r})$ after taking the Fourier transform of $V_{\rm exch}$ (note: $1/V_c \int \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})\mathrm{d}^3\boldsymbol{k} = \delta(\boldsymbol{r})$) and yields (for singlet excitons with $S=0$)

$$\Delta_{\rm LT} = \frac{2e^2}{\varepsilon_0}\frac{\hbar^2}{m^2}\frac{|P_{cv}|^2|\phi_{\nu 0}(0)|^2}{E_{\nu 0}^2}\,.$$

With $E_{\nu 0} \simeq E_g$ one finds by comparison between the two obtained expressions for $\Delta_{\rm LT}$

$$f_{\nu 0} = \frac{1}{m}\frac{|P_{cv}|^2|\phi_{\nu 0}(0)|^2}{E_{\nu 0}}$$

in accordance with (10.43).

10.6: Use the expansion of $\boldsymbol{A}(\boldsymbol{r},t)$ with $a_{\lambda\boldsymbol{\kappa}}(t) = a_{\lambda\boldsymbol{\kappa}}\mathrm{e}^{\mathrm{i}\omega(\kappa)t}$ to write the two contributions of $\mathcal{H}_{\rm rad}$ as

$$\left(\frac{\partial}{\partial t}\boldsymbol{A}(\boldsymbol{r},t)\right)^2 = \frac{\hbar}{2\varepsilon_0 V}\sum_{\lambda,\kappa}\sum_{\lambda',\kappa'}\boldsymbol{e}_{\lambda\kappa}\cdot\boldsymbol{e}_{\lambda'\kappa'}\big(\omega(\boldsymbol{\kappa})\omega(\boldsymbol{\kappa}')\big)^{1/2}$$
$$\times\big(a_{\lambda\boldsymbol{\kappa}}(t) - a^\dagger_{\lambda-\boldsymbol{\kappa}}(t)\big)\big(a_{\lambda'\boldsymbol{\kappa}'}(t) - a^\dagger_{\lambda'-\boldsymbol{\kappa}'}(t)\big)\mathrm{e}^{\mathrm{i}(\boldsymbol{\kappa}+\boldsymbol{\kappa}')\cdot\boldsymbol{r}}$$

and

$$c^2\big(\nabla\times\boldsymbol{A}(\boldsymbol{r},t)\big)^2 = -\frac{\hbar}{2\varepsilon_0 V}\sum_{\lambda,\kappa}\sum_{\lambda',\kappa'}(\boldsymbol{\kappa}\times\boldsymbol{e}_{\lambda\kappa})\cdot(\boldsymbol{\kappa}'\times\boldsymbol{e}_{\lambda'\kappa'})$$
$$\times\big(a_{\lambda\boldsymbol{\kappa}}(t) + a^\dagger_{\lambda-\boldsymbol{\kappa}}(t)\big)\big(a_{\lambda'\boldsymbol{\kappa}'}(t) + a^\dagger_{\lambda'-\boldsymbol{\kappa}'}(t)\big)\mathrm{e}^{\mathrm{i}(\boldsymbol{\kappa}+\boldsymbol{\kappa}')\cdot\boldsymbol{r}}$$

and perform the volume integral with

$$\frac{1}{V}\int \mathrm{e}^{\mathrm{i}(\boldsymbol{\kappa}+\boldsymbol{\kappa}')\cdot\boldsymbol{r}}\mathrm{d}^3\boldsymbol{r} = \delta_{\boldsymbol{\kappa},-\boldsymbol{\kappa}'}\,.$$

With $\boldsymbol{e}_{\lambda\boldsymbol{\kappa}}\cdot\boldsymbol{e}_{\lambda'\boldsymbol{\kappa}} = \delta_{\lambda,\lambda'}$ and $(\boldsymbol{\kappa}\times\boldsymbol{e}_{\lambda\kappa})\cdot(-\boldsymbol{\kappa}\times\boldsymbol{e}_{\lambda'\kappa})) = -\kappa^2\delta_{\lambda,\lambda'}$ for transverse unit vectors this reduces with $\omega(\boldsymbol{\kappa}) = \omega(-\boldsymbol{\kappa}) = c\kappa$ to

$$\mathcal{H}_{\rm rad} = \sum_{\lambda,\boldsymbol{\kappa}}\frac{1}{2}\hbar\omega(\boldsymbol{\kappa})\big(a_{\lambda\boldsymbol{\kappa}}a^\dagger_{\lambda\boldsymbol{\kappa}} + a^\dagger_{\lambda\boldsymbol{\kappa}}a_{\lambda\boldsymbol{\kappa}}\big) = \sum_{\lambda,\boldsymbol{\kappa}}\hbar\omega(\boldsymbol{\kappa})\big(a^\dagger_{\lambda\boldsymbol{\kappa}}a_{\lambda\boldsymbol{\kappa}} + \frac{1}{2}\big)\,.$$

10.7: In quasi-equilibrium one has to find only the solution for the off-diagonal elements of the density matrix, because the diagonal elements are the equilibrium distribution functions (Fermi–Dirac distribution). Therefore, one finds from

$$\frac{\mathrm{d}}{\mathrm{d}t}\bar{\rho}_{cv}(\boldsymbol{k},t) = \frac{\mathrm{i}}{\hbar}d_{cv}E(t)\mathrm{e}^{\mathrm{i}(\epsilon_{c\boldsymbol{k}}-\epsilon_{v\boldsymbol{k}})t}\,(f_{v\boldsymbol{k}} - f_{c\boldsymbol{k}})$$

with

$$E(t) = \frac{1}{2\pi}\int E(\omega)\mathrm{e}^{-\mathrm{i}\omega t}\mathrm{d}\omega$$

and integration over t

$$\bar{\rho}_{cv}(\boldsymbol{k},t) = \frac{1}{2\pi\hbar}\int \mathrm{d}\omega\frac{d_{cv}E(\omega)\mathrm{e}^{\mathrm{i}(\epsilon_{c\boldsymbol{k}}-\epsilon_{v\boldsymbol{k}}-\omega)t}}{\epsilon_{c\boldsymbol{k}}-\epsilon_{v\boldsymbol{k}}-\omega-\mathrm{i}\gamma}\,(f_{v\boldsymbol{k}} - f_{c\boldsymbol{k}})\,.$$

The dielectric polarization is obtained by

$$\begin{aligned}\boldsymbol{P}(t) &= \mathrm{Tr}\left(\bar{\rho}(t)\bar{d}(t)\right)\\ &= \frac{1}{V}\sum_{\boldsymbol{k}}\left(\bar{\rho}_{cv}(t)\bar{d}_{vc}(t)+\bar{\rho}_{vc}(t)\bar{d}_{cv}(t)\right)\\ &= \frac{1}{2\pi\hbar V}\sum_{\boldsymbol{k}}\int \mathrm{d}\omega\frac{|d_{cv}|^2(f_{v\boldsymbol{k}}-f_{c\boldsymbol{k}})}{\epsilon_{c\boldsymbol{k}}-\epsilon_{v\boldsymbol{k}}-\omega-\mathrm{i}\gamma}E(\omega)\mathrm{e}^{-\mathrm{i}\omega t}+c.c.\end{aligned}$$

and the dielectric susceptibility with $\chi(\omega)=P(\omega)/E(\omega)$ is

$$\begin{aligned}\chi(\omega) = -\frac{1}{V}\sum_{\boldsymbol{k}}|d_{cv}|^2(f_{v\boldsymbol{k}}-f_{c\boldsymbol{k}})\Big(&\frac{1}{\hbar(\epsilon_{v\boldsymbol{k}}-\epsilon_{c\boldsymbol{k}}+\omega+\mathrm{i}\gamma)}\\ &-\frac{1}{\hbar(\epsilon_{c\boldsymbol{k}}-\epsilon_{v\boldsymbol{k}}+\omega+\mathrm{i}\gamma)}\Big).\end{aligned}$$

Finally one recovers the result from Sect. 10.2 with $\varepsilon_2(\omega)=\mathrm{Im}\chi(\omega)/\varepsilon_0$.

10.8: We demonstrate here the calculation only for one term, the others follow in similar way. The example is $[\alpha^\dagger_{\boldsymbol{k}}\alpha_{\boldsymbol{k}}, \sum_{\bar{\boldsymbol{k}},\boldsymbol{k}';\boldsymbol{q}\neq\boldsymbol{0}} v_{\boldsymbol{q}}\alpha^\dagger_{\bar{\boldsymbol{k}}+\boldsymbol{q}}\alpha^\dagger_{\boldsymbol{k}'-\boldsymbol{q}}\alpha_{\boldsymbol{k}'}\alpha_{\bar{\boldsymbol{k}}}]$. The commutator is evaluated by using the fermion commutation rules when changing the order of the operators:

$$\begin{aligned}&[\alpha^\dagger_{\boldsymbol{k}}\alpha_{\boldsymbol{k}}, \alpha^\dagger_{\bar{\boldsymbol{k}}+\boldsymbol{q}}\alpha^\dagger_{\boldsymbol{k}'-\boldsymbol{q}}\alpha_{\boldsymbol{k}'}\alpha_{\bar{\boldsymbol{k}}}] = \alpha^\dagger_{\boldsymbol{k}}\alpha_{\boldsymbol{k}}\alpha^\dagger_{\bar{\boldsymbol{k}}+\boldsymbol{q}}\alpha^\dagger_{\boldsymbol{k}'-\boldsymbol{q}}\alpha_{\boldsymbol{k}'}\alpha_{\bar{\boldsymbol{k}}} - \leftrightarrow\\ &= \underbrace{\delta_{\boldsymbol{k},\bar{\boldsymbol{k}}+\boldsymbol{q}}\alpha^\dagger_{\boldsymbol{k}}\alpha^\dagger_{\boldsymbol{k}'-\boldsymbol{q}}\alpha_{\boldsymbol{k}'}\alpha_{\bar{\boldsymbol{k}}}}_{(1)} - \alpha^\dagger_{\boldsymbol{k}}\alpha^\dagger_{\bar{\boldsymbol{k}}+\boldsymbol{q}}\alpha_{\boldsymbol{k}}\alpha^\dagger_{\boldsymbol{k}'-\boldsymbol{q}}\alpha_{\boldsymbol{k}'}\alpha_{\bar{\boldsymbol{k}}} - \leftrightarrow\\ &= (1) + \underbrace{\delta_{\boldsymbol{k},\bar{\boldsymbol{k}}+\boldsymbol{q}}\alpha^\dagger_{\bar{\boldsymbol{k}}+\boldsymbol{q}}\alpha^\dagger_{\boldsymbol{k}}\alpha_{\boldsymbol{k}'}\alpha_{\bar{\boldsymbol{k}}}}_{(2)} - \alpha^\dagger_{\bar{\boldsymbol{k}}+\boldsymbol{q}}\alpha^\dagger_{\boldsymbol{k}}\alpha^\dagger_{\boldsymbol{k}'-\boldsymbol{q}}\alpha_{\boldsymbol{k}}\alpha_{\boldsymbol{k}'}\alpha_{\bar{\boldsymbol{k}}} - \leftrightarrow\\ &= (1)+(2) + \underbrace{\delta_{\boldsymbol{k},\boldsymbol{k}'}\alpha^\dagger_{\bar{\boldsymbol{k}}+\boldsymbol{q}}\alpha^\dagger_{\boldsymbol{k}'-\boldsymbol{q}}\alpha_{\bar{\boldsymbol{k}}}\alpha_{\boldsymbol{k}}}_{(3)} - \alpha^\dagger_{\bar{\boldsymbol{k}}+\boldsymbol{q}}\alpha^\dagger_{\boldsymbol{k}'-\boldsymbol{q}}\alpha_{\boldsymbol{k}'}\alpha^\dagger_{\boldsymbol{k}}\alpha_{\bar{\boldsymbol{k}}}\alpha_{\boldsymbol{k}} - \leftrightarrow\\ &= (1)+(2)+(3) - \underbrace{\delta_{\boldsymbol{k},\bar{\boldsymbol{k}}}\alpha^\dagger_{\bar{\boldsymbol{k}}+\boldsymbol{q}}\alpha^\dagger_{\boldsymbol{k}'-\boldsymbol{q}}\alpha_{\boldsymbol{k}'}\alpha_{\boldsymbol{k}}}_{(4)} + \alpha^\dagger_{\bar{\boldsymbol{k}}+\boldsymbol{q}}\alpha^\dagger_{\boldsymbol{k}'-\boldsymbol{q}}\alpha_{\boldsymbol{k}'}\alpha_{\bar{\boldsymbol{k}}}\alpha^\dagger_{\boldsymbol{k}}\alpha_{\boldsymbol{k}} - \leftrightarrow .\end{aligned}$$

In the last line, the last two terms cancel each other and one obtains the four contributions (1)–(4) which under the sum combine to the final result

$$\begin{aligned}[\alpha^\dagger_{\boldsymbol{k}}\alpha_{\boldsymbol{k}} \ , \sum_{\bar{\boldsymbol{k}},\boldsymbol{k}';\boldsymbol{q}\neq\boldsymbol{0}} v_{\boldsymbol{q}}\alpha^\dagger_{\bar{\boldsymbol{k}}+\boldsymbol{q}}\alpha^\dagger_{\boldsymbol{k}'-\boldsymbol{q}}\alpha_{\boldsymbol{k}'}\alpha_{\bar{\boldsymbol{k}}}] &=\\ = \sum_{\boldsymbol{k}';\boldsymbol{q}\neq 0} v_{\boldsymbol{q}}&\left(\alpha^\dagger_{\boldsymbol{k}}\alpha^\dagger_{\boldsymbol{k}'-\boldsymbol{q}}\alpha_{\boldsymbol{k}-\boldsymbol{q}}\alpha_{\boldsymbol{k}'} - \alpha^\dagger_{\boldsymbol{k}+\boldsymbol{q}}\alpha^\dagger_{\boldsymbol{k}'-\boldsymbol{q}}\alpha_{\boldsymbol{k}}\alpha_{\boldsymbol{k}'}\right) .\end{aligned}$$

The thermal expectation values of these terms are found in (10.115).

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