Solutions of Selected Problems and Answers

Chapter 1

Problem 1.5s

The sphere and the probability distribution have both inversion and rotation symmetry; the first implies $\langle x \rangle = \langle y \rangle = \langle z \rangle = 0$ and the second in combination with the first implies

$$\Delta x^2 = \left\langle x^2 \right\rangle = \Delta y^2 = \left\langle y^2 \right\rangle = \Delta z^2 = \left\langle z^2 \right\rangle = \frac{1}{3} \left\langle r^2 \right\rangle .$$

Hence,

$$\langle \varepsilon_k \rangle = \frac{1}{2m} 3 \Delta p_x^2 \geq \frac{3}{2m} \frac{\hbar^2}{4} \frac{1}{\Delta x^2} = \frac{9\hbar^2}{8m \left\langle r^2 \right\rangle}.$$

For a uniform probability, within the sphere of radius r_0 and volume $V = (4\pi/3)\, r_0^3$, $\left\langle r^2 \right\rangle = (3/5)\, r_0^2 = (3/5)\, (3/4\pi)^{2/3}\, V^{2/3} = 0.2309\, V^{2/3}$. Thus $\langle \varepsilon_k \rangle = 4.87\, \hbar^2/mV^{2/3}$.

Problem 1.9s

The quantity λ_{m} must depend on:

(a) $\hbar$, since black body's radiation is of quantum nature
(b) c, since it is an electromagnetic phenomenon
(c) $k_{\mathrm{B}}T$, since T is the only parameter in the spectral distribution of this radiation; furthermore, absolute temperature is naturally associated with Boltzmann's constant, k_{B}, as a product $k_{\mathrm{B}}T$ with dimensions of energy

Out of $\hbar, c, k_{\mathrm{B}}T$, there is only one combination with dimensions of length $\hbar c/k_{\mathrm{B}}T$ (remember that $\hbar c$ has dimensions of energy times length). Hence,

$$\lambda_{\mathrm{m}} = c_1 \frac{\hbar c}{k_{\mathrm{B}}T},$$

where the numerical constant $c_1 = 1.2655$

Problem 1.10s

The scattering cross-section has dimensions of length square. The photon scattering by electron must depend on:

(a) The electron charge, $-e$, since, if this charge was zero, there would be no interaction and no scattering.
(b) The velocity of light, since we are dealing with an electromagnetic phenomenon.
(c) The mass of the electron, m_e, since if the mass was infinite, the electron would not oscillate under the action of the photon electromagnetic field and would not emit radiation.
(d) The energy of the photon, $\hbar\omega$.

The quantity $e^2/4\pi\varepsilon_0 m_e c^2$ has dimensions of length (since $e^2/4\pi\varepsilon_0 r$ has dimensions of energy). Hence, the cross-section, σ, is of the form

$$\sigma = \left(\frac{e^2}{4\pi\varepsilon_0 m_e c^2}\right)^2 f\left(\frac{\hbar\omega}{m_e c^2}\right),$$

where the function f of the dimensionless quantity $\hbar\omega/m_e c^2$ cannot be determined from dimensional analysis; it turns out that $f(x)$ is a monotonically decreasing function of x with $f(0) = 8\pi/3$, and $f(\infty) = 0$. (The formula for σ is known as the Klein–Nishina formula).

Problem 1.11s

The natural linewidth, ΔE, has dimensions of energy. It must depend on:

(a) The dipole moment $p = e \cdot r$ (as suggested by the question).
(b) The velocity of light, c since the decay is due to the emission of a photon.
(c) The frequency of the emitted photon, since only an oscillating dipole emits radiation.

Hence, by finding the only combination of p, c, ω with dimensions of energy, we obtain

$$\Delta E = c_1 \frac{e^2 r^2 \omega^3}{4\pi\varepsilon_0 c^3} \text{ and the lifetime } t_l = \frac{\hbar}{\Delta E} = \frac{4\pi\varepsilon_0 \hbar c^3}{c_1 e^2 r^2 \omega^3},$$

where the "constant" c_1 depends on the details of the initial and the final atomic level, since actually r^2 is the square of the matrix element of an appropriate projection of $\boldsymbol{r}$ between the initial and the final states. We expect that, for the transition 2p to 1s in hydrogen, r^2 to be of the order of a_B^2. Choosing, arbitrarily, $c_1 = 1$ and $r^2 = a_B^2$, while $\hbar\omega = 13.6\left(1 - \frac{1}{4}\right)$ eV $= 10.2$ eV we find for this transition

$$t_l \simeq 1.17 \times 10^{-9}\text{s},$$

while a detailed advanced calculation gives $t_l = 1.59 \times 10^{-9}$s.

Problem 1.12s

The effective absolute temperature, T, would appear as the product $k_{\mathrm{B}}T$ of dimensions of energy. It must depend on:

(a) The product GM, where G is the gravitational constant. The reason is that the strong gravitational field responsible for this radiation depends on the product GM.
(b) Planck's constant $\hbar$, since the phenomenon is of quantum origin.
(c) The velocity of light, c, since we are dealing with electromagnetic radiation.

The reader may convince himself that out of GM, $\hbar$ and c there is only one combination to give dimensions of energy, namely, $\hbar c^3/GM$. Hence

$$k_{\mathrm{B}}T = c_1 \hbar c^3/GM,$$

where the numerical constant c_1 turns out to be equal to $1/8\pi$.

Problem 1.13s

It is more convenient for dimensional analysis to employ the G-CGS system (to get rid of ε_0 and μ_0). The skin depth will depend on:

(a) The frequency ω (see the statement of the problem).
(b) The velocity of light c (EM phenomenon).
(c) The conductivity σ (we are dealing with a good conductor). But $[\sigma] = \left[e^2/\hbar a_{\mathrm{B}}\right] = [t]^{-1}$. Hence,

$$\delta = c\sqrt{\frac{1}{\omega\sigma}}\, f\left(\frac{\omega}{\sigma}\right); \text{it turns out that } f\left(\frac{\omega}{\sigma}\right) = \frac{1}{\sqrt{2\pi}}.$$

Chapter 2

Problem 2.3s

According to the book by Karplus and Porter [C65], the minimum of the curve appears at $d = 0.74\,\mathrm{A} = 1.4$ a.u. and it is equal to $-4.75\,\mathrm{eV}$. Assuming that at $d' = 5$ a.u., the energy is still given by the van der Waals, we have

$$\varepsilon_{\bar{d}=5} = 6.48/d'^6\text{a.u.} = 6.48/5^6\,\text{a.u.} = 11.3\,\text{meV}.$$

At $d' = 0.5\,a.u.$, the total energy (excluding the proton–proton repulsion) is expected to be slightly higher than the total electronic energy of the He atom. The latter energy is equal to minus the sum of the first and the second ionization potential of He, i.e., $-24.587 - 54.418\,\mathrm{eV} = -79\,\mathrm{eV}$. To this energy we must add $2 \times 13.6\,\mathrm{eV}$ to be consistent with our choice of the zero of energy.

Thus the total energy at $d' = 0.5$ a.u. is higher than $-79 + 27.2 + \frac{e^2}{4\pi\varepsilon_0 d'} = -51.8 + \frac{27.2}{0.5}\,\mathrm{eV} = 2.6\,\mathrm{eV}$.

In Fig. 2.5, we plot the experimental curve and the two points we estimated above.

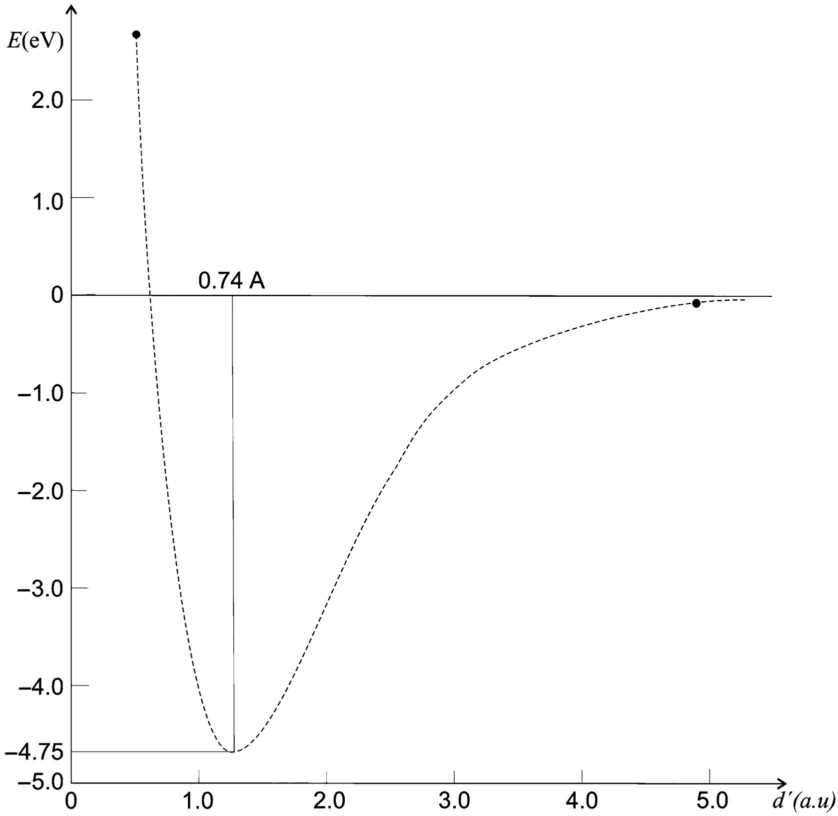

Fig. 2.5. Interaction energy of two hydrogen atoms vs their separation

Problem 2.5s

$$|\psi(r)|^2 = Ae^{-2r/a}, \quad \left\langle \frac{1}{\mathrm{r}} \right\rangle = \int_0^\infty 4\pi r^2 \mathrm{d}r\, |\psi|^2 \frac{1}{r}$$

$$= \frac{\int_0^\infty \mathrm{d}r r e^{-2r/a}}{\int_0^\infty \mathrm{d}r r^2 e^{-2r/a}} = \frac{1/\left(2/a\right)^2}{2/\left(2/a\right)^3} = \frac{1}{a},$$

$$\left\langle r^2 \right\rangle = \frac{\int_0^\infty \mathrm{d}r r^4 e^{-2r/a}}{\int_0^\infty \mathrm{d}r r^2 e^{-2r/a}} = \frac{4!/\left(2/a\right)^5}{2!/\left(2/a\right)^3} = 4 \times 3 \left(\frac{a}{2}\right)^2 = 3a^2,$$

$$\left\langle \frac{p^2}{2m} \right\rangle = -\frac{\hbar^2}{2m}\int \psi \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}\psi}{\mathrm{d}r}\right)4\pi r^2 \mathrm{d}r = -\frac{4\pi\hbar^2}{2m}\int \psi \frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}\psi}{\mathrm{d}r}\right)\mathrm{d}r$$

$$= -\frac{\hbar^2}{2m}\frac{\int_0^\infty \mathrm{e}^{-r/a}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}}{\mathrm{d}r}\mathrm{e}^{-r/a}\right)dr}{\int_0^\infty \mathrm{d}r r^2 \mathrm{e}^{-2r/a}} = \frac{\hbar^2}{2m}\frac{a/4}{2a^3/8} = \frac{\hbar^2}{2ma^2},$$

$$\langle\varepsilon\rangle = \frac{\hbar^2}{2ma^2} - \frac{e^2}{4\pi\varepsilon_0 a}, \quad \frac{\partial\langle\varepsilon\rangle}{\partial a} = 0 \Rightarrow a = \frac{4\pi\varepsilon_0\hbar^2}{e^2 m} = a_\mathrm{B},$$

$$\Delta r = \sqrt{\langle r^2\rangle} = \sqrt{3}a_\mathrm{B}, \quad \Delta p_i^2 = \frac{1}{3}\left\langle p^2\right\rangle = \frac{1}{3}\frac{\hbar^2}{a^2},$$

$$\Delta x_i^2 = \frac{1}{3}\left\langle r^2\right\rangle = \frac{3}{3}a^2 = a^2, \quad \Delta p_i^2\Delta x_i^2 = \frac{1}{3}\hbar^2,$$

vs. $\Delta p_i^2 \Delta x_i^2 \geq \frac{\hbar^2}{4}$.

Problem 2.6s

Solving the system

$$\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2, \quad \boldsymbol{R} = (m_1\boldsymbol{r}_1 + m_2\boldsymbol{r}_2)/(m_1+m_2),$$

with respect to $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, we find

$$\boldsymbol{r}_1 = \boldsymbol{R} + \frac{m_2}{M}\boldsymbol{r}, \quad \boldsymbol{r}_2 = \boldsymbol{R} - \frac{m_1}{M}\boldsymbol{r}.$$

Hence, taking into account that $\boldsymbol{p}_1 = m_1\dot{\boldsymbol{r}}_1$, $\boldsymbol{p}_2 = m_2\dot{\boldsymbol{r}}_2$, we have

$$\frac{\boldsymbol{p}_1^2}{2m_1} = \frac{m_1\dot{\boldsymbol{R}}^2}{2} + \frac{\mu^2\dot{\boldsymbol{r}}^2}{2m_1} + \mu\dot{\boldsymbol{R}}\dot{\boldsymbol{r}}, \quad \frac{\boldsymbol{p}_2^2}{2m_2} = \frac{m_2\dot{\boldsymbol{R}}^2}{2} + \frac{\mu^2\dot{\boldsymbol{r}}^2}{2m_2} - \mu\dot{\boldsymbol{R}}\dot{\boldsymbol{r}}.$$

Summing the two equations we find

$$\frac{\boldsymbol{p}_1^2}{2m_1} + \frac{\boldsymbol{p}_2^2}{2m_2} = \frac{1}{2}M\dot{\boldsymbol{R}}^2 + \frac{1}{2}\mu\dot{\boldsymbol{r}}^2 = \frac{\boldsymbol{P}^2}{2M} + \frac{\boldsymbol{p}^2}{2\mu}, \text{ QED.}$$

Problem 2.8s

From virial theorem $E = \left(1 + \frac{2}{\beta}\right)\bar{V}$, where $V(x) \sim \pm|x|^\beta$. According to the correspondence principle (valid for large n), to go from the level n to level $n+1$, $\bar{V}$ must go from $\bar{V}(x)$ to $\bar{V}(x+\delta x)$, where $\delta x = \lambda$; but $\lambda^{-2} \sim E_\mathrm{K} \sim E$. Thus

$$\delta E \equiv E(n+1) - E(n) \sim \frac{\partial\bar{V}}{\partial x}\lambda \sim \frac{\partial\bar{V}}{\partial x}\frac{1}{\sqrt{E}}.$$

But

$$\delta E \simeq (\mathrm{d}E/\mathrm{d}n) = \alpha E/n \sim E/E^{1/a} = E^{1-(1/a)}, \quad \text{since}\, E \sim n^a,$$

$$\frac{\partial\bar{V}}{\partial x}\lambda \simeq \left(|\beta|\,|x|^\beta/|x|\right)\lambda \sim \bar{V}^{1-(1/\beta)}E^{-1/2}.$$

Substituting in $\delta E \sim (\partial \bar{V}/\partial x)\lambda$ the last two relations and taking into account that $E \sim \bar{V}$, we have

$$E^{1-\frac{1}{a}} \sim V^{1-\frac{1}{\beta}} E^{-\frac{1}{2}} \sim E^{1-\frac{1}{\beta}-\frac{1}{2}},$$

or

$$\frac{1}{a} = \frac{1}{2} + \frac{1}{\beta} \Rightarrow a = \left(\frac{1}{2} + \frac{1}{\beta}\right)^{-1}. \tag{1}$$

In spite of the hand-waving character of "deriving" (1), the latter is valid (for every n) for $\beta = 2$ (harmonic potential) and for $\beta = -1$ (Coulomb potential), since the exact results are $a = 1$ and $a = -2$ respectively.

The WKB approach (see Q34, p.447) gives that $|E| \sim \left(n + \frac{1}{2}\right)^a$.

Problem 2.11s

We introduce the quantities q and k as follows:

$$\hbar^2 q^2/2m \equiv \varepsilon_\mathrm{b} \text{ and } \hbar^2 k^2/2m \equiv |\varepsilon| - \varepsilon_\mathrm{b}.$$

Then the ground state has the form:

$$\psi = AJ_0\left(kr\right), r \leq a; \psi = BK_0\left(qr\right), r \geq a; \tag{1}$$

($K_0(z) = \frac{\mathrm{i}\pi}{2} H_0^{(1)}(\mathrm{i}z)$ is the modified Bessel function of zero-order; see Table H.18). The continuity of the logarithmic derivative ψ'/ψ at $r = a$ leads to the following relation

$$\frac{kJ_0'\left(ka\right)}{J_0\left(ka\right)} = \frac{qK_0'\left(qa\right)}{K_0\left(qa\right)}, \tag{2}$$

where the prime denote differentiation with respect to the corresponding argument ka or qa respectively. For small values of ε_b and $|\varepsilon|$ (in comparison with $E_0 \equiv \hbar^2/ma^2$), ka and qa are much smaller than one. Expanding $J_0\left(ka\right)$ and $K_0\left(qa\right)$ we have

$$J_0\left(ka\right) = 1 - \frac{1}{4}(ka)^2 + \mathcal{O}\left(k^4 a^4\right), \tag{3}$$

$$K_0\left(qa\right) = -\left[\ln\left(\frac{qa}{2}\right) + \gamma\right]\left[1 + \frac{(qa)^2}{4}\right] + \frac{(qa)^2}{4} + \mathcal{O}\left[\ln\left(\frac{qa}{2}\right) q^4 a^4\right].$$

Substituting in (2) we have

$$-\frac{k^2 a^2}{2} = -\frac{1}{-\ln\left(\frac{1}{2} e^{\gamma} qa\right)}. \tag{4}$$

Taking into account that $q^2 a^2 = 2\varepsilon_\mathrm{b} / E_0$ and $k^2 a^2 = 2(|\varepsilon| - \varepsilon_\mathrm{b})/ E_0 \simeq 2|\varepsilon|/ E_0$, we obtain the relation

$$\varepsilon_\mathrm{b} \simeq \frac{2}{e^{2\gamma}} E_0 \exp\left(-\frac{2E_0}{|\varepsilon|}\right).$$

Chapter 3

Problem 3.1s

According to (3.1) the viscosity η is equal to $\mu_s t$, where μ_s is the shear modulus and t is a characteristic time of motion of each water molecule; t is expected to be of the order of the period of molecular vibration T in ice: $t = c_1 T = 2\pi c_1 / \omega$, where $\omega = \left(c_2 \hbar / m_e a_B^2 \bar{r}_w^2\right) \sqrt{m_e / m_w}$ and c_1, c_2 are numerical constants of the order of one. Substituting $m_w = 18 \times 1823\, m_e$ and $\bar{r}_w = (2.68 \times 18)^{1/3} = 3.64$ we have $\omega = c_2 1.72 \times 10^{13}\,\text{rad/s}$. The shear modulus μ_s (in ice) is expected to be around $0.3\,B$ where B is the bulk modulus of water, where $B \simeq 0.2\hbar^2 / m_e a_B^5 \bar{r}_w^5 = 9.2 \times 10^9\,\text{N/m}^2$ (the numerical coefficient was taken 0.2 and not 0.6 as usually, because the hydrogen bond is much weaker than the strong bonds for which the 0.6 is a reasonable choice). Hence, the result for η is

$$\eta = (2\pi c_1 / c_2)(0.3 \times 9.2 \times 10^9 / 1.72 \times 10^{13}) = (c_1 / c_2) 10^{-3}\,\text{kg/ms},$$

which coincides with the experimental result if $c_1 = c_2$.

Problem 3.2s

H_2O has larger cohesive energy, because H_2O possesses a dipole moment (being non-linear), while CO_2 is non-polar (being a symmetric linear molecule).

Problem 3.12s

Consider a rotation of a Bravais Lattice, by an angle θ, around the axis z, of an orthogonal Cartesian system, passing through a lattice point. The matrix $\sum(\theta)$ implementing this rotation has the form

$$\sum(\theta) = \begin{vmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{vmatrix}. \tag{1}$$

Now we denote the same rotation in the system $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$ by the matrix $\sum'(\theta)$. If $\sum'(\theta)$ is compatible with the translational symmetry of the lattice, each lattice point $\sum_i n_i \boldsymbol{a}_i$ will be mapped to another lattice point $\sum_i n'_i \boldsymbol{a}_i$: $[n'_i] = \sum'(\theta)\,[n_i]$; where $[n'_i]$ and $[n_i]$ are column matrices. For $\{n'_i\}$ $(i = 1, 2, 3)$ to be integers, for any set of three integers n_1, n_2, n_3 the matrix elements of $\sum'(\theta)$, must be integers. Since $\sum(\theta)$ and $\sum'(\theta)$ describe the same rotation in different coordinate systems, they must be related by a transformation of the form

$$\sum'(\theta) = S^{-1} \sum(\theta) S, \tag{2}$$

where S is a 3×3 matrix, connecting the two coordinate systems. By taking the trace of (2), we have

$$\mathrm{Tr}\sum{}'(\theta) = \mathrm{Tr} S^{-1}\sum(\theta) S = \mathrm{Tr} S S^{-1}\sum(\theta) = \mathrm{Tr}\sum(\theta). \qquad (3)$$

The $\mathrm{Tr}\sum(\theta) = 2\cos\theta + 1$ and the $\mathrm{Tr}\sum{}'(\theta)$ is an integer, since all matrix elements of $\sum{}'(\theta)$ are integers. Hence

$$2\cos\theta = \text{integer},$$

from which it follows that $\theta = 2\pi/n$, $n = 1, 2, 3, 4, 6$.

Chapter 4

Problem 4.7ts

For Cu, $\zeta = 2.57$, $\bar{r}_c = 1.113$, $\eta = 0.6025$, $a = 4.429 + 6.2687 = 10.70$, $\gamma = 1.97 + 5.944 = 7.916$, $\bar{r}_a = 2.70$, $B = 1.16\,\mathrm{Mbar}$, $P_\mathrm{P} = 294\dfrac{\gamma}{4\pi\bar{r}_a^4} = \dfrac{185.2}{\bar{r}_a^4} = 3.48\,\mathrm{Mbar}$.

Problem 4.1s

Binding energies in eV(Th.: Theory: Exp.: Experiment) Na (Th. 4.92; Exp. 6.25), K (Th. 4.07; Exp. 5.27), Mg (Th. 19.98; Exp. 24.19), Ca (Th. 15.73; Exp. 19.82), Fe (Th. 56.29; Exp. 59.02), Al (Th. 52.49; Exp. 56.65), Ti (Th. 69.36, Exp. 96.01).

Problem 4.2s

Debye temperature in degrees K according to the RJM for some solids:

$$\mathrm{Al}\,(419)\,,\ \mathrm{Cu}\,(300)\,,\ \mathrm{Au}\,(142)\,,\ \mathrm{Fe}\,(497)\,,\ \mathrm{Pb}\,(80)\,,\ \mathrm{Mg}\,(344)\,,\ \mathrm{Be}\,(1322)\,.$$

Problem 4.3s

Hint: Combine (C.25) with (4.100). At $T \geq \Theta_\mathrm{D}$ use (4.51) for B and (4.66) for Θ_D.

Problem 4.7s

The constant electronic charge density is $\rho = -3\zeta e \,/\, 4\pi\left(r_a^3 - r_c^3\right)$, $r_c \leq r \leq r_a$; from Gauss theorem the electric field $\varepsilon(r)$ is $4\pi\varepsilon_0\varepsilon(r) r^2 = (4\pi\,/\,3)\rho\left(r^3 - r_c^3\right)$. The potential $\phi(r) = -\int \varepsilon(r)\mathrm{d}r$ is $4\pi\varepsilon_0\phi(r) = -(2\pi\,/\,3)\rho r^2 - \left(4\pi\rho r_c^3/3r\right) +$

const. The const. is determined from $4\pi\varepsilon_0\phi(r_a) = -\zeta e / r_a$: $const = -3\zeta e r_a^3 / 2\left(r_a^3 - r_c^3\right)$. The classical electronic Coulomb self-energy is

$$E_{e-e} = \frac{1}{2}\int_{r_c}^{r_a} \phi(r)\rho(r)\mathrm{d}^3r = \frac{3}{2}\frac{\zeta^2 e^2}{4\pi\varepsilon_0(1-x^2)^2 r_a}\left[\frac{4}{10} - x^3 + \frac{6}{10}x^5\right], \quad x = \frac{r_c}{r_a}.$$

The electrostatic Coulomb electron-ion interaction is

$$E_{e-i} = \rho\int_{r_c}^{r_a} \mathrm{d}^3r\frac{\zeta e}{4\pi\varepsilon_0 r} = -\frac{3}{2}\frac{\zeta^2 e^2\left(r_a^2 - r_c^2\right)}{4\pi\varepsilon_0\left(r_a^3 - r_c^3\right)}.$$

Adding E_{e-e} and E_{e-i}, we obtain the classical electrostatic energy per atom in agreement with the given formula.

Chapter 5

Problem 5.4s

Values of $\hbar\omega_{pf}$ (in eV) for some solids according to (5.27).

Li (8.39) , Na (6.62) , K (4.87) , Rb (4.45) , Mg (11.21) , Al (14.98) , Ag (9.33) .

Problem 5.9s

For Si and from Table 4.4 (p. 98), we have $c_\mathrm{l} = 8945\,\mathrm{m/s}$ and $c_\mathrm{t} = 5341\,\mathrm{m/s}$. We shall choose $\langle c\rangle \simeq 7500\,\mathrm{m/s}$. The Debye temperature $\Theta_\mathrm{D} = 645\,\mathrm{K}$, so that $T / \Theta_\mathrm{D} \simeq 300 / 645 = 0.465$ and $C_\mathrm{V} \simeq 0.82 \times 3N_\mathrm{a}k_\mathrm{B}$; $V / N_\mathrm{a} = 20\,\mathrm{A}^3$; $\ell_\mathrm{ph} \simeq 300\,\mathrm{A}$. The result, according to (5.134), is $K_\mathrm{ph} \simeq 127\,\mathrm{Wm^{-1}K^{-1}} = 1.27\,\mathrm{Wcm^{-1}K^{-1}}$ vs. $1.48\,\mathrm{Wcm^{-1}K^{-1}}$ experimentally.

Problem 5.11s

The Fourier transform of $f(\boldsymbol{r}) = \exp\left(-k_\mathrm{s}r\right)/r$ is

$$\begin{aligned}\tilde{f}(\boldsymbol{k}) &= \int \mathrm{d}^3r\exp\left(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}\right)f(\boldsymbol{r}) \\ &= 2\pi\int_{-1}^{1}\mathrm{d}\left(\cos\theta\right)\exp\left(-\mathrm{i}kr\cos\theta\right)\mathrm{d}r r^2 f(r) \\ &= (4\pi/k)\int_0^\infty \mathrm{d}r\sin kr\exp\left(-k_\mathrm{s}r\right) = 4\pi/\left(k^2 + k_\mathrm{s}^2\right).\end{aligned}$$

Problem 5.13s

The resistivity in SI is $\rho = \upsilon_{\mathrm{F}} / \varepsilon_0 \omega_{\mathrm{pf}}^2 \ell$, where $\ell^{-1} = n_{\mathrm{s}} \int \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}(1-\cos\theta)\mathrm{d}\Omega$. We have $k^2 = 4k_{\mathrm{F}}^2 \sin^2(\theta/2) = 2k_{\mathrm{F}}^2(1-\cos\theta)$, $2k\mathrm{d}k = -2k_{\mathrm{F}}^2\mathrm{d}(\cos\theta)$, $\mathrm{d}\Omega = -2\pi\mathrm{d}(\cos\theta) = 2\pi k\mathrm{d}k / k_{\mathrm{F}}^2$. Moreover, $\mathrm{d}\sigma / \mathrm{d}\Omega = (m^2 / 4\pi^2\hbar^4)(e^2 n_{\mathrm{e}} / \varepsilon_0)^2 \left(|\mathbf{k}\cdot\boldsymbol{u}| / k^2\varepsilon(k)\right)^2 = \left(m^2 e^4 n_{\mathrm{e}}^2 / 4\pi^2\hbar^4\varepsilon_0^2\right) (V\hbar\omega_k < n_k > / B)/(k^2\varepsilon(k))^2 = \left(\lambda_0 k_{\mathrm{s}}^4/\rho_{\mathrm{FV}}\right) (m^2/4\pi^2\hbar^4) \times (V\hbar\omega_k < n_k >)/(k_2^2\varepsilon(k))^2$. We took into account that $\lambda_0 / \rho_{\mathrm{FV}} = E_{\mathrm{s}}^2 / B$ and $E_{\mathrm{s}} = e^2 n_{\mathrm{e}} / \varepsilon_0 k_{\mathrm{s}}^2$. Substituting in the expression for ℓ^{-1} we have $\ell^{-1} = \left(\lambda_0 k_{\mathrm{s}}^4 / \rho_{\mathrm{FV}}\right)(m^2/4\pi^2\hbar^4)V^{-1}V\hbar \int \omega_k < n_k > \left(k^2/2k_{\mathrm{F}}^2\right) \left(2\pi k\mathrm{d}k/k_{\mathrm{F}}^2\right)/(k^2\varepsilon(k))^2 = \left(\lambda_0 k_{\mathrm{s}}^4 m^2 / 4\pi k_{\mathrm{F}}^4\hbar^4\rho_{\mathrm{FV}}\right) \times \int \mathrm{d}k k^3\hbar\omega_k < n_k > / (k^2\varepsilon(k))^2$ or, by defining $y \equiv \beta\hbar\bar{c}k$, $\ell^{-1} = (\lambda_0 m^2 k_{\mathrm{s}}^4/4\pi\hbar^4 k_{\mathrm{F}}^4\rho_{\mathrm{FV}})(2^4 k_{\mathrm{F}}^4/y_0^4) \int \mathrm{d}y y^3\hbar\omega_k \frac{1}{k^4\varepsilon^2(k)}\frac{1}{e^y-1}$, where $y_0 = 2\beta\hbar\bar{c}k_{\mathrm{F}}$. We have taken into account that $E_{\mathrm{F}} = \hbar^2 k_{\mathrm{F}}^2/2m$, $E_{\mathrm{F}}\rho_{\mathrm{FV}} = (3/4)n_{\mathrm{e}} = (3/4)(k_{\mathrm{F}}^3/3\pi^2) = k_{\mathrm{F}}^3/4\pi^2$, and $k^2\varepsilon(k) = k^2 + k_{\mathrm{s}}^2 = k_{\mathrm{s}}^2[1 + (k^2/k_{\mathrm{s}}^2)]$ and we have

$$\ell^{-1} = \frac{\lambda_o m}{8\pi\hbar}\frac{4\pi^2}{p_{\mathrm{F}}}\frac{16k_{\mathrm{B}}T}{y_0^4}\int_0^{y_0}\frac{\mathrm{d}y y^4}{[1+(2by^2/y_0^2)]^2(e^y-1)},$$

where $k^2/k_{\mathrm{s}}^2 = (k^2/k_{\mathrm{F}}^2)(k_{\mathrm{F}}^2/k_{\mathrm{TF}}^2 f) = (2y^2/y_0^2)(2k_{\mathrm{F}}^2/k_{\mathrm{TF}}^2 f)$ and $f(k/k_f)$ is given by (D.28). We write $b \equiv 2k_{\mathrm{F}}^2/k_{\mathrm{TF}}^2 f$. Thus

$$\rho = \frac{\upsilon_{\mathrm{F}}}{\varepsilon_0\omega_{\rho\mathrm{f}}^2\ell} = \frac{m\upsilon_{\mathrm{F}}}{p_{\mathrm{F}}}\frac{8\pi^2\lambda_0}{4\pi\varepsilon_0\hbar\omega_{\mathrm{pf}}^2}\frac{4k_{\mathrm{B}}T}{y_0^4}\int_0^{y_0}\frac{\mathrm{d}y\, y^4}{[1+(2by^2/y_0^2)]^2(e^y-1)},$$

which coincides with (5.59) since $m\upsilon_{\mathrm{F}} \equiv p_{\mathrm{F}}$.

Problem 5.15s

$$m\dot{\boldsymbol{v}} = -e\boldsymbol{E} - \frac{e\boldsymbol{v}\times\boldsymbol{B}}{c},$$
$$m\boldsymbol{B}\times\dot{\boldsymbol{v}} = -e\boldsymbol{B}\times\boldsymbol{E} - \frac{e}{c}\boldsymbol{B}\times(\boldsymbol{v}\times\boldsymbol{B}),$$
$$\boldsymbol{B}\times(\boldsymbol{v}\times\boldsymbol{B}) = \boldsymbol{v}B^2 - \boldsymbol{B}(\boldsymbol{v}\cdot\boldsymbol{B}),$$
$$m\boldsymbol{B}\times\dot{\boldsymbol{v}} = -e\boldsymbol{B}\times\boldsymbol{E} - \frac{e}{c}\left[\boldsymbol{v}B^2 - \boldsymbol{B}(\boldsymbol{v}\cdot\boldsymbol{B})\right],$$
$$\frac{e}{c}B^2\boldsymbol{v} = -m\boldsymbol{B}\times\dot{\boldsymbol{v}} - e\boldsymbol{B}\times\boldsymbol{E} + \frac{e}{c}(\boldsymbol{v}\cdot\boldsymbol{B})\boldsymbol{B},$$
$$\boldsymbol{v} = -\frac{mc}{e}\frac{1}{B^2}\boldsymbol{B}\times\dot{\boldsymbol{v}} - \frac{c}{B^2}\boldsymbol{B}\times\boldsymbol{E} + \frac{1}{B^2}(\boldsymbol{v}\cdot\boldsymbol{B})\boldsymbol{B},$$
$$\boldsymbol{v} = -\frac{mc}{e}\frac{1}{B}\boldsymbol{B}_0\times\dot{\boldsymbol{v}} - \frac{c}{B}\boldsymbol{B}_0\times\boldsymbol{E} + (\boldsymbol{v}\cdot\boldsymbol{B}_0)\boldsymbol{B}_0,$$
$$\boldsymbol{v} = -\frac{mc}{eB}\boldsymbol{B}_0\times\dot{\boldsymbol{v}} + \boldsymbol{v}_0 + (\boldsymbol{v}\cdot\boldsymbol{B}_0)\boldsymbol{B}_0,$$
$$\boldsymbol{v}_\perp = -\frac{mc}{eB}\boldsymbol{B}_0\times\dot{\boldsymbol{v}}_\perp + \boldsymbol{v}_0, \boldsymbol{v}_\parallel = (\boldsymbol{v}\cdot\boldsymbol{B}_0)\boldsymbol{B}_0 = \mathrm{Const.}$$

Chapter 6

Problem 6.5s

We implement the successive transformations shown in Fig. 6.16a and at each stage we calculate the matrix elements of the Hamiltonian

$$\chi_{n-1}^{1} = \frac{1}{\sqrt{2}}\left(\mathrm{s}_{n-1} + \mathrm{p}_{x,n-1}\right), \quad \chi_{n}^{2} = \frac{1}{\sqrt{2}}\left(\mathrm{s}_{n} - \mathrm{p}_{x,n}\right),$$
$$\chi_{n}^{1} = \frac{1}{\sqrt{2}}\left(\mathrm{s}_{n} + \mathrm{p}_{x,n}\right), \quad \chi_{n+1}^{2} = \frac{1}{\sqrt{2}}\left(\mathrm{s}_{n+1} - \mathrm{p}_{x,n+1}\right).$$

For the matrix elements of $\hat{H}$ we have

$$\left\langle \chi_i^1 \middle| \hat{H} \middle| \chi_i^1 \right\rangle = \left\langle \chi_i^2 \middle| \hat{H} \middle| \chi_i^2 \right\rangle = \frac{\varepsilon_{\mathrm{p}} + \varepsilon_{\mathrm{s}}}{2}, \quad i = n-1,\, n,\, n+1,$$
$$\left\langle \chi_i^1 \middle| \hat{H} \middle| \chi_i^2 \right\rangle = \left\langle \chi_i^2 \middle| \hat{H} \middle| \chi_i^1 \right\rangle = -\frac{\varepsilon_{\mathrm{p}} - \varepsilon_{\mathrm{s}}}{2} = -V_1, \quad i = n-1,\, n,\, n+1,$$
$$\begin{aligned}\left\langle \chi_{n-1}^1 \middle| \hat{H} \middle| \chi_n^1 \right\rangle &= \frac{1}{2}\Big[\left\langle s_{n-1} \middle| \hat{H} \middle| s_n \right\rangle + \left\langle s_{n-1} \middle| \hat{H} \middle| p_{x,n} \right\rangle + \left\langle p_{x,n-1} \middle| \hat{H} \middle| s_n \right\rangle \\ &\quad + \left\langle p_{x,n-1} \middle| \hat{H} \middle| p_{x,n} \right\rangle\Big] \\ &= \frac{\hbar^2}{2md^2}\left[-1.32 + 1.42 - 1.42 + 2.22\right] = 0.45\,\frac{\hbar^2}{md^2}.\end{aligned}$$

Similarly, $\left\langle \chi_n^2 \middle| \hat{H} \middle| \chi_{n+1}^2 \right\rangle = \frac{\hbar^2}{2md^2}\left[-1.32 - 1.42 + 1.42 + 2.22\right] = 0.45\,\frac{\hbar^2}{md^2}$,

$$\left\langle \chi_n^1 \middle| \hat{H} \middle| \chi_{n+1}^2 \right\rangle = \frac{\hbar^2}{2md^2}\left[-1.32 - 1.42 - 1.42 - 2.22\right] = -3.19\,\frac{\hbar^2}{md^2},$$
$$\begin{aligned}\psi_{bn-1,n} &= \frac{1}{\sqrt{2}}\left(\chi_{n-1}^1 + \chi_n^2\right), \quad \psi_{bn,n+1} = \frac{1}{\sqrt{2}}\left(\chi_n^1 + \chi_{n+1}^2\right), \\ \psi_{a,n-1,n} &= \frac{1}{\sqrt{2}}\left(\chi_{n-1}^1 - \chi_n^2\right), \quad \psi_{an,n+1} = \frac{1}{\sqrt{2}}\left(\chi_n^1 - \chi_{n+1}^2\right), \\ H_{n,n+1}^{bb} &\equiv \left\langle \psi_{bn-1,n} \middle| \hat{H} \middle| \psi_{bn,n+1} \right\rangle \\ &= \frac{1}{2}\Big[\left\langle \chi_{n-1}^1 \middle| \hat{H} \middle| \chi_n^1 \right\rangle + \left\langle \chi_n^2 \middle| \hat{H} \middle| \chi_n^1 \right\rangle + \left\langle \chi_n^2 \middle| \hat{H} \middle| \chi_{n+1}^2 \right\rangle\Big] \\ &= \frac{1}{2}\left[0.45\,\hbar^2/md^2 - V_1 + 0.45\,\hbar^2/md^2\right] = \frac{1}{2}\left[0.9\,\hbar^2/md^2 - V_1\right], \\ H_{n,n+1}^{aa} &= \frac{1}{2}\left[0.45\,\hbar^2/md^2 + V_1 + 0.45\,\hbar^2/md^2\right] = \frac{1}{2}\left[0.9\,\hbar^2/md^2 + V_1\right], \\ H_{n,n+1}^{ab} &= \frac{1}{2}\left[0.45\,\hbar^2/md^2 - V_1 - 0.45\,\hbar^2/md^2\right] = V_1/2.\end{aligned}$$

Problem 6.6s

The bonding or antibonding molecular orbitals are linear combinations of χ^1_{nc} and χ^2_{n+1a} atomic hybrids (see Fig. 6.17):

$\psi_{bn,n+1} = c_1\chi^1_{nc} + c_2\chi^2_{n+1a}$ with a similar expression $\psi_{an,n+1}$. Equation (1), $\hat{H}\psi_{bn,n+1} = \varepsilon\psi_{bn,n+1}$, in the basis χ^1_{nc} and χ^2_{n+1a} reads

$$\begin{pmatrix} \varepsilon_{hc} - \varepsilon_{b,a} & V_{2h} \\ V_{2h} & \varepsilon_{ha} - \varepsilon_{b,a} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0, \tag{4}$$

where $\varepsilon_{hc} = \varepsilon + V_{3h}$, $\varepsilon_{ha} = \varepsilon - V_{3h}$ are given by (6.81)-(6.83) and $V_{2h} = -3.19\hbar^2/md^2$. By setting the determinant equal to zero we find the eigenenergies ε_b and ε_a as given by (6.77) and (6.78). From (1) we have that $c_1/c_2 = V_{2h}/\left(\varepsilon_{b,a} - \varepsilon_{hc}\right) = V_{2h}/\left(\mp\sqrt{V_{2h}^2 + V_{3h}^2} - V_{3h}\right) = \pm\left(|V_{2h}|/\sqrt{V_{2h}^2 + V_{3h}^2}\right)/\left(1 \pm a_p\right) = \pm\sqrt{1 - a_p^2}/\left(1 \pm a_p\right) = \pm\left[\left(1 - a_p^2\right)/\left(1 \pm a_p\right)^2\right]^{1/2} = \left[\left(1 \mp a_p\right)/\left(1 \pm a_p\right)\right]^{1/2}$ where the upper signs are for the bonding and the lower for the antibonding. Taking into account the requirement of normalization it follows that

$$\begin{aligned} c_1 &= \frac{1}{\sqrt{2}}\left(1 - a_p\right)^{1/2}, \quad c_2 = \frac{1}{\sqrt{2}}\left(1 + a_p\right)^{1/2}, \text{bonding}, \\ c_1 &= \frac{1}{\sqrt{2}}\left(1 + a_p\right)^{1/2}, \quad c_2 = -\frac{1}{\sqrt{2}}\left(1 - a_p\right)^{1/2}, \text{ antibonding}. \end{aligned}$$

Problem 6.7s

Hint: Follow a similar to 6.5s step by step procedure and take into account that ψ_b and ψ_a are given by (6.79) and (6.80).

Problem 6.8s

As it was mentioned in Problem 6.3 the Hamiltonian in the basis g_{iak} is diagonal in k; thus in the intermediate expressions we are going to omit the index k. From (6.41) we have

$$\begin{aligned} &\left\langle g_{sc}\left|\hat{H}\right|g_{sc}\right\rangle = \varepsilon_{sc}, \quad \left\langle g_{sc}\left|\hat{H}\right|g_{sa}\right\rangle = V_{ss\sigma}\left(1 + \mathrm{e}^{2\mathrm{i}kd}\right), \quad \left\langle g_{sc}\left|\hat{H}\right|g_{pc}\right\rangle = 0, \\ &\left\langle g_{sc}\left|\hat{H}\right|g_{pa}\right\rangle = V_{sp\sigma}\left(-1 + \mathrm{e}^{2\mathrm{i}kd}\right), \quad \left\langle g_{sa}\left|\hat{H}\right|g_{sa}\right\rangle = \varepsilon_{sa}, \\ &\left\langle g_{sa}\left|\hat{H}\right|g_{pc}\right\rangle = V_{sp\sigma}\left(1 - \mathrm{e}^{-2\mathrm{i}kd}\right), \quad \left\langle g_{sa}\left|\hat{H}\right|g_{pa}\right\rangle = 0, \\ &\left\langle g_{pc}\left|\hat{H}\right|g_{pc}\right\rangle = \varepsilon_{pc}, \quad \left\langle g_{pc}\left|\hat{H}\right|g_{pa}\right\rangle = V_{pp\sigma}\left(1 + \mathrm{e}^{2\mathrm{i}kd}\right). \end{aligned}$$

Thus the 4×4 Hamiltonian matrix is:

$$\begin{array}{c|cccc|}
 & sc & sa & pc & pa \\
sc & \varepsilon_{sc} & V_{ss\sigma}\left(1+\mathrm{e}^{2\mathrm{i}kd}\right) & 0 & V_{sp\sigma}\left(-1+\mathrm{e}^{2\mathrm{i}kd}\right) \\
sa & V_{ss\sigma}\left(1+\mathrm{e}^{-2\mathrm{i}kd}\right) & \varepsilon_{sa} & V_{sp\sigma}\left(1-\mathrm{e}^{-2\mathrm{i}kd}\right) & 0 \\
pc & 0 & V_{sp\sigma}\left(1-\mathrm{e}^{2\mathrm{i}kd}\right) & \varepsilon_{ps} & V_{pp\sigma}\left(1+\mathrm{e}^{2\mathrm{i}kd}\right) \\
pa & V_{sp\sigma}\left(-1+\mathrm{e}^{-2\mathrm{i}kd}\right) & 0 & V_{pp\sigma}\left(1+\mathrm{e}^{-2\mathrm{i}kd}\right) & \varepsilon_{pa}
\end{array} .$$

For $\sin kd = 0$, i.e. $kd = 0$ or π, the above 4×4 breaks into two uncoupled 2×2 matrices, one involving the s states only and the other the p states only. These can be diagonalized immediately giving the following eigenvalues:

$$E_{v\ell} = \bar{\varepsilon}_s - \sqrt{V_{3s}^2 + 4V_{ss\sigma}^2} \quad s\text{-character},$$

$$E_{c\ell} = \bar{\varepsilon}_s + \sqrt{V_{3s}^2 + 4V_{ss\sigma}^2} \quad s\text{-character},$$

$$E_{vu} = \bar{\varepsilon}_p - \sqrt{V_{3p}^2 + 4V_{pp\sigma}^2} \quad p\text{-character},$$

$$E_{cu} = \bar{\varepsilon}_p + \sqrt{V_{3p}^2 + 4V_{pp\sigma}^2} \quad p\text{-character},$$

where

$$\bar{\varepsilon}_s = \left(\varepsilon_{cs} + \varepsilon_{sa}\right)/2, \quad V_{3s} = \left(\varepsilon_{sc} - \varepsilon_{sa}\right)/2, \quad \bar{\varepsilon}_p = \left(\varepsilon_{ps} + \varepsilon_{pa}\right)/2,$$
$$V_{3p} = \left(\varepsilon_{pc} - \varepsilon_{pa}\right)/2.$$

The gap E_{g} is equal to

$$E_{\mathrm{g}} = E_{c\ell} - E_{vu} = \sqrt{V_{3s}^2 + 4V_{ss\sigma}^2} + \sqrt{V_{3p}^2 + 4V_{pp\sigma}^2} - \left(\bar{\varepsilon}_{\mathrm{p}} - \bar{\varepsilon}_{\mathrm{s}}\right),$$

(assuming that $E_{c\ell} > E_{vu}$; if $E_{vu} > E_{c\ell}$the gap is equal to minus the above expression). According to this analysis the band edges of the VB and the CB are obtained by the following graphical analysis (Fig. 6.19):

The resulting gap is larger than that given by (6.50).

Using the values for GaAs (from table B.3 and for $d = 2.45A$) we have

$$\bar{\varepsilon}_s = -15.23, \quad V_{3s} = 3.68, \quad V_{ss\sigma} = 1.674,$$
$$\bar{\varepsilon}_p = -7.325, \quad V_{3p} = 1.655, \quad V_{pp\sigma} = 2.815,$$
$$E_{v\ell} = -20.205\,\mathrm{eV}, \quad E_{c\ell} = -10.255\,\mathrm{eV}, \quad E_{vu} = -13.1932\,\mathrm{eV},$$
$$E_{cu} = -1.457\,\mathrm{eV},$$
$$E_{\mathrm{g}} = 2.938\,\mathrm{eV},$$

while the approach shown in Fig. 6.17 gives

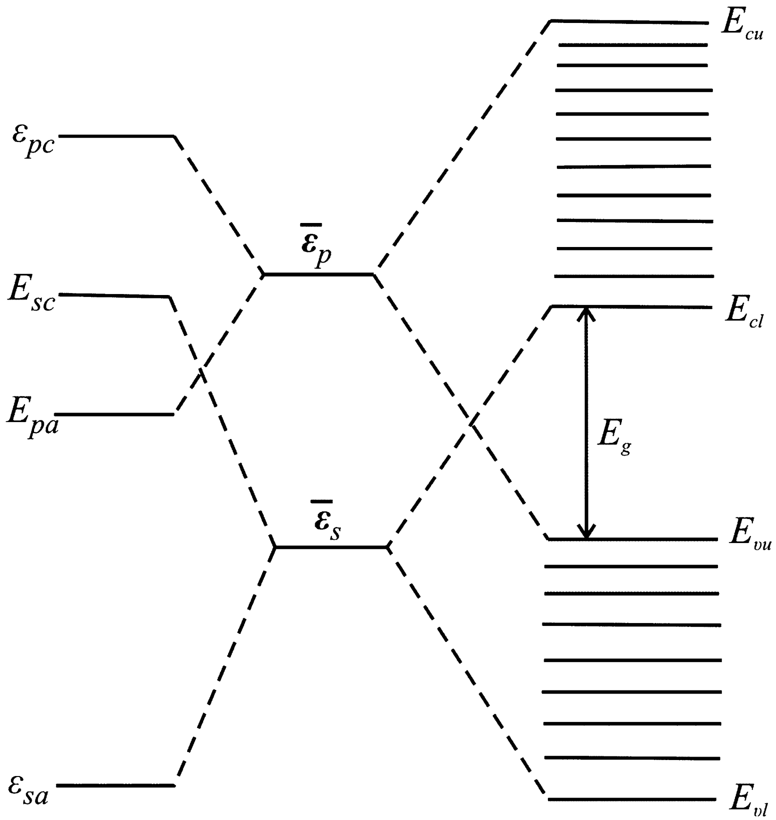

Fig. 6.19. The band edges, $E_{v\ell}$, E_{vu}, $E_{c\ell}$, E_{cu} of a one–dimensional compound semiconductor assuming that they correspond to $\sin kd = 0$; for $\sin kd = 0$ the s-states decoupled from the p-states, so that the bottoms of both the VB and the CB are of s- character, while the tops of both the VB and the CB are of p- character.

$E_{v\ell} \simeq -19.68\,\text{eV}, E_{c\ell} \simeq -10.78\,\text{eV}, E_{vu} \simeq -12.58\,\text{eV}, E_{cu} \simeq -2.075\,\text{eV}$, $E_\text{g} = 1.85\,\text{eV}$, vs. $E_\text{g} \simeq 1.52\,\text{eV}$ experimentally.

In the case of an elemental "semiconductor" for which $V_{3s} = V_{3p} = 0$, we have that the coefficients $c_{sa} = c_{sc}\exp(-ikd)$ and $c_{pa} = c_{pc}\exp(-\text{i}kd)$; thus the 4×4 matrix reduces to a 2×2 matrix as follows

$$\begin{array}{lcc} & sc & pc \\ sc & \varepsilon_s + 2V_{ss\sigma}\cos kd & 2iV_{sp\sigma}\sin kd \\ pc & -2iV_{sp\sigma}\sin kd & \varepsilon_p + 2V_{pp\sigma}\cos kd. \end{array}$$

Problem 6.10s

By performing the integration (since $\sum_k \to (L/2\pi)\int \text{d}k$) we obtain the following result

$$2\sum\nolimits_{k\le k_{\mathrm{F}}} E(k) = N\left[\varepsilon - \frac{2\left|V_2+V_2'\right|}{\pi}E\left(\lambda\right)\right], \tag{2}$$

where $E\left(\lambda\right)$ is the complete elliptic integral of second kind, $E\left(\lambda\right) \equiv \int_0^{\pi/2} \mathrm{d}\phi\sqrt{1-\lambda^2\sin^2\phi}$, and $\lambda = 4V_2V_2'/\left(V_2+V_2'\right)^2$. Assume that $V_2 = V_0\left(\frac{a}{2}-x\right)$ and $V_2' = V_0\left(\frac{a}{2}+x\right)$ where $V_0\left(y\right) \equiv -c/y^2$ and x is small. We call $U\left(x\right)$ the value of $2\sum_{k\le k_{\mathrm{F}}} E(k)$ for small x and $\delta U \equiv U\left(0\right) - U\left(x\right)$. Make the appropriate expansions and show that

$$\delta U = \frac{8}{\pi}\left|V_0\left(\frac{a}{2}\right)\right|\left[1+\ln\left(\frac{a}{|x|}\right)\right]\frac{4x^2}{a^2}. \tag{3}$$

Equation (3) shows that the dimerization of the model given by (6.11) and (6.12) by a small amount x lowers the total electronic energy by an amount of the order $x^2\ln\left(1/\left|x\right|\right)$. If any other energy (such as the elastic energy) contributing to the total energy changes by an amount of the order x^2, then we can conclude that the dimerization lowers the total energy and hence, the model given by (6.11) and (6.12) with one electron per atom is unstable against lattice distortion (**Peierls instability**).

Chapter 7

Problem 7.1s

Let us calculate, e.g., the matrix element $\left\langle g_{os}\left|\hat{H}\right| g_{1px}\right\rangle$. The summation over the primitive cell vectors $\boldsymbol{R}$ in (6.49) involves the ones for which $\boldsymbol{R}+\boldsymbol{d}_1$ are nearest neighbors of the atom "0" located at $\boldsymbol{R} = 0$ (see Fig. 7.1); $\boldsymbol{d}_1 = (a/4)\left(1,1,1\right)$ is the position of the atom "1" at the primitive cell $\boldsymbol{R} = 0$. Out of the twelve nearest neighbors $\mathbf{R}$ of $\boldsymbol{R} = 0$ only the following, $(a/2)\left(0\bar{1}\bar{1}\right)$, $(a/2)\left(\bar{1}0\bar{1}\right)$, $(a/2)\left(\bar{1}\bar{1}0\right)$ have $\left|\boldsymbol{R}+\boldsymbol{d}_1\right| = \left|\boldsymbol{d}_1\right|$ and hence, are nearest neighbors of atom "0" located at $\boldsymbol{R} = 0$. Thus, the four nearest neighbors of atom "0" are located at $\boldsymbol{d}_1 = \boldsymbol{O}+\boldsymbol{d}_1$, $\boldsymbol{d}_2 = (a/2)\left(0\bar{1}\bar{1}\right)+\boldsymbol{d}_1 = (a/4)\left(1\bar{1}\bar{1}\right)$, $\boldsymbol{d}_3 = (a/2)\left(\bar{1}0\bar{1}\right)+\boldsymbol{d}_1 = (a/4)\left(\bar{1}1\bar{1}\right)$, and $\boldsymbol{d}_4 = (a/2)\left(\bar{1}\bar{1}0\right)+\boldsymbol{d}_1 = (a/4)\left(\bar{1}\bar{1}1\right)$. To obtain a more symmetrical expression we define $\bar{c}_{1a}$ from the relation $c_{1a} = \bar{c}_{1a}\exp\left(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_1\right)$ (see (6.42)) so that all off-diagonal matrix elements will be multiplied by $\exp\left(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_1\right)$. The matrix elements $\left\langle\phi_{oos}\left|\hat{H}\right|\phi_{R1p_x}\right\rangle$ are given by (F.6) and (F.8), where $\ell = 1/\sqrt{3}, 1/\sqrt{3}, -1/\sqrt{3}, -1/\sqrt{3}$ for $\boldsymbol{d}_1, \boldsymbol{d}_2, \boldsymbol{d}_3, \boldsymbol{d}_4$ respectively. Thus with these conventions we have

$$\left\langle g_{os}\left|\hat{H}\right| g_{1p_x}\right\rangle = E_{sp}g_1\left(\boldsymbol{k}\right),$$

where $E_{sp} = \left(1.42/\sqrt{3}\right)\hbar^2/md^2 = 0.82\,\hbar^2/md^2$ and

$$g_1\left(\boldsymbol{k}\right) \equiv \exp\left(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_1\right)+\exp\left(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_2\right)-\exp\left(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_3\right)-\exp\left(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_4\right).$$

In a similar way we obtain all other matrix elements. The final result for the 8×8 matrix equation is the following:

$$\begin{vmatrix} \varepsilon_{so}-E & E_{ss}g_o & 0 & 0 & 0 & E_{sp}g_1 & E_{sp}g_2 & E_{sp}g_3 \\ E_{ss}g_o^* & \varepsilon_{s1}-E & -E_{sp}g_1^* & -E_{sp}g_2^* & -E_{sp}g_3^* & 0 & 0 & 0 \\ 0 & -E_{sp}g_1 & \varepsilon_{po}-E & 0 & 0 & E_{xx}g_o & E_{xy}g_3 & E_{xy}g_2 \\ 0 & -E_{sp}g_2 & 0 & \varepsilon_{po}-E & 0 & E_{xy}g_3 & E_{xx}g_o & E_{xy}g_1 \\ 0 & -E_{sp}g_3 & 0 & 0 & \varepsilon_{po}-E & E_{xy}g_2 & E_{xy}g_1 & E_{xx}g_o \\ E_{sp}g_1^* & 0 & E_{xx}g_o^* & E_{xy}g_3^* & E_{xy}g_2^* & \varepsilon_{p1}-E & 0 & 0 \\ E_{sp}g_2^* & 0 & E_{xy}g_3^* & E_{xx}g_o^* & E_{xy}g_1^* & 0 & \varepsilon_{p1}-E & 0 \\ E_{sp}g_3^* & 0 & E_{xy}g_2^* & E_{xy}g_1^* & E_{xx}g_o^* & 0 & 0 & \varepsilon_{p1}-E \end{vmatrix} \begin{vmatrix} c_{so} \\ \bar{c}_{s1} \\ c_{xo} \\ c_{yo} \\ c_{zo} \\ \bar{c}_{x1} \\ \bar{c}_{y1} \\ \bar{c}_{z1} \end{vmatrix} = 0,$$

where $E_{ss} \equiv V_{ss\sigma} = -1.32\,\hbar^2/md^2$, $E_{xx} = \frac{1}{3}V_{pp\sigma} + \frac{2}{3}V_{pp\pi} = 0.32\,\hbar^2/md^2$, and $E_{xy} = \frac{1}{3}V_{pp\sigma} - \frac{1}{3}V_{pp\pi} = 0.95\,\hbar^2/md^2$; moreover,

$$\begin{aligned} g_0(\boldsymbol{k}) &= \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_1) + \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_2) + \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_3) + \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_4), \\ g_2(\boldsymbol{k}) &= \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_1) - \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_2) + \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_3) - \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_4), \\ g_3(\boldsymbol{k}) &= \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_1) - \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_2) - \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_3) + \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}_4). \end{aligned}$$

The eigenfunctions $\psi_{\boldsymbol{k}}$ are of the form $\psi_k = \sum_a c_{0a}\,|g_{0a\boldsymbol{k}}\rangle + \sum_a \bar{c}_{1a}\,|g_{1a\boldsymbol{k}}\rangle$. Notice that for $\boldsymbol{k}=0$, $g_0 = 4$ and $g_1 = g_2 = g_3 = 0$, so that the 8×8 breaks into four 2×2 systems (one for s and three identical ones for the $p's$).

Problem 7.4s

We choose the atom "0" in Fig. 7.1 to be the anion and the atom "1" to be the cation. By a similar calculation as in Problem 6.6s, we find that the bonding and the antibonding molecular orbitals between atoms "0" and "1" are:

$$\begin{aligned} \psi_b^{(01)} &= \frac{1}{\sqrt{2}}\left[(1+a_p)^{1/2}\chi_o^1 + (1-a_p)^{1/2}\chi_1^1\right], \\ \psi_a^{(01)} &= \frac{1}{\sqrt{2}}\left[(1-a_p)^{1/2}\chi_o^1 - (1+a_p)^{1/2}\chi_1^1\right]. \end{aligned}$$

Similarly, the bonding and the antibonding orbitals between atoms "1" and "2" in Fig. 7.1 are

$$\begin{aligned} \psi_a^{(12)} &= \frac{1}{\sqrt{2}}\left[(1-a_p)^{1/2}\chi_2^2 - (1+a_p)^{1/2}\chi_1^2\right], \\ \psi_b^{(12)} &= \frac{1}{\sqrt{2}}\left[(1+a_p)^{1/2}\chi_2^2 + (1-a_p)^{1/2}\chi_1^2\right]. \end{aligned}$$

Let us calculate

$$H_c^{bb} = \left\langle \psi_b^{(01)} \middle| \hat{H} \middle| \psi_b^{(12)} \right\rangle = \tfrac{1}{2}\left[\left(1-a_p^2\right)^{1/2}\left\langle \chi_o^1 \middle| \hat{H} \middle| \chi_1^2 \right\rangle + \left(1-a_p^2\right)^{1/2} \left\langle \chi_1^1 \middle| \hat{H} \middle| \chi_2^2 \right\rangle + (1-a_p)\left\langle \chi_1^1 \middle| \hat{H} \middle| \chi_1^2 \right\rangle\right].$$

To proceed, we have to calculate $\left\langle \chi_0^1 \left| \hat{H} \right| \chi_1^2 \right\rangle$, which by symmetry is equal to $\left\langle \chi_1^1 \left| \hat{H} \right| \chi_2^2 \right\rangle$. (The matrix element, $\left\langle \chi_1^1 \left| \hat{H} \right| \chi_1^2 \right\rangle = -V_{1c} = -(\varepsilon_p - \varepsilon_s)/4$) according to (F.65)). The matrix element $\left\langle \chi_0^1 \left| \hat{H} \right| \chi_1^2 \right\rangle$ can be obtained either by employing the analysis in s, p_x, p_y, p_z as given in (F.60) and the mirror image of (F.61) (see also Fig. 7.1) or, more conveniently, by choosing the x' axis along the χ_0^1 orbital and the y' axis in the plane defined by the three atoms "0", "1", "2" in Fig. 7.1. Then $\chi_0^1 = \left[s + \sqrt{3}p_{x'}\right]/2$, $\chi_1^1 = \left[s - \sqrt{3}p_{x'}\right]/2$ and $\chi_1^2 = [s + \lambda_{x'}p_{x'} + \lambda_{y'}p_{y'}]$. The orthogonality of χ_1^1 and χ_1^2 requires that $\lambda_{x'} = 1/\sqrt{3}$ and the sp^3 condition, $\lambda_{x'}^2 + \lambda_{y'}^2 = 3$, determines $\lambda_{y'} = -\sqrt{8/3}$. Hence,

$$\begin{aligned}\left\langle \chi_0^1 \left| \hat{H} \right| \chi_1^2 \right\rangle &= \tfrac{1}{4}\left[V_{ss\sigma} + \tfrac{1}{\sqrt{3}}V_{sp\sigma} + \sqrt{3}V_{ps\sigma} + V_{pp\sigma}\right] \\ &= \tfrac{1}{4}\left[-1.32 + \tfrac{1.42}{\sqrt{3}} - \sqrt{3}\times 1.42 + 2.22\right]\tfrac{\hbar^2}{md^2} \\ &= -0.185\,\hbar^2/md^2.\end{aligned}$$

Thus the final result for H_c^{bb} is

$$H_c^{bb} = -\frac{1-a_p}{2}V_{1c} - \Lambda';\ \Lambda' = 0.185\frac{\sqrt{1-a_p^2}\hbar^2}{md^2},$$

which coincides with (7.14). In a similar way we obtain $\hat{H}_a^{bb}, \hat{H}_c^{aa}$ and $\hat{H}_a^{aa}$; a_p is given by (F.30) with V_2 and V_3 replaced by V_{2h} and V_{3h} respectively.

Problem 7.6s

Notice that $v_{\boldsymbol{k}} = \hbar^{-1}\nabla_k\varepsilon_{\boldsymbol{k}}$ and that $\varepsilon_{\boldsymbol{k}}v_{\boldsymbol{k}} = (2\hbar)^{-1}\nabla_k\varepsilon_{\boldsymbol{k}}^2$. The integral of the gradient of a periodic function, $f(\boldsymbol{k})$, such as $\varepsilon_{\boldsymbol{k}}$ or $\varepsilon_{\boldsymbol{k}}^2$, over the BZ is zero. To prove this define

$$I(\boldsymbol{q}) = \int_{\mathrm{BZ}} \mathrm{d}^3k\, f(\boldsymbol{k}+\boldsymbol{q}),$$

and notice that $I(\boldsymbol{q})$ does not depend on $\boldsymbol{q}$. (To show this, change variable to $\boldsymbol{k}' = \boldsymbol{k}+\boldsymbol{q}$ so that $I(\boldsymbol{q}) = \int_{\mathrm{pc}} \mathrm{d}^3k' f(\boldsymbol{k}')$, where pc is a primitive cell; but the integral of a periodic function over a primitive cell is the same no matter how the primitive cell is chosen). Then take the gradient of $I(q)$:

$$\nabla_k I(\boldsymbol{q}) = 0 = \int_{\mathrm{BZ}} \mathrm{d}^3k\nabla_k f(\boldsymbol{k}+\boldsymbol{q});\quad QED.$$

Chapter 8

Problem 8.7s

For Schottky defects, the energy U due to the presence of N_{S} defects is $U = N_{\mathrm{S}}\varepsilon_{\mathrm{V}}$; the entropy $\mathrm{S} = k_{\mathrm{B}}\ln\Delta\Gamma$, where $\Delta\Gamma$ is the number of ways for the N_{S}

defects to be placed at the N_L lattice sites:

$$\Delta\Gamma = N_L!/N_S!\,(N_L - N_S)! \simeq N_L^{N_L}/N_S^{N_S}\,(N_L - N_S)^{(N_L - N_S)}\,.$$

Thus the minimization condition $\partial G/\partial N_S = 0$ leads to $\varepsilon_v = -k_B T\,[\ln N_s - \ln (N_L - N_S)]\,(N_S/N_L \ll 1)$.

For Frenkel defects we have to combine the $N_L!/N_F!\,(N_L - N_F)!$ ways of placing the N_F vacancies in the N_L lattice sites with the $N_I!/N_F!\,(N_I - N_F)!$ ways of placing the N_F atoms in the N_I interstitial sites. From this point on the procedure is to minimize the Gibbs free energy $G = U - TS = N_F\varepsilon_F - k_B T \ln \Delta\Gamma$, taking into account that $N_F/N_L \ll 1$ and $N_F/N_I \ll 1$.

Problem 8.8s

The bound state eigenenergy does not belong to the spectrum of the unperturbed Hamiltonian. This implies that the operator $\varepsilon_b - \hat{H}_0$ never becomes zero and that the only solution of $\hat{H}_0\,|\,\chi\rangle = \varepsilon_b\,|\,\chi\rangle$ is the trivial one, $|\,\chi\rangle = 0$. Thus the only possibility, if any, to have a non-zero $|\,\psi\rangle$ in (B.59) for $E = \varepsilon_b$ and $|\,\chi\rangle = 0$ is for the operator

$$\left[1 - \hat{G}_0(E)\hat{H}_1\right]^{-1},$$

to blow up; given the form of $\hat{H}_1$, the only non-zero matrix elements of this operator are the ones between any $\langle n|$ and the $|0\rangle$ orbital. Expanding the operator in a power series and taking the matrix element $\langle n|,\,|0\rangle$ we obtain

$$\left\langle n \left| \left[1 - \hat{G}_0\,(E)\,\hat{H}_1\right]^{-1} \right| 0 \right\rangle = \delta_{n0} - \varepsilon G_{n0} \frac{1}{1 + \varepsilon G_{00}},$$

where

$$G_{n0}\,(E) = \left\langle n \left| \hat{G}_0\,(E) \right| 0 \right\rangle = \left\langle n \left| \frac{1}{E - \hat{H}_0} 0 \right| \right\rangle = \sum_{\boldsymbol{k}} \frac{\langle n\,|\,\boldsymbol{k})\,(\,\boldsymbol{k}|\,0\,\rangle}{E - E\,(\boldsymbol{k})},$$

and $\hat{H}_0\,|\,\boldsymbol{k}) = E\,(\mathbf{k})\,|\,\boldsymbol{k})$, i.e. $|\,\boldsymbol{k})$ are the eigenstates and $E\,(\boldsymbol{k})$ are the eigenenergies of $\hat{H}_0$. The sum over $\boldsymbol{k}$ can be simplified by introducing the DOS, $\rho\,(E') = \sum_{\boldsymbol{k}} \delta\,(E' - E\,(\boldsymbol{k}))$, as follows

$$\begin{aligned} G_{n0}\,(E) &= \int \mathrm{d}E' \sum_{\boldsymbol{k}} \delta\,(E' - E\,(\boldsymbol{k}))\,\frac{\langle n\,|\,\boldsymbol{k})\,(\boldsymbol{k}\,|0\,)}{E - E\,(\boldsymbol{k})} \\ &= \int \delta E' \frac{1}{E - E'} \sum_{\boldsymbol{k}} \delta\,(E' - E\,(\boldsymbol{k})) \times \langle n\,|\,\boldsymbol{k})\,(\boldsymbol{k}\,|0\,)\,. \end{aligned}$$

By choosing $\langle n| = \langle 0|$ we have

$$G_{00}\,(E) = \int \frac{\mathrm{d}E'}{E - E'} \frac{\rho\,(E')}{V}, \text{ since } \langle 0\,|\,k)\,(k\,|\,0\rangle = 1/V\,.$$

Hence, the bound eigenenergy ε_{b} is given as solution of the equation $1 + \varepsilon G_{00}(E) = 0$, or equivalently

$$\frac{1}{\varepsilon} = -\frac{1}{V}\int_{E_{\mathrm{l}}}^{E_{\mathrm{u}}} \frac{\mathrm{d}E' \rho(E')}{E - E'} = -\int_{E_{\mathrm{l}}}^{E_{\mathrm{u}}} \frac{\mathrm{d}E' \rho_0(E')}{E - E'}; \quad \rho_0(E') = \frac{1}{V}\rho(E'),$$

where E_l is the lower and E_u is the upper band edge.

Show that $G_{00}(E)$ is negative with negative slope for $E < E_{\mathrm{l}}$; moreover, as E approaches E_{l} from below, $G_{00}(E)$ blows up as $-(E_\ell - E)^{-1/2}$ when $\rho_0(E') \to (E' - E_{\mathrm{l}})^{-1/2}$, or as $\ln(E_{\mathrm{l}} - E)$ if $\rho_0(E)$ goes to a constant as $E' \to E_{\mathrm{l}}$; finally $G_{00}(E)$ goes to a negative constant as $E' \to E_{\mathrm{l}}^-$, if $\rho_0(E') \to (E' - E_{\mathrm{l}})^a$ with $a > 0$.

Chapter 9

Problem 9.1s

The phase of the incoming wave at the point $\boldsymbol{R}$ relative to that of the origin is $\phi_{\boldsymbol{R}i} - \phi_{oi} = \boldsymbol{k}_i \cdot \boldsymbol{R}$. The phase of the scattered wave at the point $\boldsymbol{R}$ is delayed relative to that at the origin by $\phi_{\boldsymbol{R}f} - \phi_{of} = -\boldsymbol{k}_f \cdot \boldsymbol{R}$ (the minus sign because of the delay). Hence, the scattered wave by a scatterer at $\boldsymbol{R}$ has a phase difference $\Delta\phi$ relative to that in the origin given by

$$\Delta\phi = \phi_{Ri} - \phi_{0i} + \phi_{\boldsymbol{R}f} - \phi_{0f} = \boldsymbol{k}_i \cdot \boldsymbol{R} - \boldsymbol{k}_f \cdot \boldsymbol{R} = \boldsymbol{k} \cdot \boldsymbol{R}.$$

Problem 9.2s

If we choose to work with the *cubic unit* cell of the *bcc* lattice (instead of the primitive cell), the vectors of the direct lattice are $a(n_1\boldsymbol{i} + n_2\boldsymbol{j} + n_3\boldsymbol{k})$ and that of the reciprocal are $(2\pi/a)(m_1\boldsymbol{i} + m_2\boldsymbol{j} + m_3\boldsymbol{k})$. There are two atoms per cubic unit cell, one at the origin and the other at $\boldsymbol{r} = (a/2)(\mathbf{i} + \boldsymbol{j} + \boldsymbol{k})$. Hence, the structure factor of the cubic unit cell is

$$S_{\mathrm{G}} = g[1 + \exp(-\mathrm{i}\boldsymbol{G} \cdot \boldsymbol{r})] = g[1 + \exp(-\mathrm{i}\pi(m_1 + m_2 + m_3))],$$

where g is the atomic form factor. Notice that if, $m_1+m_2+m_3$ is odd, $S_{\boldsymbol{G}} = 0$. Thus only $\boldsymbol{G}'s$ such that $m_1 + m_2 + m_3$ is even contribute to S_G giving $2g$.

If we choose to work with the primitive cell of the *bcc* we have

$$\boldsymbol{R}_n = (a/2)[(-n_1 + n_2 + n_3)\boldsymbol{i} + (n_1 - n_2 + n_3)\boldsymbol{j} + (n_1 + n_2 - n_3)\boldsymbol{k}],$$
$$\boldsymbol{G}_m = \frac{2\pi}{a}[(m_2 + m_3)\boldsymbol{i} + (m_3 + m_1)\boldsymbol{j} + (m_1 + m_2)\boldsymbol{k}].$$

In this case all $\boldsymbol{G}'s$ contribute, and $S_{\boldsymbol{G}} = g$; however, the sum of their Cartesian component is $2(m_1 + m_2 + m_3)$, i.e. always even. The cubic unit cell will give $2g$ since there are two primitive cells per cubic cell. Thus both approaches give the same result. The reader may work out the **fcc** case with four primitive cells per cubic unit cell.

Problem 9.3s

The distance between two points lying in two consecutive direct lattice planes along the direction of the basic vector $\boldsymbol{a}_1$ is $|\boldsymbol{a}_1|$; then the distance d_{p} between these two planes is $\boldsymbol{a}_1 \cdot \boldsymbol{n}$ where $\boldsymbol{n}$ is a vector of magnitude one normal to both planes. But $\boldsymbol{n} = \mathbf{G}/|\boldsymbol{G}|$ where $\boldsymbol{G}(m_1, m_2, m_3)$ is a vector of the reciprocal lattice normal to the plane with Miller indices, m_1, m_2, m_3. Hence, the distance $d_{\mathrm{p}} = \mathbf{a}_1 \cdot \boldsymbol{G}/|\boldsymbol{G}| = 2\pi m_1/|\boldsymbol{G}|$, or $|\boldsymbol{G}| = 2\pi m_1/d_{\mathrm{p}}$ QED.

Problem 9.5s

In Fig. 9.10 below we plot the phonon dispersion $\pm\hbar\omega(q)$ vs. q in the repeated zone scheme (continuous curves) and the parabolas $\varepsilon_{\mathrm{f}} - \varepsilon_{\mathrm{i}} = \left(\hbar^2/2m\right)(k_{\mathrm{i}} \pm q)^2 - \varepsilon_{\mathrm{i}}$ for the neutron (dashed curves). The intersection of solid and the dashed curves, gives the values of q which satisfy both (9.26) and (9.27).

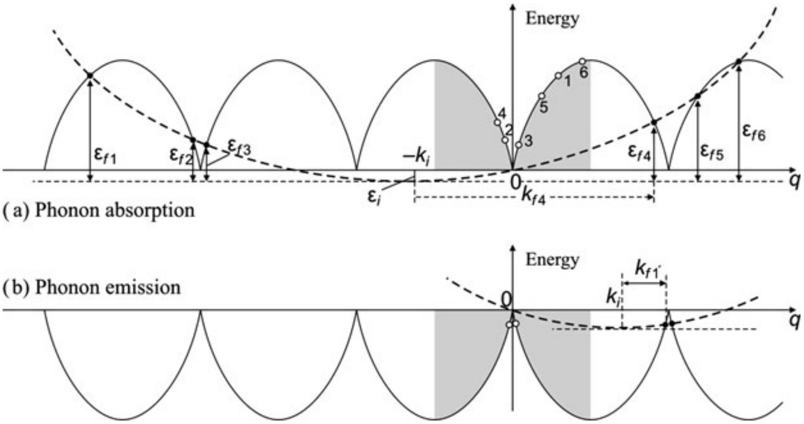

Fig. 9.10. Phonon dispersion, $\hbar\omega$ vs q, in the repeated zone scheme (continuous lines) and the neutron parabolas $\varepsilon_f - \varepsilon_i$ vs $(k_i \pm q)^2$ (dashed lines). The intersections of the continuous lines with the dashed lines provide the energies and the wavenumbers for absorbed and emitted phonons

Problem 9.7s and 9.9s

Let $|\lambda\rangle$ be a normalized eigenfunction of the hermitean non negative operator $a_Q^+ a_Q$: $a_Q^+ a_Q |\lambda\rangle = \lambda |\lambda\rangle$, where λ is the corresponding eigenvalue $(\lambda \geq 0)$. Consider the state $a_{Q'} |\lambda\rangle$ and act on it by $a_Q^+ a_Q$: $a_Q^+ a_Q a_{Q'} |\lambda\rangle = \left(a_{Q'} a_Q^+ a_Q - \delta_{QQ'} a_Q\right) |\lambda\rangle = a_{Q'} \lambda |\lambda\rangle - \delta_{QQ'} a_Q |\lambda\rangle = \lambda a_{Q'} |\lambda\rangle - \delta_{QQ'} a_Q |\lambda\rangle = (\lambda - \delta_{QQ'}) a_{Q'} |\lambda\rangle$. Thus the state $a_Q |\lambda\rangle$ is also an eigenstate of $a_Q^+ a_Q$ with an eigenvalue $\lambda - 1$; moreover, the state $a_Q^n |\lambda\rangle$ is also an eigenstate for $a_Q^+ a_Q$ with eigenvalue $\lambda - n$ where n is any natural number. Since the eigenvalues of $a_Q^+ a_Q$ are non negative, it follows that these eigenvalues are $n = 0, 1, 2, \ldots$, because, otherwise, $a_Q^+ a_Q$ would have negative eigenvalues.

We found that $a_Q\,|n\rangle = \chi_n\,|n-1\rangle$, where $|n-1\rangle$ is normalized and χ_n is the normalization factor. We have $\left\langle n\left|a_Q^+ a_Q\right|n\right\rangle = n = \chi_n^2\,\langle n-1|\,n-1\rangle = \chi_n^2$. Hence

$$a_Q\,|n\rangle\ = \sqrt{n}\,|n-1\rangle\ .$$

Similarly we can show that $a_Q^+\,|n\rangle\ = \chi_n'\,|n+1\rangle$ and that $\chi_n' = \sqrt{n+1}$.

Problem 9.12s

We assume central forces and cubic symmetry. Let $\mathcal{V}(R)$ be the potential energy between an atom at the origin and one located at the lattice point $\boldsymbol{R}$. The change Δ in the total potential energy due to displacements $\boldsymbol{u}(\boldsymbol{R})$ is

$$\Delta = \frac{1}{2}\sum_{\boldsymbol{R}}(\partial^2 V/\partial R^2)(\delta R)^2,$$

where $\delta R^2 = \left[\boldsymbol{R}\cdot(\boldsymbol{u}(\boldsymbol{R})-\boldsymbol{u}(0))\,/R\right]^2 = \Big\{R_x^2\,(u_x(\boldsymbol{R})-u_x(0))^2 + R_y^2\,(u_y(\boldsymbol{R}) - u_y(0))^2 + R_xR_y\,(u_x(\boldsymbol{R})-u_x(0))\,(u_y(\boldsymbol{R})-u_y(0)) + R_yR_x\,(u_y(\boldsymbol{R})-u_y(0))\,(u_x(\boldsymbol{R})-u_x(0))\Big\}\,/R^2$ assuming displacements in the x, y plane. It follows that the spring constants $\kappa_{ij}(\boldsymbol{R}) = -D_{ij}(\boldsymbol{R})$ are proportional to R_iR_j: $D_{ij}(\boldsymbol{R}) = -A\,R_iR_j$. Substituting in (9.63) we have

$$\begin{aligned} c_{12} \equiv c_{xxyy} &= \frac{-1}{8V_{\rm pc}}\sum_{\boldsymbol{R}}\left[R_xD_{xy}R_y + R_xD_{xy}R_y + R_xD_{xy}R_y + R_xD_{xy}R_y\right] \\ &= \frac{A}{2V_{\rm pc}}\sum_{\mathbf{R}}R_x^2R_y^2. \end{aligned}$$

Similarly

$$\begin{aligned} c_{44} \equiv c_{xyxy} &= -\tfrac{1}{8V_{\rm pc}}\sum_{\boldsymbol{R}}\left[R_xD_{yy}R_x + R_yD_{xy}R_x + R_xD_{yx}R_y + R_yD_{xx}R_y\right] \\ &= \tfrac{A}{8V_{\rm pc}}\sum_{\boldsymbol{R}}\left[R_x^2R_y^2 + R_y^2R_x^2 + R_x^2R_y^2 + R_y^2R_x^2\right] = \tfrac{A}{2V_{pc}}\sum_{\boldsymbol{R}}R_x^2R_y^2 = c_{12}. \end{aligned}$$

(For a more general treatment of Cauchy's relations see the book by Born and Huang [AW64], p. 136).

Problem 9.13s

The force, $\boldsymbol{F}_i$ exercised on the atom 0 at the center by the spring i ($i = 1,\ldots 8$) is the product of the unit vector $\boldsymbol{n}_i = \cos\theta_i\boldsymbol{i} + \sin\theta_i\boldsymbol{j}$ in the direction of the spring i, times the elongation of the spring i along the direction $\boldsymbol{n}_i$, $\boldsymbol{n}_i\cdot(\boldsymbol{u}_i-\boldsymbol{u}_0)$, times the spring constant:

$\boldsymbol{F}_i = \kappa_i\boldsymbol{n}_i\cdot(\boldsymbol{u}_i-\boldsymbol{u}_o)\boldsymbol{n}_i = \kappa_i[\cos\theta_i(u_{ix}-u_{0x}) + \sin\theta_i(u_{iy}-u_{0y})][\cos\theta_i\boldsymbol{i} + \sin\theta_i\boldsymbol{j}]$; $\kappa_i = \kappa$, if i odd, $\kappa_i = \kappa'$, if i even.

Newton's equation for the ℓ component ($\ell = x, y$) of the displacement $\boldsymbol{u}_0$ is

$$
\begin{aligned}
-m\omega^2 u_{0x} = \kappa(u_{1x} - u_{0x}) + \frac{1}{2}\kappa'(u_{2x} - u_{0x} + u_{2y} - u_{0y}) \\
+ \frac{1}{2}\kappa'(u_{4x} - u_{0x} - u_{4y} + u_{0y}) + \kappa(u_{5x} - u_{0x}) \\
+ \frac{1}{2}\kappa'(u_{6x} - u_{0x} + u_{6y} - u_{0y}) + \frac{1}{2}\kappa'(u_{8x} - u_{0x} - u_{8y} + u_{0y}),
\end{aligned} \tag{1}
$$

where $\cos^2\theta_i = 1/2$ and $\cos\theta_i \cdot \sin\theta_i = \pm 1/2$, for even i; there is an equation similar to (1) for the u_{0y} component.

Employing Bloch theorem, $\boldsymbol{u}_i = \boldsymbol{u}_0 \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}_i)$, and the following relations:

$$
\begin{aligned}
\boldsymbol{k} \cdot \boldsymbol{R}_1 = k_x a, \;\; \boldsymbol{k} \cdot \mathbf{R}_2 = k_x a + k_y a, \;\; \boldsymbol{k} \cdot \boldsymbol{R}_3 = k_y a, \;\; \boldsymbol{k} \cdot \boldsymbol{R}_4 = -k_x a + k_y a, \\
\boldsymbol{k} \cdot \boldsymbol{R}_5 = -k_x a, \;\; \boldsymbol{k} \cdot \mathbf{R}_6 = -k_x a - k_y a, \;\; \boldsymbol{k} \cdot \boldsymbol{R}_7 = -k_y a, \\
\text{and } \boldsymbol{k} \cdot \boldsymbol{R}_8 = k_x a - k_y a,
\end{aligned} \tag{2}
$$

we obtain from (1), by setting $\omega_0^2 = \kappa/m$ and $\omega_0'^2 = \kappa'/m$:

$$
\begin{aligned}
\left[\omega^2 - 2\omega_0^2 (1 - \cos k_x a) - \omega_0'^2 (2 - \cos(k_x a + k_y a) - \cos(k_x a - k_y a))\right] u_{ox} \\
+\omega_0'^2 \left[\cos(k_x a + k_y a) - \cos(k_x a - k_y a)\right] u_{oy} = 0.
\end{aligned} \tag{3}
$$

Similarly, for the y-component we have

$$
\begin{aligned}
\omega_0'^2 \left[\cos(k_y a + k_x a) - \cos(k_y a - k_x a)\right] u_{0x} \\
+ \left[\omega^2 - 2\omega_0^2 (1 - \cos k_y a) - \omega_0'^2 (2 - \cos(k_y a + k_x a) - \cos(k_y a - k_x a))\right] u_{0y} = 0.
\end{aligned} \tag{4}
$$

Setting the determinant of (3) and (4) equal to zero we obtain a quadratic equation for ω^2, the solutions of which give the two eigenfrequencies. Plot with the help of the computer the eigenfrequencies vs. $\boldsymbol{k}$ as $\boldsymbol{k}$ follows the line segments, ΓX, XM, MΓ . Plot also the contours $\omega = \omega_1(\boldsymbol{k})$ and $\omega = \omega_2(\boldsymbol{k})$ for various values of ω. Notice that, for $\boldsymbol{k}$ along ΓX, (3) and (4) decouple and the solutions are either pure longitudinal or pure transverse. Along ΓM also the solutions are pure LA or pure TA. The sound velocities for $\boldsymbol{k}$ along ΓX or along ΓM are:

$c_{\mathrm{l}} = a\sqrt{\omega_0^2 + \omega_0'^2}$, $c_{\mathrm{t}} = a\omega_0'$ and $c_{\mathrm{l}} = a\sqrt{\frac{1}{2}\omega_0^2 + 2\omega_0'^2}$, $c_{\mathrm{t}} = a\omega_0/\sqrt{2}$ respectively.

Problem 9.16s

We have shown that $2W = \left\langle (\boldsymbol{k} \cdot \boldsymbol{u})^2 \right\rangle = \left\langle k^2 u^2 \cos^2\theta \right\rangle = \frac{1}{3}k^2 \left\langle u^2 \right\rangle$; we took into account that $\boldsymbol{k}$ is constant and that the average of $\cos^2\theta$ over all solid angles is 1/3. But twice the potential energy $\frac{1}{2}\kappa\left\langle u^2\right\rangle$ is equal to the total vibrational energy ε per atom. Hence, $2W = \frac{1}{3}k^2\left\langle u^2\right\rangle = \frac{1}{3}k^2\varepsilon/\kappa$; but $\omega_{\mathrm{D}}^2 = c_1\kappa/M$, where c_1 is a numerical constant of the order of one and M is the mass of each atom. Thus

$$2W = \frac{c_1}{3}\frac{1}{{\omega_{\mathrm{D}}}^2 M}k^2\varepsilon. \tag{1}$$

For low temperatures $T \ll \Theta_{\mathrm{D}}$, $\varepsilon = (9/8)\hbar\omega_{\mathrm{D}}$, while for $T \gtrsim \Theta_{\mathrm{D}}$, $\varepsilon = 3k_{\mathrm{B}}T$. Hence

$$2W = \frac{3c_1}{8}\frac{\hbar^2k^2/M}{\hbar\omega_{\mathrm{D}}}, \quad T \ll \Theta_{\mathrm{D}}, \tag{2}$$

$$2W = c_1\frac{k^2k_{\mathrm{B}}T}{\omega_{\mathrm{D}}^2 M} = c_1\frac{\hbar^2k^2/M}{\hbar\omega_D}\frac{T}{\Theta_{\mathrm{D}}}, \quad T \ll \Theta_{\mathrm{D}}. \tag{3}$$

The exact asymptotic expressions for the Debye model are obtained by setting $c_1 = 2$ in (2) and $c_1 = 3$ in (3).

Chapter 10

Problem 10.2s

We change the integration to summation over the $\boldsymbol{k}'s$ of the 1^{st} BZ, according to (B.19); then we use the identity $(x + \mathrm{i}s)^{-1} \to P(x^{-1}) - \mathrm{i}\pi\delta(x)$, as $s \to 0^+$.Thus, we end up with $\rho_n(E) = \sum_{\boldsymbol{k}}\delta(E - E_n(\boldsymbol{k}))$, which is valid by the definition of $\rho_n(E)$.

Problem 10.4s

The full answer can be found in the book by E. N. Economou [DSL153], pp.422–425.

Problem 10.5s

According to (10.42) m_c^* is proportional to $\left|\partial A\left(E, k_z\right)/\partial E\right|$ where A is the area enclosed by the curve resulting from the intersection of the constant energy surface $E = \frac{1}{2}\sum_{ij}\gamma_{ij}q_iq_j + \varepsilon_0$ and the plane $q_z = 0$, where $\boldsymbol{q} = \boldsymbol{k} - \boldsymbol{k}_0$; the tensor γ_{ij} is related to the mass tensor as follows: $\gamma_{ij} = \hbar^2(M^{-1})_{ij}$. The equation of the closed curve, $\frac{1}{2}\gamma_{xx}q_x^2 + \frac{1}{2}\gamma_{yy}q_y^2 + \gamma_{xy}q_xq_y = E - \varepsilon_o$, can be brought to a diagonal form $\frac{1}{2}\tilde{\gamma}_{xx}\tilde{q}_x^2 + \frac{1}{2}\tilde{\gamma}_{yy}\tilde{q}_y^2 = E - \varepsilon_o + c$ by a rotation plus translation transformation; c is a constant. This is the equation of an ellipse with semiaxes $a^2 = 2|E - \varepsilon_o + c|/\tilde{\gamma}_{xx}$ and $b^2 = 2\left|E - \varepsilon_o + c\right|/\tilde{\gamma}_{yy}$; its enclosed area is $A = \pi ab = 2\pi|E - \varepsilon_o + c|/\sqrt{\tilde{\gamma}_{zz}\tilde{\gamma}_{yy}}$ and $|\partial A/\partial E| = 2\pi/\sqrt{\tilde{\gamma}_{xx}\tilde{\gamma}_{yy}}$. The rotation preserves the determinant so that $\tilde{\gamma}_{xx}\tilde{\gamma}_{yy} = \gamma_{xx}\gamma_{yy} - \gamma_{xy}^2$; but, because $\gamma M = \hbar^2$, we have that $\gamma_{xx}\gamma_{yy} - \gamma_{xy}^2 = \hbar^4 M_{z\,z}/\det|M_{ij}|$. hence, $m_c^* = (\hbar^2/2\pi)\,|\partial A \,/\, \partial E| = |\det(M)/M_{z\,z}|^{1/2}$.

Chapter 11

Problem 11.3s

See the book by S. Flügge [Q26], problem 81, pp. 210–213.

Problem 11.5s

Equation (11.75), by employing the identity $\nabla' \cdot (f_1(\boldsymbol{r}')\nabla' f_2(\boldsymbol{r}')) = f_1(\boldsymbol{r}')$ $\nabla'^2 f_2(\boldsymbol{r}') + \nabla' f_1(\boldsymbol{r}') \cdot \nabla' f_2(\boldsymbol{r}')$ and the equations (11.43) and (11.16), turns out to be identical to (11.47). From (11.75) we have by employing Gauss theorem

$$\int d\boldsymbol{S}' G_o(\boldsymbol{r}-\boldsymbol{r}') \cdot \nabla'\psi(\boldsymbol{r}') = \int d\boldsymbol{S}'\psi(\boldsymbol{r}') \cdot \nabla' G_0(\boldsymbol{r}-\boldsymbol{r}'), \qquad (1)$$

where $d\boldsymbol{S}'$ is the infinitesimal element of the area of the sphere $|\boldsymbol{r}'| = r_0$ pointing along the direction $\boldsymbol{r}'$. Setting: $\boldsymbol{r} = \rho, \theta, \phi$, $\boldsymbol{r}' = \rho', \theta', \phi'$, and $\rho = \rho' = r_0$, we have $\mathrm{d}\boldsymbol{S}' \cdot \nabla'\psi(\boldsymbol{r}') = r_0^2 \mathrm{d}\Omega'(\partial\psi(\boldsymbol{r}')/\partial\rho')$ and $d\boldsymbol{S}' \cdot \nabla' G_0(\boldsymbol{r}-\boldsymbol{r}') = r_o^2 d\Omega'(\partial G(\boldsymbol{r}-\boldsymbol{r}')/\partial\rho')$; substituting in (1), (11.49) follows (with the renaming $\rho', \theta', \phi', \mathrm{d}\Omega' \leftrightarrow \rho, \theta, \phi, \mathrm{d}\Omega$).

Problem 11.9s

The interaction energy, $U_{\mathrm{ie}} = \int V_i\,(\boldsymbol{r})\,n(\boldsymbol{r})\mathrm{d}^3 r$, in view of (11.77) and (11.78) can be written as follows

$$U_{\mathrm{ie}} = \frac{1}{V}\sum_{\boldsymbol{q},\boldsymbol{k}} V_{\mathrm{i}\,\boldsymbol{q}} n_{\boldsymbol{k}} \int \mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{k})\cdot\boldsymbol{r}} \mathrm{d}^3 r = \sum_{\boldsymbol{q}} V_{\mathrm{i}\,\boldsymbol{q}} n_{-\boldsymbol{q}} = -\frac{1}{e}\sum_{\boldsymbol{q}} V_{\mathrm{i}\,\boldsymbol{q}} \rho_{-\boldsymbol{q}}, \qquad (1)$$

since the integral is equal to $V\delta_{-\boldsymbol{q},\boldsymbol{k}}$. The ionic potential $V_{\mathrm{i}}(\boldsymbol{r})$ can be written as follows: $V_i(\boldsymbol{r}) = (-e/4\pi\varepsilon_0)\int \mathrm{d}^3 r' \rho_i(\boldsymbol{r}')/\,|\boldsymbol{r}-\boldsymbol{r}'|$. Writing both $\rho_i(\boldsymbol{r}')$ and $|\boldsymbol{r}-\mathbf{r}'|^{-1}$ in terms of their Fourier transforms, $\rho_i(\boldsymbol{r}') = \frac{1}{\sqrt{V}}\sum_{\boldsymbol{q}} \rho_{\mathrm{i}\boldsymbol{q}} \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}')$ and $|\boldsymbol{r}-\boldsymbol{r}'|^{-1} = \frac{1}{V}\sum_{\boldsymbol{k}} \frac{4\pi}{k^2}\exp\left(\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')\right)$, we obtain

$$V_{\mathrm{i}}(\boldsymbol{r}) = -\frac{4\pi e}{4\pi\varepsilon_0\sqrt{V}}\sum_{\boldsymbol{q}} (\rho_{\mathrm{i}\boldsymbol{q}}/q^2)e^{i\boldsymbol{q}\cdot\boldsymbol{r}}. \qquad (2)$$

Comparing (11.77) and (2), we find that $V_{\mathrm{i}\boldsymbol{q}} = -4\pi e\rho_{\mathrm{i}\,\boldsymbol{q}}/4\pi\varepsilon_0 q^2$; substituting this expression for $V_{\mathrm{i}\boldsymbol{q}}$ in (11.78), (11.79) follows.

Chapter 12

Problem 12.5s

The potential energy $V_{\mathrm{i}}(d')$, which is the quantity in brackets in (12.23), can be written as follows by taking into account (12.21), (12.18), and the identity $d'^{-1} \equiv (2/\pi d') \int_0^\infty \mathrm{d}k(\sin kd')/k$

$$V_{\mathrm{i}}\,(d) = -\frac{2e^2\zeta^2}{4\pi\varepsilon_0\pi d'}\int_0^\infty \mathrm{d}k \sin kd' \left[\frac{(\cos^2 kr_{\mathrm{c}})\tilde{f}(k)-1}{k}\right]. \tag{1}$$

In arriving at (1) we have set $1-\varepsilon^{-1} \equiv \tilde{f}$ and we have used the empty-core pseudopotential given by (11.4). The integrand in (1) is an even function; so we can extend the integration from $-\infty$ to $+\infty$ by dividing by two. Next we write: $\sin kd' = [\exp(\mathrm{i}kd') - \exp(-\mathrm{i}kd')]/2\mathrm{i}$; in the integral over $\exp(-\mathrm{i}kd')$ we change variables from k to $-k$, and this integral becomes identical to the one involving $\exp(\mathrm{i}kd')$. Thus the end result is

$$V_{\mathrm{i}}(d') = -\frac{e^2\zeta^2}{4\pi\varepsilon_0 i\pi d'}\int_{-\infty}^\infty \mathrm{d}k\mathrm{e}^{\mathrm{i}kd'}\left[\frac{\cos^2 kr_{\mathrm{c}}\tilde{f}(k)-1}{k}\right]. \tag{2}$$

If we choose the Thomas–Fermi expression for $\varepsilon(k)$ we have that $\tilde{f}(k) = k_{\mathrm{TF}}^2/(k^2+k_{\mathrm{TF}}^2)$; then the integral in (2) can be calculated by closing the integration path with an infinite semicircle in the upper complex plane (which gives no contribution for $d' > 2r_{\mathrm{c}}$) and by employing the residue theorem at the pole $k = \mathrm{i}k_{\mathrm{TF}}$ (the $k = 0$ is not a pole because $\cos^2 kr_{\mathrm{c}}\tilde{f}(k) = 1 + O(k^2)$ *as* $k \to 0$). The residue is $-\frac{1}{2}\exp(-k_{\mathrm{TF}}d')\cosh^2 k_{\mathrm{TF}}r_{\mathrm{c}}$ and, thus, (12.25) is obtained.

In the case where the RPA dielectric function is used we perform first two successive integrations by parts in (1) by setting $\sin kd' = -(1/d')d(\cos kd')/\mathrm{d}k$ and $\cos kd' = (1/d')d(\sin kd')/\mathrm{d}k$, so that the RPA singularity at $k = 2k_{\mathrm{F}}$ would give rise to two poles at $k = \pm 2k_{\mathrm{F}}$; then we do the same transformations which took us from (1) to (2). We have at the end the following result:

$$V_{\mathrm{i}}(d') = \frac{1}{4\pi\varepsilon_0}\frac{e^2\zeta^2}{\mathrm{i}\pi d'^3}\int_{-\infty}^\infty \mathrm{d}k\mathrm{e}^{\mathrm{i}kd'}\frac{\mathrm{d}^2}{\mathrm{d}k^2}\left[\frac{\cos^2 kr_{\mathrm{c}}\tilde{f}(k)-1}{k}\right]. \tag{3}$$

The quantity $\tilde{f} \equiv 1-\varepsilon^{-1}$, given the expression $\varepsilon = 1+(k_{\mathrm{TF}}/k^2)f$, becomes $\tilde{f} = \frac{k_{\mathrm{TF}}^2 f}{k^2+k_{\mathrm{TF}}^2 f}$, where f is given by (D.28). The most singular part of the integrand in (3), for real k, is due to the second derivative of f. Thus, for

$k^2 \simeq (2k_\mathrm{F})^2$, we have

$$\frac{\mathrm{d}^2}{\mathrm{d}k^2}\left[\frac{\cos^2 kr_\mathrm{c}\tilde{f}(k)-1}{k}\right] \simeq \frac{\cos^2 2k_\mathrm{F}r_\mathrm{c}}{2k_\mathrm{F}}\frac{1}{\varepsilon^2(2k_\mathrm{F})}\frac{1}{\pi a_\mathrm{B}k_\mathrm{F}}\frac{1}{2(2k_\mathrm{F})}\left[\frac{1}{k-2k_\mathrm{F}}+\frac{1}{k+2k_\mathrm{F}}\right]. \tag{4}$$

In arriving at (4) we use the relation, $k_\mathrm{TF}^2 = 4k_\mathrm{F}/\pi a_\mathrm{B}$. Substituting (4) in (3) and performing the integration by the residue theorem we find

$$V_\mathrm{i}(d') = \frac{e^2\zeta^2}{4\pi\varepsilon_0}\frac{\cos 2k_\mathrm{F}d'}{d'^3}\frac{\cos^2 2k_\mathrm{F}r_\mathrm{c}}{(2k_\mathrm{F})^2}\frac{1}{\varepsilon^2(2k_\mathrm{F})}\frac{1}{\pi a_\mathrm{B}k_\mathrm{F}}. \tag{5}$$

Replacing $\cos^2 2k_\mathrm{F}r_\mathrm{c}$ from the relation, $\tilde{v}_{\mathrm{i}A}(2k_\mathrm{F}) = -4\pi\zeta e^2 n_\mathrm{a}\cos 2k_\mathrm{F}r_\mathrm{c}/4\pi\varepsilon_0\,(2k_\mathrm{F})^2$, taking into account that $n_\mathrm{a} = k_\mathrm{F}^3/3\pi^2\zeta$ and $\tilde{v} = v_i/\varepsilon$, we obtain finally (12.24).

Chapter 13

Problem 13.2ts

To solve the system

$$\begin{vmatrix} E-E^{(0)} & V & \cdots & V \\ V & E-E^{(0)} & \cdots & V \\ \vdots & \vdots & & \vdots \\ V & V & \cdots & E-E^{(0)} \end{vmatrix} \begin{vmatrix} c_1 \\ c_2 \\ \vdots \\ c_\mathrm{N} \end{vmatrix} = 0, \tag{1}$$

we try solutions of the form $c_n = c_o\exp(\mathrm{i}\phi n)$ with $c_{N+1} = c_1$, so that $\phi = (2\pi/N)\ell$, $\ell = 1,2,\ldots,N$. The solution corresponding to $\ell = N$ is $c_1 = c_2 = \ldots = c_N$ with eigenenergy $E = E^{(0)} - (N-1)V$. For all other solutions we have

$$V\mathrm{e}^{\mathrm{i}\phi} + V\mathrm{e}^{2\mathrm{i}\phi} + \ldots + (E-E^{(0)})\mathrm{e}^{\mathrm{i}n_0\phi} + \ldots + V\mathrm{e}^{\mathrm{i}N\phi} = 0. \tag{2}$$

We add and subtract the quantity $V\exp(\mathrm{i}\phi n_0)$ so that (2) becomes

$$(E-E^{(0)}-V)\mathrm{e}^{\mathrm{i}\phi n_0} + V\sum_{n=1}^{N}\mathrm{e}^{\mathrm{i}\phi n}. \tag{3}$$

But the sum is equal to $\exp(\mathrm{i}\phi)\left[\mathrm{e}^{\mathrm{i}N\phi}-1\right]/\left[\mathrm{e}^{\mathrm{i}\phi}-1\right] = 0$. Thus the other $N-1$ eigensolutions are all degenerate corresponding to the eigenenergy

$$E = E^{(0)} + V.$$

Problem 13.6ts

Let x' be the axis joining the misaligned atoms 0 and 1. The axis x' makes an angle θ with the original axis x joining the atoms 0 and 1 when they were aligned. The hybrid orbital $\chi_0^1 = \frac{1}{2}(|s\rangle_o + \sqrt{3}\,|p_x\rangle_o)$ for atom 0 is written in the new axes x' *and* y' $\chi_0^1 = \frac{1}{2}\left[|\,s\rangle_o + \sqrt{3}\cos\theta\,|p_{x'}\rangle_o - \sqrt{3}\sin\theta\,\big|p_{y'}\rangle_o\right]$. Similarly the hybrid for atom 1 is $\chi_1^{\bar{1}} = \frac{1}{2}\left[|s\rangle_1 - \sqrt{3}\cos\theta\,|p_{x'}\rangle_1) + \sqrt{3}\sin\theta\,\big|p_{y'}\rangle_1\right]$. Thus the matrix element $\left\langle \chi_0^1 \middle| \hat{H} \middle| \chi_1^{\bar{1}} \right\rangle$ is equal to

$$\frac{1}{4}\left[V_{ss\sigma} - 2\sqrt{3}\cos\theta\,V_{sp\sigma} - 3\cos^2\theta\,V_{pp\sigma} - 3\sin^2\theta\,V_{pp\pi}\right], \qquad (4)$$

vs.

$$\frac{1}{4}\left[V_{ss\sigma} - 2\sqrt{3}V_{sp\sigma} - 3V_{pp\sigma}\right], \quad \text{for } V_{2h}. \qquad (5)$$

Taking into account that for small θ, $\cos\theta \simeq 1 - \theta^2/2$, $\sin^2\theta = 1 - \cos^2\theta = \theta^2$, we have for the difference (5) – (4) $= \frac{\theta^2}{4}\left[-\sqrt{3}V_{sp\sigma} - 3V_{pp\sigma} + 3V_{pp\pi}\right] = -2.75\frac{\hbar^2}{md^2}\theta^2$. Thus $\frac{(5)-(4)}{V_{2h}} = \frac{2.75}{3.22}\,\theta^2 = 0.85\,\theta^2$.

Problem 13.7ts

The energy per bond Δ divided by the volume per bond $V_0 = a^3/16$ is related to the bulk modulus B as follows $\Delta/V_0 = \frac{1}{2}B(\delta V/V_0)^2$ but $\delta V/V_0 = 3\delta d/d_0$ so that $\Delta/V_0 = \frac{9}{2}B(\delta d/d_0)^2$ or $\Delta = \frac{1}{2}\frac{9Ba^3}{16}(\delta d/d_0)^2$. Comparing with (13.26) we obtain (13.27). For a derivation of (13.28) see Harrison [SS76], p. 195, and for a derivation of (13.29) see Harrison [SS76], p. 197–200.

Chapter 14

Problem 14.1ts

The zero point energy per atom must depend on $\hbar$ (due to its quantum nature), on the mass m_a (since it is due to vibrations of atoms), and on σ and ε, which are the two parameters characterizing the interaction energy. The mass must enter as a factor $m_{\mathrm{a}}^{-1/2}$ because of the vibrational character of the phenomenon. Out of the three quantities $\hbar$, σ, ε the only combination to produce mass is the following: $\hbar^2/\varepsilon\sigma^2$. Hence, $U_i^{(0)}/N_{\mathrm{a}} = c_1\varepsilon\sqrt{\hbar^2/\varepsilon\sigma^2 m_{\mathrm{a}}} = c_1(\hbar/\sigma)\sqrt{\varepsilon/m_{\mathrm{a}}}$.

Problem 14.2s

The Debye temperature Θ_{D} is given by (14.10) and the zero point motion by (14.11). We need the value of f which depends on the ratio $x = \mu_{\mathrm{s}}/B$ (see

(4.67)). For $x = 0.32$, 0.445, and 0.49, $f = 0.636$, 0.745, and 0.78 respectively. We expect the smaller values of f to be associated with the lighter noble gas atoms and the larger ones with the heavier. We chose f as shown in the table below:

	f	Θ_D, theory	Θ_D, exp	$U_i^{(0)}/N_a$ theory (meV)	U_c/N_a, theory (meV)	U_c/N_a exp (meV)
Ne	0.6	68	75	6.6	20.4	20
Ar	0.7	83	92	8.0	81	80
Kr	0.75	66	72	6.4	114.6	116
Xe	0.8	62	64	6	166	170

Problem 14.5s

In Fig. 14.4, we plot schematically the phase diagram in the P, T plane.

For noble gases the difference between B.P. and F.P. (under normal pressure) is very small (between 2.5 K and 4 K). Hence, taking into account the freezing temperatures and Fig. 14.4, we expect the triple point temperatures to be approximately 24.5 K, 83.8 K, 115.8 K and 161.4 K, for Ne, Ar, Ar, Kr, and Xe respectively (experimental values 24.5561, 83.8058, 115.8, 161.4); the triple point pressure is expected to be lower than the normal pressure of 100 kPa (experimental values 50 kPa, 68.95 kPa, 72.92 kPa, 81.59 kPa for Ne,

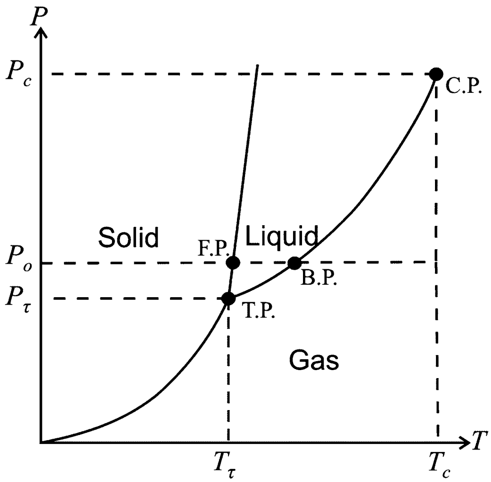

Fig. 14.4. Schematic phase diagram for a typical substance. T.P. is the triple point where the three phases (solid, liquid, gas) coexist. C.P. is the critical point where the liquid/gas coexistence line terminates. The solid/liquid coexistence curve is almost vertical. The freezing point (F.P.) and the boiling point (B.P.) under normal pressure are also shown.

Ar, Kr, and Xe respectively). Can you obtain the slope of the liquid/gas coexistence line as to estimate how much below the normal pressure the triple point pressure is?

Chapter 15

Problem 15.2s

We classify the 17 orbitals (or combination of orbitals) into columns of similarly behaving ones under rotation around the z-axis as shown below (see also Fig. 15.12)

$$\begin{array}{llllll} d\{\ d_{3z^2-r^2} & d_{zx} & d_{zy} & d_{xy} & d_{x^2-y^2} & \\ p\left\{\begin{array}{l} p_{3z} \\ \frac{1}{\sqrt{2}}(p_{1z}+p_{2z}) \\ \\ \end{array}\right. & \begin{array}{l} p_{1x} \\ p_{2x} \\ p_{3x} \end{array} & \begin{array}{l} p_{1y} \\ p_{2y} \\ p_{3y} \end{array} & & \frac{1}{\sqrt{2}}(p_{1z}-p_{2z}) & . \\ s\left\{\begin{array}{l} s_3 \\ \frac{1}{\sqrt{2}}(s_1+s_2) \end{array}\right. & & & & \frac{1}{\sqrt{2}}(s_1-s_2) & \end{array} \tag{1}$$

The advantage of this classification is that any matrix element of the Hamiltonian between orbitals belonging to different columns is zero. Notice also that the combinations $(1/\sqrt{2})(s_1 \pm s_2)$ and $(1/\sqrt{2})(p_{1z} \pm p_{2z})$, obey Bloch's theorem in spite of 1 and 2 being non Bravais lattice points; the reason is that $\exp[\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}+\boldsymbol{d}_1)] = \exp[\mathrm{i}\boldsymbol{k}\cdot(\mathbf{R}+\boldsymbol{d}_2)] == \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R})$ as a result of our choice for $\boldsymbol{k}$ to be along the z-direction.

Let us proceed with the calculation of a few representative matrix elements of the form $\sum_{\boldsymbol{R}} \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_n)\left\langle 0,a\left|\hat{H}\right|\boldsymbol{R}_n,\beta\right\rangle$. As an example, consider the case where $|\alpha\rangle = d_{3z^2-r^2}$ and $|\beta\rangle = (s_1+s_2)/\sqrt{2}$. The only non-zero matrix elements $\left\langle 0,\alpha\left|\hat{H}\right|\boldsymbol{R}_n,\beta\right\rangle$ in this case are for $\boldsymbol{R}_n = 0$ and for $\boldsymbol{R}_n = -a(\boldsymbol{x}_0 + \boldsymbol{y}_0)$ (the last one corresponds to $(s_{1'}+s_{2'})/\sqrt{2}$), where $1'$ and $2'$ are symmetric of 1 and 2 with respect to the origin. If we call V_{sd} the matrix element, $\left\langle s\left|\hat{H}\right|d_{3z^2-r^2}\right\rangle$, we have

$$\begin{aligned} \sum\nolimits_{\boldsymbol{R}} \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_n)\left\langle 0,d_{3z^2-r^2}\left|\hat{H}\right|\boldsymbol{R}_n,(s_1+s_2)/\sqrt{2}\right\rangle &= (2/\sqrt{2})[V_{\mathrm{sd}}+V_{\mathrm{sd}}] \\ &= (4/\sqrt{2})V_{\mathrm{sd}}. \end{aligned}$$

Next we must express V_{sd} in terms of the first matrix element shown in Fig. 15.9. This can be achieved by the so called Slater–Koster relations[1]which are the analogs of F.7 to F.10 for d orbitals; these relations express matrix

[1] J.C. Slater and G.F. Koster, Phys. Rev. **94**, 1498 (1954). The Slater-Koster relations are reproduced in the book by Harrison [SS76], p. 481 and the book by Papaconstantopoulos [SS81].

elements of the form $\left\langle \alpha \middle| \hat{H} \middle| \beta \right\rangle$ involving at least one d orbital in terms of those in Fig. 15.9 and the direction cosines ℓ, m, n of the vector going from the center of $|\alpha\rangle$ to the center of $|\beta\rangle$. In the present case $V_{\mathrm{sd}} = -\frac{1}{2}V_{\mathrm{sd}\sigma} = (3.16/2)\hbar^2 r_{\mathrm{d}}^{3/2}/md^{7/2} = 0.0479$. Thus$\left(4/\sqrt{2}\right) V_{\mathrm{sd}} = 0.136\,\mathrm{a.u.} = 3.69\,\mathrm{eV}$. ($r_d = 1.08\,\mathrm{A}$ for Ti and $d_{\mathrm{TiO}} = 1.95\,\mathrm{A}$).

As another example consider the case $|\alpha\rangle = \mathrm{d}_{3z^2-r^2}$ and $|\beta\rangle = \mathrm{p}_{3z}$. Then $\sum_{\boldsymbol{R}} \left\langle 0, d_{3z^2-r^2} \middle| \hat{H} \middle| \boldsymbol{R}, p_{3z} \right\rangle = V_{\mathrm{d}p}^{+} + V_{\mathrm{d}p}^{-}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} = \mathrm{e}^{-\mathrm{i}\boldsymbol{k}d}(V_{dp}^{+}\mathrm{e}^{\mathrm{i}\boldsymbol{k}d} + V_{dp}^{-}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}d}) = \mathrm{e}^{-\mathrm{i}\boldsymbol{k}d}V_{dp}^{+}(\mathrm{e}^{\mathrm{i}\boldsymbol{k}d} - \mathrm{e}^{-\mathrm{i}\boldsymbol{k}d}) = -\mathrm{e}^{-\mathrm{i}\boldsymbol{k}d}2\mathrm{i}V_{\mathrm{pd}\sigma}\sin kd$ where $\boldsymbol{k} = 0, 0, k$, $\boldsymbol{R} = -a(0, 0, 1)$, $kd = ka/2$, $d = d_{\mathrm{Ti-O}}$. We can get rid of the factor $\exp(-\mathrm{i}kd)$ by redefining the corresponding coefficient, c_{3p_z}. Continuing this way we obtain the 5×5 Hamiltonian for each $\boldsymbol{k} = (0, 0, k)$ corresponding to the first column in (1)

	$d_{3z^2-r^2}$	p_{3z}	$\frac{1}{\sqrt{2}}(p_{1z}+p_{2z})$	s_3	$\frac{1}{\sqrt{2}}(s_1+s_2)$
$d_{3z^2-r^2}$	ε_d	$-2\mathrm{i}V_{pd\sigma}\sin kd$	0	$2V_{pd\sigma}\cos kd$	$-\sqrt{2}V_{sd\sigma}$
p_{3z}	$2\mathrm{i}V_{pd\sigma}\sin kd$	ε_p	$2\sqrt{2}E_{x,x}\cos kd$	0	0
$\frac{1}{\sqrt{2}}(p_{1z}+p_{2z})$	0	$2\sqrt{2}E_{x,x}\cos kd$	ε_p	0	0
s_3	$2V_{pd\sigma}\cos kd$	0	0	ε_s	0
$\frac{1}{\sqrt{2}}(s_1+s_2)$	$-\sqrt{2}V_{sd\sigma}$	0	0	0	ε_s

, (2)

where $E_{x,x} = (V_{pp\sigma} + V_{pp\pi})/2$, taken as $0.153\,\mathrm{eV}$. (These atoms are second nearest neighbors).

The 4×4 Hamiltonian corresponding to the second column of (1) is (the third column is the same)

	d_{zx}	p_{1x}	p_{2x}	p_{3x}
d_{zx}	ε_d	0	0	$-2\mathrm{i}V_{pd\pi}\sin kd$
p_{1x}	0	ε_p	$4E_{x,x}$	$4E_{x,x}\cos kd$
p_{2x}	0	$4E_{x,x}$	ε_p	0
p_{3x}	$2\mathrm{i}V_{pd\pi}\sin kd$	$4E_{x,x}\cos kd$	0	ε_p

. (3)

Finally the 3×3 Hamiltonian matrix corresponding to the last column in (1) is

	$d_{x^2-y^2}$	$\frac{1}{\sqrt{2}}(p_{1z}-p_{2z})$	$\frac{1}{\sqrt{2}}(s_1-s_2)$
$d_{x^2-y^2}$	ε_d	0	$\sqrt{6}V_{sd\sigma}$
$\frac{1}{\sqrt{2}}(p_{1z}-p_{2z})$	0	ε_p	0
$\frac{1}{\sqrt{2}}(s_1-s_2)$	$\sqrt{6}V_{sd\sigma}$	0	ε_s

. (4)

The matrix (4) is independent of k and can by diagonalized analytically yielding

$$E_1 = \varepsilon_p$$
$$E_{2,3} = \frac{1}{2}(\varepsilon_s + \varepsilon_d) \pm \sqrt{\frac{1}{4}(\varepsilon_s - \varepsilon_d)^2 + 6V_{sd\sigma}^2}.$$

The one element fourth column gives, obviously

$$E_4 = \varepsilon_{\mathrm{d}}.$$

The 4×4 shown in (3) can be diagonalized analytically at $k = 0$ and at $k = \pi/a$ yielding

$$E_{5,6}(0) = \varepsilon_d, \qquad \mathrm{E}_{5,6}(\pi/a) = \tfrac{1}{2}(\varepsilon_d + \varepsilon_p) + \left[\tfrac{1}{4}(\varepsilon_d - \varepsilon_p)^2 + 4V_{pd\pi}^2\right]^{1/2},$$
$$E_{7,8}(0) = \varepsilon_p, \qquad \mathrm{E}_{7,8}(\pi/a) = \tfrac{1}{2}(\varepsilon_d + \varepsilon_p) - \left[\tfrac{1}{4}(\varepsilon_d - \varepsilon_p)^2 + 4V_{pd\pi}^2\right]^{1/2},$$
$$E_{9,10}(0) = \varepsilon_p + 4\sqrt{2}E_{x,x}, \qquad E_{9,10}(\pi/a) = \varepsilon_p + 4E_{x,x},$$
$$\mathrm{E}_{11,12}(0) = \varepsilon_p - 4\sqrt{2}E_{x,x}. \qquad E_{11,12}(\pi/a) = \varepsilon_p - 4E_{x,x}.$$

Finally the 5×5 shown in (2) yields at $k = 0$

$$E_{13}(0) = \varepsilon_s,$$
$$E_{14}(0) = \varepsilon_p + 4\sqrt{2}E_{x,x},$$
$$E_{15}(0) = \varepsilon_p - 4\sqrt{2}E_{x,x},$$
$$E_{16}(0) = \tfrac{1}{2}(\varepsilon_d + \varepsilon_s) + \left[\tfrac{1}{4}(\varepsilon_d - \varepsilon_s)^2 + 6V_{sd\sigma}^2\right]^{1/2},$$
$$\mathrm{E}_{17}(0) = \tfrac{1}{2}(\varepsilon_d + \varepsilon_s) - \left[\tfrac{1}{4}(\varepsilon_d - \varepsilon_s)^2 + 6V_{sd\sigma}\right]^{1/2}.$$

The reader may attempt to diagonalize the 5×5 Hamiltonian matrix also for $k = \pi/a$.

Chapter 16

Problem 16.1ts

The system $\boldsymbol{x}_{\boldsymbol{K}}, \boldsymbol{y}_{\boldsymbol{K}}, \mathbf{K}$ is an orthogonal one. Hence, $\boldsymbol{K} = |\boldsymbol{K}|\,\boldsymbol{K}_0 = |\boldsymbol{K}|\,(\boldsymbol{x}_{\boldsymbol{K}} \times \boldsymbol{y}_{\boldsymbol{K}})$. Similarly, $\boldsymbol{K}' = \left|\boldsymbol{K}'\right|(\boldsymbol{x}_{\boldsymbol{K}'} \times \boldsymbol{y}_{\boldsymbol{K}'})$. $\boldsymbol{K}' \times \mathbf{H}_{\boldsymbol{K}'} = \left|\boldsymbol{K}'\right|(\boldsymbol{x}_{\boldsymbol{K}'} \times \boldsymbol{y}_{\boldsymbol{K}'}) \times (H_{\boldsymbol{K}'x'}\boldsymbol{x}_{\boldsymbol{K}'} + H_{\boldsymbol{K}'y'}\boldsymbol{y}_{\boldsymbol{K}'}) = \left|\boldsymbol{K}'\right|(H_{\boldsymbol{K}'x'}\boldsymbol{y}_{\boldsymbol{K}'} - H_{\boldsymbol{K}'y'}\boldsymbol{x}_{\boldsymbol{K}'})$. By multiplying the last expression by $\boldsymbol{K}\times$ we have.

$$|\boldsymbol{K}|\left|\boldsymbol{K}'\right|(\boldsymbol{x}_{\boldsymbol{K}} \times \boldsymbol{y}_{\boldsymbol{K}}) \times (H_{\boldsymbol{K}'x'}\boldsymbol{y}_{\boldsymbol{K}'} - H_{\boldsymbol{K}'y'}\boldsymbol{x}_{\boldsymbol{K}'})$$

$$|\boldsymbol{K}|\left|\boldsymbol{K}'\right|[\boldsymbol{y}_{\boldsymbol{K}}(\boldsymbol{x}_{\boldsymbol{K}} \cdot \boldsymbol{y}_{\boldsymbol{K}'})H_{\boldsymbol{K}'x'} - \boldsymbol{x}_{\boldsymbol{K}}(\boldsymbol{y}_{\boldsymbol{K}} \cdot \boldsymbol{y}_{\boldsymbol{K}'})H_{\boldsymbol{K}'x'} \qquad (1)$$

$$+\boldsymbol{x}_{\boldsymbol{K}}(\boldsymbol{y}_{\boldsymbol{K}} \cdot \boldsymbol{x}_{\boldsymbol{K}'})H_{\boldsymbol{K}'y'} - \boldsymbol{y}_{\boldsymbol{K}}(\boldsymbol{x}_{\boldsymbol{K}} \cdot \boldsymbol{x}_{\boldsymbol{K}'})H_{\boldsymbol{K}'y'}].$$

Substituting (1) in (16.15) and equating the $\boldsymbol{x}_K$ coefficients on both sides, we have

$$\sum\nolimits_{\boldsymbol{K}'} a_{\boldsymbol{K}-\boldsymbol{K}}{}' \left|\boldsymbol{K}\right| \left|\boldsymbol{K}'\right| \left[(\boldsymbol{y}_{\boldsymbol{K}} \cdot \boldsymbol{y}_{\boldsymbol{K}'})H_{\boldsymbol{K}'x'} - (\boldsymbol{y}_{\boldsymbol{K}} \cdot \boldsymbol{x}_{\boldsymbol{K}'})H_{\boldsymbol{K}'y'}\right] = \frac{\omega^2}{c^2} H_{\boldsymbol{K}x}. \quad (2)$$

Similarly, by equating the $\boldsymbol{y}_{\boldsymbol{K}}$ coefficients, we obtain

$$\sum\nolimits_{\boldsymbol{K}'} a_{\boldsymbol{K}-\boldsymbol{K}}{}' \left|\boldsymbol{K}\right| \left|\boldsymbol{K}'\right| \left[-(\boldsymbol{x}_{\boldsymbol{K}} \cdot \boldsymbol{y}_{\boldsymbol{K}'})H_{\boldsymbol{K}'x'} + (\boldsymbol{x}_{\boldsymbol{K}} \cdot \boldsymbol{x}_{\boldsymbol{K}'})H_{\boldsymbol{K}'y'}\right] = \frac{\omega^2}{c^2} H_{\boldsymbol{K}y}. \quad (3)$$

Equations (2) and (3) can be written in the compact form (16.18) with $M_{\boldsymbol{K}\boldsymbol{K}'}$ given by (16.19).

Problem 16.2ts

$$E_{\mathrm{K}} = \frac{1}{2}\rho_0 S r \delta\dot{r}^2 = \frac{1}{2}\rho_0 S r \omega^2 \delta r^2, E_{\mathrm{P}} = \frac{1}{2}\delta P S \delta r, \delta P = \frac{P_i}{V_i}\delta V_i, \delta V_i = 4\pi r^2 \delta r,$$

$$E_{\mathrm{P}} = \frac{1}{2}\frac{P_i}{V_i} 4\pi r^2 \delta r\, S\, \delta r = \frac{1}{2}\frac{B_i}{\rho_i}\frac{\rho_i}{\frac{4\pi}{3} r^3} 4\pi r^2 S\, \delta r^2 = \frac{1}{2} c_i^2 3\rho_i \frac{1}{r}\, S\, \delta r^2.$$

Setting $E_{\mathrm{K}} = E_{\mathrm{P}}$, we obtain $\rho_0 r \omega^2 = c_i^2 3\rho_i \frac{1}{r}$, or $\frac{\omega^2 r^2}{c_i^2} = \frac{3\rho_i}{\rho_0}$.

Problem 16.5ts

From (16.33), we have $u = \frac{c^2}{4\pi\omega}\frac{k}{v}(1+x)\frac{{E_0}^2}{\mu} = \frac{c^2}{4\pi\omega}\frac{k}{v}(1+x)\frac{{H_0}^2}{\varepsilon}$; $\omega = v \cdot k = c \cdot k/n$,

$$x = (\omega/n)/(\partial\omega/\partial n) \text{ and } n^2(1+x) = \frac{1}{2}\left[\left(\varepsilon\mu + \omega\mu\frac{\partial\varepsilon}{\partial\omega}\right) + \left(\varepsilon\mu + \omega\varepsilon\frac{\partial\mu}{\partial\omega}\right)\right],$$

$$\begin{aligned} u &= \frac{1}{4\pi} n^2 (1+x)\frac{{E_0}^2}{\mu} = \frac{n^2}{4\pi}(1+x)\frac{{H_0}^2}{\varepsilon} = \frac{1}{8\pi}\left[\left(\varepsilon\mu + \omega\mu\frac{\partial\varepsilon}{\partial\omega}\right)\frac{{E_0}^2}{\mu}\right.\\ &\quad \left. + \left(\varepsilon\mu + \omega\varepsilon\frac{\partial\mu}{\partial\omega}\right)\frac{{H_0}^2}{\varepsilon}\right]\\ &= \frac{1}{8\pi}\left[\varepsilon{E_0}^2 + \omega\frac{\partial\varepsilon}{\partial\omega}{E_0}^2 + \mu{H_0}^2 + \omega\frac{\partial\mu}{\partial\omega}{H_0}^2\right] = \frac{1}{8\pi}\left[\frac{\partial(\omega\varepsilon)}{\partial\omega}E_0^2 + \frac{\partial(\omega\mu)}{\partial\omega}H_0^2\right]. \end{aligned}$$

Chapter 17

Problem 17.6ts

The power P produced by a photovoltaic is $P = (FF)I_{\mathrm{L}}V_0$. The voltage V_0 is a fraction of E_{g}/e: $V_0 = a_1 E_{\mathrm{g}}/e$, where, usually, $a_1 \simeq 2/3$. The current I_{L} is proportional to j_{L} given by (17.81). Hence

$$P = (FF)a_1(E_g/e)a_2\frac{e}{\hbar}\int\limits_{E_g/\hbar}^{\infty} d\omega\frac{I(\omega)}{\omega},$$

where $a_2 < 1$ and $I(\omega) = A\omega^3/(e^{\beta\hbar\omega} - 1)$ with A a known universal constant. Thus

$$P = (FF)a_1a_2\frac{A\,E_g}{\hbar^4\beta^3}\int\limits_{\beta E_g}^{\infty}\frac{dxx^2}{e^x - 1}, \text{ and}$$

$$P_t = \frac{A}{(\beta\hbar)^4}\int\limits_0^{\infty}\frac{dxx^3}{e^x - 1}, \text{ so that}$$

$$\eta = (FF)a_1a_2(E_g\beta)\frac{I_1}{I_0}; \quad I_1 = \int\limits_{\beta E_g}^{\infty} dxx^2(e^x - 1)^{-1}, \text{ and}$$

$I_0 = \int\limits_0^{\infty} dxx^3(e^x - 1)^{-1} = \pi^4/15$. To maximize η with respect to E_g is equivalent to maximize

$$\Gamma = y\int\limits_y^{\infty} dxx^2(e^x - 1)^{-1}, \text{ where } y = \beta E_g :$$

$d\Gamma/dy = 0 \Rightarrow \int\limits_y^{\infty}\frac{dxx^2}{e^x-1} = \frac{y^3}{e^y-1}$. By plotting both sides we found the solution to be $y = 2.166$. Hence, $E_g = (5800/11600)2.166\,\text{eV} = 1.083\,\text{eV}$. For this value of y, $\eta = (FF)a_1a_2 \times 2.166 \times 1.316/(\pi^4/15) = (FF)a_1a_2 \times 0.44 \lesssim 22\%$. This upper limit of about 22% is not unrealistic for optimal E_g, although the values of the latter are higher than our crude estimate of 1.08 eV and vary between 1.2 and 1.6eV depending, among other factors, on the shape of the solar spectrum at the surface of the Earth.

Problem 17.1s

From each point of a diamond lattice, located at the sides $\boldsymbol{R}_n$ of the **fcc** lattice, four bonds emerge in the directions (111), $(\bar{1}\bar{1}1)$, $(1\bar{1}\bar{1})$ and $(\bar{1}1\bar{1})$. Hence, a plane normal to the direction (111) will cut a minimum of one bond per lattice point of the 2-D hexagonal lattice shown in Fig. 17.8. Hence, the minimum number of bonds cut by (111) planes per unit area is $1/(\sqrt{3}a^2/4) = 4/\sqrt{3}a^2$ and the corresponding energy cost for creating such a surface is $(E_c/2)(4/\sqrt{3}a^2) = 2E_c/\sqrt{3}a^2 = \sqrt{3}E_c/8d^2$ per unit area, where E_c is the cohesive energy per atom.

For the direction (100) two bonds, the (111) and the $(1\bar{1}\bar{1})$ have positive dot product with the vector (100), while the other two, the $(\bar{1}\bar{1}1)$ and the $(\bar{1}1\bar{1})$ have negative. Hence, two bonds are on the one side of the lattice plane (100) and the other two on the other side. It follows that the minimum number of bonds that the (100) plane will cut, will be two per lattice point of the square lattice shown in Fig. 17.8. Hence, the bonds cut per unit area is $2/(a^2/2) = 4/a^2$ and the surface energy (per unit area) is $2E_c/a^2 = 3E_c/8d^2$. Thus the ratio of the two surface energies $E_{100}/E_{111} = \sqrt{3}$.

For the direction $(1,1,0)$ the dot products with the vectors (111), $(\bar{1}\bar{1}1)$, $(1\bar{1}\bar{1})$ and $(\bar{1}1\bar{1})$ are 2, -2, 0, 0, which means that two bonds are on the lattice plane (110) and the other two are on each side of this plane. The fact that two diamond lattice points, the $\boldsymbol{d}_1 = (1\bar{1}\bar{1})(a/4)$ and $\boldsymbol{d}_2 = (\bar{1}1\bar{1})(a/4)$, are on the (110) **fcc** plane without belonging to the **fcc** 2D rectangular lattice[2] shown in Fig. 17.8, shows that the diamond (110) 2D lattice results from the rectangular **fcc** lattice by inserting a two atom basis with one atom located at the lower left corner of the rectangular lattice shown in Fig. 17.8 and the other located at the point $-(a/4)\boldsymbol{x}_0 + (a\sqrt{2}/4)\boldsymbol{y}_0$ relative to the rectangular lattice. For each of the two atoms in the basis we have to cut one bond, so that the minimum number of bonds cut for the (110) surface of the diamond lattice per unit are is $2/(\sqrt{2}a^2/2) = 2\sqrt{2}/a^2$. Hence, the surface energy per unit area is $\sqrt{2}E_c/a^2 = 3\sqrt{2}E_c/16d^2$. The final result is $E_{100} : E_{110} : E_{111} = 2 : \sqrt{2} : (2/\sqrt{3})$.

Problem 17.2s

Let the surface and the volume of a regular octahedron of edge length a be S and V, where

$$\begin{aligned} S &= 2\sqrt{3}a^2, \\ V &= \frac{1}{3}\sqrt{2}a^3. \end{aligned}$$

Truncated octahedron: The volume V_1 of each of the six pyramids cut off the octahedron is

$$V_1 = \frac{1}{6}\sqrt{2}b^3 \Rightarrow V_t = V\,(a) - 6V_1 = \frac{1}{3}\sqrt{2}a^3 - \sqrt{2}b^3.$$

The truncated octahedron surface is decreased by $6 \times \sqrt{3}b^2$ but is increased by $6b^2$. Thus

$$S_t = \underbrace{2\sqrt{3}a^2 - 6\sqrt{3}b^2}_{E_{111}} + \underbrace{6b^2}_{E_{100}}.$$

The surface energy for the truncated octahedron is $E_t = 2\sqrt{3}E_{111}\left(a^2 - 3b^2\right) + 6b^2E_{100}$.

[2] Their difference $\boldsymbol{d}_1 - \boldsymbol{d}_2 = (1,1,0)(a/2)$ belongs to this 2-D rectangular lattice.

We must minimize E_t with respect to b *under* constant volume:

$$V_\mathrm{t} = \mathrm{const} \Rightarrow \mathrm{d}V_\mathrm{t}/\mathrm{d}b = 0.$$
$$\mathrm{d}V_\mathrm{t}/\mathrm{d}b = 0 \Rightarrow \sqrt{2}a^2(\mathrm{d}a/\mathrm{d}b) = 3\sqrt{2}b^2 \Rightarrow \mathrm{d}a/\mathrm{d}b = 3b^2/a^2. \text{ Thus}$$
$$\mathrm{d}E_\mathrm{t}/\mathrm{d}b = 0 \Rightarrow 2\sqrt{3}E_{111}\left(2a(3b^2/a^2) - 6b\right) + 12bE_{100} = 0,$$
$$2\sqrt{3}E_{111}\left(6\frac{b}{a} - 6\right) + 12E_{100} = 0, \quad \frac{b}{a} = 1 - \frac{E_{100}}{\sqrt{3}E_{111}}. \tag{1}$$

In arriving at the last equation, it was implicitly assumed that $2b \le a$ (otherwise our formulas for the volume and the surface of truncated octahedron are invalid). This inequality combined with (1) implies that $E_{100} \ge \sqrt{3}E_{111}/2$; actually, as it was argued in problem 17.1s, it is expected that $E_{100} \simeq \sqrt{3}E_{111}$. If, $E_{100} \ge \sqrt{3}E_{111}$, then $b = 0$ and the regular octahedron would have the lower surface energy; if $E_{100} = (\sqrt{3} - x)E_{111}$ with x positive and small, then $b/a = x/\sqrt{3}$, the surface energy of a truncated octahedron would be $2\sqrt{3}E_{111}a^2\left(1 - \frac{x^3}{\sqrt{3}}\right)$, while the surface energy of a regular octahedron *of equal volume with the truncated one* would be $2\sqrt{3}E_{111}a^2\left(1 - \frac{x^3}{\sqrt{3}}\right)^{2/3}$, i.e., higher than that of the truncated octahedron.

Chapter 18

Problem 18.9ts

We write $x \equiv (\varepsilon_n - \Sigma)g_o$ and we have $\varepsilon_n(1-x)^{-1} = \varepsilon_n(1+x+x^2+x^3+\dots) = \varepsilon_n + \varepsilon_n^2 g_0 - g_0\varepsilon_n\Sigma + \varepsilon_n^3 g_0^2 - 2\varepsilon_n^2 g_0^2\Sigma + g_0^2\varepsilon_n\Sigma^2 + \varepsilon_n g_0^3(\varepsilon_n^3 - 3\varepsilon_n^2\Sigma + 3\varepsilon_n\Sigma^2 - \Sigma^3) + \mathcal{O}(w^6)$. The odd powers of ε_n would give zero contributions to the integral (18.74). Keeping terms up to 4$^{\text{th}}$ order in w and performing the integrations shown in (18.74) we have

$$\Sigma = w^2 g_0 - 2w^2 g_0^2\Sigma + \mu_4 g_0^3 + \mathcal{O}(w^6) = w^2 g_0 - (2w^4 - \mu_4)g_0^3 + \mathcal{O}(w^6).$$

Problem 18.11ts

Figure 18.13 shows that, for $D \le 2$, β is negative. Hence, $\mathrm{d}G/\mathrm{d}L$ is negative and, as a result, as $L \to \infty$, $G \to 0$. In this case, strictly speaking a truly metallic behavior is not possible. On the other hand for $D > 2$ and $G > G_\mathrm{c}$ a truly metallic behavior is realized. A metallic behavior is definitely possible for $D = 2$ in the presence of magnetic forces.

Problem 18.12ts

Taking into account that $\beta = (L/Q)(\mathrm{d}Q/\mathrm{d}L)$ and that $Q = \hbar G/e^2 = (\hbar/e^2)\sigma L^{D-2}$ and substituting in (18.102) we end up with the following simple differential equation

$$\frac{d\sigma}{dL} = -\frac{\Gamma_{\mathrm{D}}}{L^{D-1}}, \Gamma_{\mathrm{D}} = A_{\mathrm{D}} e^2/\hbar,$$

which gives

$$\sigma = \sigma_0 + \tfrac{\Gamma_{\mathrm{D}}}{D-2} L^{2-D}, \quad D \neq 2,$$
$$\sigma = \sigma_0 - \Gamma_2 \ln \tfrac{L}{L_e}, \quad D = 2.$$

Problem 18.1s

To prove the relation, $s = -k_{\mathrm{B}}[p \ln p + (1-p)\ln(1-p)]$, where $p = p_{AB} + p_{BA}$ and $1-p = p_{AA} + p_{BB}$, we have to show first that the probability p of a bond to be AB or BA is independent of what is happening in a nearest neighbor bond. This is indeed the case, if $x = 0.5$. To show this, consider three consecutive sites 1, 2, 3 and check whether the probability for the bond 2, 3 to be AB or BA depends on what is happening in the bond 1, 2. If the latter is AA, BB, AB or BA the probability for the bond 2, 3 to be either AB or BA is respectively $p_{B/A} = p$, $p_{A/B} = p$, $p_{A/B} = p$, $p_{B/A} = p$. Having established that the bonds are statistically independent we can use (C.30) with P_I taking two values: p and $1-p$. To obtain the equilibrium value of p we minimize the free energy $f \equiv \langle \varepsilon \rangle - Ts = \frac{1}{2}[(1-p)(U_{AA}+U_{BB})/N] + \frac{1}{2}[p(U_{AB}+U_{BA})/N] - Ts$. Thus $\partial f/\partial p = u + k_B T[\ln p - \ln(1-p)] = 0 \Rightarrow p = (e^{\beta u}+1)^{-1}; \beta = 1/k_{\mathrm{B}}T$.

Problem 18.4s

We have to calculate the integral, $g_0(E) = \frac{2}{\pi B^2}\int_{-B}^{B} \frac{\mathrm{d}E'(B^2-E'^2)^{1/2}}{E-E'}$. Change variables to $E' = B\sin\theta \Rightarrow \mathrm{d}E' = B\cos\theta d\theta$, $(B^2 - E'^2)^{1/2} = B(1 - \sin^2\theta)^{1/2} = B\cos\theta$; $E \equiv Bz$. Thus $g_0(E) = \frac{2}{\pi B}\int_{-\pi/2}^{\pi/2} \frac{\mathrm{d}\theta\cos^2\theta}{z-\sin\theta} = \frac{1}{\pi B} \int_{-\pi}^{\pi} \frac{\mathrm{d}\theta\cos^2\theta}{z-\sin\theta}$. Setting $w = \exp(i\theta)$ we have $\mathrm{d}w = \mathrm{i}w\mathrm{d}\theta$ and $g_0(E) = \frac{1}{2\pi B} \int_{c_0} \frac{\mathrm{d}w(w+w^{-1})^2}{2\mathrm{i}w\left(z-\frac{1}{2i}(w-w^{-1})\right)} = \frac{1}{2\pi B}\int_{c_0}\frac{\mathrm{d}w(w+w^{-1})^2}{2\mathrm{i}zw-w^2+1}$, where the contour c_0 of integration is along the unit circle in the complex w plane, as shown in Fig. 18.16 below. However, in order to apply the residue theorem, we have to avoid the singularity at $w=0$ by following the contour $c_0+c_1+c_2+c_3$, i.e., the contour $c_0 + c_2$ (since the contributions of c_1 and c_3 cancel each other) (Fig. 18.16). Hence,

$$g_0 = \frac{-1}{2\pi B}\int_{c_0+c_2} \frac{dw(w+w^{-1})^2}{(w-w_1)(w-w_2)} - \frac{1}{2\pi B}\int_{c_2} dw(w+w^{-1})^2(1-2\mathrm{i}zw+\mathcal{O}(w^2)), \tag{1}$$

where w_1, w_2 are the roots of $w^2 - 2\mathrm{i}zw - 1 = 0$, $\quad w_{1,2} = \mathrm{i}z \pm \sqrt{1-z^2}$ with $|w_1| < 1$. The first term in the *rhs* of (1) by residue theorem and in

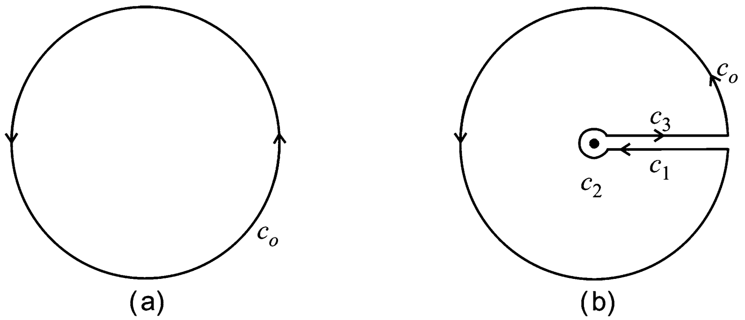

Fig. 18.16. The contour of integration (a) encloses the singular point $w = 0$, while that in (b) does not

view of $w_1 w_2 = -1$ gives $-(2\pi i/2\pi B)(w_1 - w_2) = -(2/B)i\sqrt{1-z^2}$. In the second term the only non-zero contribution, as the radius of c_2 tends to zero, comes from the product $(-2izw)w^{-2} = -2izw^{-1}$ in the integrand. Setting $w = \rho\exp(i\theta)$, $\mathrm{d}w = \mathrm{i}w\mathrm{d}\theta$ we obtain $-\frac{2z}{2\pi B}\int_{\pi}^{-\pi} d\theta = 2z/B$. Thus, finally $g_0 = \frac{2}{B}(z - \mathrm{i}\sqrt{1-z^2}) = -\frac{2\mathrm{i}}{B}w_1 = \frac{2}{B}\frac{1}{z+\mathrm{i}\sqrt{1-z^2}} = \frac{2}{E+\mathrm{i}\sqrt{B^2-E^2}}$.

Chapter19

Problem 19.1ts

From (14.12), $\ln\sigma = \ln 4.64 - 0.6\ln(IP) = \ln 4.64 - 0.6\ln(3/27.2) = 2.857 \Rightarrow \sigma = 17.418\,\text{a.u.} = 9.21\,\text{A}$; $d = 1.09\sigma = 10.043$ vs. $10.013\,\text{A}$ experimentally; $a = \sqrt{2}d = 14.203\,\text{A}$. $\tilde{a} = 4(3.4125/0.527)^2/(3/27.2) = 1509\,\text{a.u.} = 223.4\,\text{A}^3$; $\varepsilon = 0.4\tilde{\alpha}^2(IP)/\sigma^6 = 0.4(223.4)^2 3/(9.2138)^6 = 0.0979\,\text{eV}$. $E_i'/N = -8.61\varepsilon = 0.8424\,\text{eV/molecule}$. $\Lambda = \hbar/\sigma\sqrt{m_a\varepsilon} = 8.35\times10^{-4}; U_i^{(0)}/N = 37.46 f\Lambda\varepsilon = 37.46\times0.6\times8.35\times10^{-4}\times0.979\,\text{eV} = 1.83\,\text{meV}$. $U_\text{c}/N = (E_i'/N) - (U_i^{(0)}/N) = 0.8427\,\text{eV} - 1.83\,\text{meV} \simeq 0.84\,\text{eV}$, vs. $0.4\,\text{eV}$ experimentally.

Problem 19.2ts

$U_c/M_3C_{60} \simeq \left|3(\text{IP})_\text{M} - 3(\text{EA})_\text{F} - (3e^2\alpha/4\pi\varepsilon_0 d')\right|$, where $d' = (2d'_\text{tetr.} + d'_\text{oct.})/3 = \left[(2\sqrt{3}a/4) + (a/2)\right]/3 = 6.46\,\text{A} = 12.2\,\text{a.u.}$ $\quad U_\text{c}/M_3C_{60} \simeq 6.46\,\text{eV}$.

Problem 19.8ts

Because the wave functions $\Psi_{3/2}(r)$ and $\Psi_{1/2}(r)$ are even in x, y and z, the matrix elements $\left\langle \Psi_\ell(\boldsymbol{r}) \left| \frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j} \right| \Psi_m(\boldsymbol{r}) \right\rangle = 0$ for $i \neq j$, where $i, j = 1, 2, 3$ and $l, m = \frac{3}{2}, \frac{1}{2}$. Hence,

$$\langle \Psi_\ell(\boldsymbol{r})\,|S|\,\Psi_m(\boldsymbol{r}) = 0;\ l, m = \frac{3}{2}, \frac{1}{2}. \tag{19.39}$$

For the same reason the corresponding matrix element of the imaginary of R is zero; furthermore, because of symmetry,

$$\langle \Psi_\ell(\boldsymbol{r}) |R| \Psi_\ell(\boldsymbol{r}) \rangle = 0, \quad l, m = \frac{3}{2}, \ \frac{1}{2}. \tag{19.40}$$

Thus the only matrix element which is non-zero is the following

$$\tilde{R} \equiv \left\langle \Psi_{1/2}(\boldsymbol{r}) |R| \Psi_{3/2}(\boldsymbol{r}) \right\rangle = -\frac{\sqrt{3}\hbar^2}{2m}\gamma_2 \left\langle \Psi_{1/2}(\boldsymbol{r}) \left| \left(k_x^2 - k_y^2\right) \right| \Psi_{3/2}(\boldsymbol{r}) \right\rangle . \tag{19.41}$$

Problem 19.1s

The eigenfunctions of a particle moving within a spherical potential well of radius a with infinite walls are of the form $A\, j_l(kr)Y_{lm}(\theta, \varphi)$, with ka coinciding with the roots ρ_{nl} of the spherical Bessel functions j_l:$k_{nl}a = \rho_{nl}$; the ordering of $k_{nl}a$ is the same as that of the corresponding eigenenergies $\varepsilon_{nl} = \hbar^2 k_{nl}^2/2m$. The results for $k_{nl}a$ are (see [D4]): 3.14, 4.49, 5.76, 6.28, 6.98, 7.72, 8.18, 9.09, 9.35, 9.42 for 1s, 1p, 1d, 2s, 1f, 2p, 1g, 2d, 1h, 3s respectively. This ordering coincides with the one given in Section 19.2 with the single exception of the 3s being lower than 1h.

Problem 19.2s

The k_y coordinate of the point P' (which is equal to $\boldsymbol{\Gamma}P + \boldsymbol{G}$, where P is the point at which the gap closes in graphene) is $\pm 1/3$ in units of $2\pi/\sqrt{3}d$. The allowed values of k_y for the zig-zag case are ℓ'/n (in units of $2\pi/\sqrt{3}d$). Hence, the minimum value of $\delta k_y = \min\left|\frac{1}{3} - \frac{\ell'}{n}\right|\left(\frac{2\pi}{\sqrt{3}d}\right)$. For $n = 4$, $\delta k_y = (1/12)(2\pi/\sqrt{3}d)$; for $n = 7$, $\delta k_y = (1/21)(2\pi/\sqrt{3}d)$. The gap according to (11.68) is estimated to be $E_\mathrm{g} \simeq 3\,|Vd|\,\delta k_y = 3 \times 0.63 \times (\hbar^2/md^2)(2\pi/\sqrt{3})(1/12) = 2.15\,\mathrm{eV}$ for $n = 4$ and $E_\mathrm{g} = 1.23\,\mathrm{eV}$ for $n = 7$. Actually for $n = 7$ the gap is $0.2\,\mathrm{eV}$, which shows that the rolling up reduces significantly the matrix elements of the Hamiltonian. This is to be expected, since, among other reasons, the rolling up multiplies the nearest neighbor matrix element $V_{pp\pi}$ by $\cos\theta$, where $\theta = 2\pi/n$.

Chapter 20

Problem 20.2ts

See the book by Landau and Lifshitz [E15], pp. 147–150.

Problem 20.2s

Setting $H = 0$ and the derivatives $\partial\tilde{g}/\partial L_i = 0$, $i = x, y$, $\partial\tilde{g}/\partial L_z = 0$ we obtain

$$L_i(2a + 4bL^2 + b') = 0, \quad i = x, y,$$
$$L_z(2a + 4bL^2) = 0.$$

If $b' > 0$, the easy axis will be in the $z-$direction, $L_i = 0$ $(i = x, y)$ and

$$L = (-a/2b)^{1/2} = (a_1/2b)^{1/2}(T_{\text{N}} - T)^{1/2}.$$

If $b' < 0$, then $L_z = 0$ and $2a + 4bL^2 + B = 0$ or $L = (a_1/2b)^{1/2}(T_{\text{N}} - T)^{1/2}$, where $a_1 T_{\text{N}} = a_1 T'_{\text{N}} - B/2$, and $a = a_1(T - T'_{\text{N}})$. Combining the general thermodynamic relation (20.38) with the derivatives of $\tilde{g}$ with respect to H_i, $i = x, y, z$, we obtain

$$-\mu_0(\boldsymbol{H} + \boldsymbol{M}) = 2\mu_0 D(\boldsymbol{H} \cdot \ \boldsymbol{L})\boldsymbol{L} + 2\mu_0 D' L^2 \boldsymbol{H}$$
$$-\mu_0 \chi_p \boldsymbol{H} - \mu_0\gamma(H_x \boldsymbol{i} + H_y \boldsymbol{j}) - \mu_0 \boldsymbol{H}.$$

Dropping $-\mu_0\boldsymbol{H}$ from both sides and dividing by $-\mu_0$ we end up with (20.39). For $T > T_{\text{N}}$, for which $\boldsymbol{L} = 0$, we obtain (20.40) from (20.39) by dividing by H_x, H_y, H_z. To arrive at (20.41) and (20.42) we assume $B > 0$, so that $L_z \neq 0$, $L_x = L_y = 0$ and we use (20.37). If $B < 0$, then $(\boldsymbol{H} \cdot \boldsymbol{L}) \cdot \ \boldsymbol{L} = (H_x L_x + H_y L_y)(L_x \boldsymbol{i} + L_y \boldsymbol{j})$.

Problem 20.5s

See the book by Landau and Lifshitz [E15], p. 141–143.

Chapter 21

Problem 21.1s

To the Hamiltonian $\hat{H}$, we add the proton–proton repulsion $\hat{H}_{pp} = e^2/4\pi\text{e}_0 r$ so that $\hat{H}_t = \hat{H} + \hat{H}_{pp} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{ee} + \hat{H}_{1B} + \hat{H}_{2A} + \hat{H}_{pp} = \hat{H}_1 + \hat{H}_2 + \Delta\hat{H}$. The presence of $\hat{H}_{pp}$ does not change the value of J, since $\left\langle \Psi \middle| \hat{H}_{pp} \middle| \Psi \right\rangle$ is the same for $\Psi = \Psi_s$ or $\Psi = \Psi_t$. Thus

$$2J = \frac{D' + E'}{1 + \ell^2} - \frac{D' - E'}{1 - \ell^2}, \tag{1}$$

where $D' = 2E_{\text{H}} + \Delta D$, $E' = 2E_{\text{H}}\ell^2 + \Delta E$; ΔD is as in (21.8) with $\Delta\hat{H}$ replacing $\hat{H}$, and ΔE is as in (21.9) with $\Delta\hat{H}$ replacing $\hat{H}$. Substituting D', E' in (1), we obtain

$$2J = \frac{\Delta D + \Delta E}{1 + \ell^2} - \frac{\Delta D - \Delta E}{1 - \ell^2}. \tag{2}$$

All the quantities entering (2) are of the order $\exp(-2r/a_\mathrm{B})$ for large r so that $2J = (\Delta D + \Delta E)(1 - \ell^2) - (\Delta D - \Delta E)(1 + \ell^2) = 2\Delta E + O(\exp(-4r/a_\mathrm{B}))$, which coincides with (21.11), (21.12).

Problem 21.5s

We will present the general method of canonical transformation for handling situations where $\hat{H} = \hat{H}_0 + \hat{H}_1$ and $\hat{H}_1$ is a small perturbation to the Hamiltonian $\hat{H}_0$. The transformation to a new equivalent Hamiltonian $\hat{\hat{H}}$ will be implemented by a unitary transformation $\exp(-\hat{S})$ such that $\hat{\hat{H}}$ will not include terms of first order in $\hat{H}_1$.

$$\hat{\hat{H}} = e^{-\hat{S}}\hat{H}\,e^{\hat{S}}. \tag{1}$$

By expanding $\exp(-\hat{S})$ and $\exp(\hat{S})$ in power series, we have $\hat{\hat{H}} = \hat{H} + [\hat{H}, \hat{S}] + \frac{1}{2}\left[[\hat{H}, \hat{S}], \hat{S}\right] + \ldots = \hat{H}_0 + \hat{H}_1 + [\hat{H}_0, \hat{S}] + [\hat{H}_1, \hat{S}] + \ldots$. If we chose $\hat{S}$ so that $\hat{H}_1 + [\hat{H}_0, \hat{S}] = 0$ we have

$$\hat{H}_1 = -\hat{H}_0\hat{S} + \hat{S}\,\hat{H}_0, \tag{2}$$

$$\hat{S} = \hat{H}_0^{-1}\hat{S}\,\hat{H}_0 - \hat{H}_0^{-1}\hat{H}_1, \tag{3}$$

$$\hat{\hat{H}} = \hat{H}_0 + \frac{1}{2}\left[\hat{H}_1, \hat{S}\right] + O\left(\hat{H}_1^3\right). \tag{4}$$

For the Hubbard case and for $U \gg |V_2|$ we have $\hat{H}_0 = U\Sigma_i\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ and $\hat{H}_1 = V_2\Sigma_i\Sigma'_j\Sigma_\sigma\,|i\sigma\rangle\,\langle j\sigma|$. Let us symbolize by Ψ_n, $\Psi_m, \ldots$ the states (not eigenstates) of the Hubbard Hamiltonian where every site is singly occupied. For such states

$$\hat{H}_0\Psi_n = \hat{H}_0\Psi_m = \ldots = 0. \tag{5}$$

From (2), (4) and (5) we have

$$\left\langle\Psi_m\left|\hat{\hat{H}}\right|\Psi_n\right\rangle = \left\langle\Psi_m\left|\hat{S}\,\hat{H}_0\hat{S}\right|\Psi_n\right\rangle, \tag{6}$$

or, by introducing a complete set Φ_i of eigenstates of H_o,

$$\left\langle\Psi_m\left|\hat{\hat{H}}\right|\Psi_n\right\rangle = \Sigma_i\left\langle\Psi_m\left|\hat{S}\,\hat{H}_0\right|\Phi_i\right\rangle\left\langle\Phi_i\left|\hat{S}\right|\Psi_n\right\rangle. \tag{7}$$

$$\left\langle\Phi_i\left|\hat{S}\right|\Psi_n\right\rangle = -E_i^{-1}\left\langle\Phi_i\left|\hat{H}_1\right|\Psi_n\right\rangle, \text{because of (3) and (5),}$$

$$\left\langle\Psi_m\left|\hat{S}\,\hat{H}_0\right|\Phi_i\right\rangle = \left\langle\Psi_m\left|\hat{H}_1\right|\Phi_i\right\rangle, \text{because of (2) and (5).}$$

The only eigenfunctions Φ_i for which $\left\langle\Psi_m\left|\hat{H}_1\right|\Phi_i\right\rangle\left\langle\Phi_i\left|\hat{H}_1\right|\Psi_n\right\rangle$ is non-zero are the ones where Φ_i has a site doubly occupied and a nearest neighbor empty (because $\hat{H}_1$ can only take one electron from one site and transfer it to a nearest neighbor site). For all those states, $\Phi_i,\ E_i = U$. Hence

$$\begin{aligned} \left\langle \Psi_m \left| \hat{\hat{H}} \right| \Psi_n \right\rangle &= -\tfrac{1}{U} \left\langle \Psi_m \left| \hat{H}_1^2 \right| \Psi_n \right\rangle \\ &= \left\langle \Psi_m \left| \tfrac{2V_2^2}{U} \Sigma_{ij}' (\hat{s}_{i-}\hat{s}_{j+} + \hat{s}_{iz}\hat{s}_{jz}) \right| \Psi_n \right\rangle - \tfrac{N_a Z}{2} \tfrac{V_2^2}{U}. \end{aligned} \tag{8}$$

It is not so difficult to justify physically that the expression in the last line is indeed equivalent to the rhs of the previous line: If the nearest neighbor pair ij has parallel spins, $\langle \Psi_m | \hat{s}_{i-}\hat{s}_{j+} | \Psi_n \rangle = 0$, $\langle \Psi_m | (2V_2^2/U)(\hat{s}_{iz}\hat{s}_{jz} + \hat{s}_{jz}\hat{s}_{iz}) | \Psi_n \rangle = V_2^2/U$; thus the last line in (8) is zero and so $\left\langle \Psi_m \left| \hat{H}_1^2 \right| \Psi_n \right\rangle$is. If the pair ij has antiparallel spins there are two possibilities: (a) $|\Psi_n\rangle$, $|\Psi_m\rangle$ correspond to no spin flip, in which case $\langle \hat{s}_{i-}\hat{s}_{j+} + \hat{s}_{j-}\hat{s}_{i+} \rangle = 0$ and $\langle \hat{s}_{iz}\hat{s}_{jz} + \hat{s}_{jz}\hat{s}_{iz} \rangle = -\delta_{nm}/2$ so that the total energy per pair is $-2V_2^2/U$ in agreement with the results $-\left\langle \Psi_m \left| \hat{H}_1^2 \right| \Psi_n \right\rangle /U$. The factor of 2 in the latter comes because there are two intermediate states corresponding to double occupation of either in i or in j. Finally, if ij are antiparallel and there is spin flip, $|\Psi_m\rangle \neq |\Psi_n\rangle$ and $\langle \Psi_m | \hat{s}_{i-}\hat{s}_{j+} + \hat{s}_{j-}\hat{s}_{i+}) | \Psi_n \rangle$ would be one and the strength of the spin flip would be $2V_2^2/U$. The same result will be obtained from $-\left\langle \Psi_m \left| \hat{H}_1^2 \right| \Psi_n \right\rangle /U$ (The factor of two because of the two intermediate states and an extra factor -1 because of the antisymmetry of the electronic wave function). Taking into account (21.74) and (8) we have:

$$\hat{\hat{H}} = \frac{2V_2^2}{U} \sum_{i \neq j}{}' \hat{\boldsymbol{s}}_i \cdot \hat{\boldsymbol{s}}_j - \frac{N_\mathrm{a} Z}{2} \frac{V_2^2}{U}; \quad |V_2|/U \to 0.$$

in agreement with (21.63).

Problem 21.7s

From the definition of $\hat{S}_{i\pm}$, (21.70), and the commutation relations (21.69), eqns. (21.71) and (21.72) follow in a straightforward way. Thus, if $\hat{S}_z \, |S_z\rangle = S_z \, |S_z\rangle$, we have (dropping the index i)

$$\hat{S}_z \hat{S}_\pm \, |S_z\rangle = \left(\hat{S}_\pm \hat{S}_z \pm \hat{S}_\pm \right) |S_z\rangle = (S_z \pm 1) \hat{S}_\pm \, |S_z\rangle \, ; \tag{1}$$

Equation (1) means that $\hat{S}_\pm \, |S_z\rangle$ are eigenstates of $\hat{S}_z$ with eigenvalues, $\hat{S}_z \pm 1$:

$$\hat{S}_\pm \, |S_z\rangle = A_\pm(S, S_z) \, |S_z \pm 1\rangle \, .$$

Taking into account that the inner product of $\hat{S}_\pm \, |S_z\rangle$ with itself is equal to $\left\langle S_z \left| \hat{S}_\mp \hat{S}_\pm \right| S_z \right\rangle$, we have that $[A_\pm(S_z)]^2 = A_\mp(S_z \pm 1) A_\pm(S_z)$ or $A_\pm(S_z) = A_\mp(S_z \pm 1)$ (assuming reality of $A_\pm$). Furthermore, $\hat{S}_\pm \hat{S}_\mp = \hat{S}_x^2 + \hat{S}_y^2 \pm \hat{S}_z$; hence, $\hat{\boldsymbol{S}}^2 = \hat{S}_\pm \hat{S}_\mp + \hat{S}_z^2 \mp \hat{S}_z$. Acting on $|S_z\rangle$ by $\hat{\boldsymbol{S}}^2$ we have $S(S+1) \, |S_z\rangle = \left([A_\mp(S_z)]^2 + S_z^2 \mp S_z \right) |S_z\rangle$, or $[A_\mp(S_z)]^2 = S(S+1) \pm S_z - S_z^2 = (S \pm S_z)(S + 1 \mp S_z)$, which coincides with (21.73).

Chapter 22

Problem 22.1ts

Outside the superconductor $\boldsymbol{B}(\boldsymbol{r}) = \mu_0 \boldsymbol{H}(\boldsymbol{r})$; hence, since there is no external current density, $\nabla \times \boldsymbol{H} = 0 \Rightarrow \nabla \times \boldsymbol{B} = 0$. This last equation is valid in the interior of the superconductor as well, since $\boldsymbol{B}(\boldsymbol{r}) = 0$ there. Hence, $\boldsymbol{B}(\ \boldsymbol{r})$ can be written as

$$\boldsymbol{B} = -\nabla\phi, \tag{1}$$

which combined with the equation $\nabla \cdot \boldsymbol{B} = 0$ yields

$$\nabla^2\phi = 0. \tag{2}$$

The continuity of $\boldsymbol{B}_\perp$ at the surface in combination with $\boldsymbol{B} = 0$ in the interior of the superconductor implies that

$$\frac{\partial\phi}{\partial n} = 0. \tag{3}$$

At infinity, $r \to \infty$

$$\boldsymbol{B}\left(\boldsymbol{r}\right) \to \boldsymbol{B}_0. \tag{4}$$

Equations (1)–(4) uniquely determine $\boldsymbol{B}(\boldsymbol{r})$. The surface current density $\boldsymbol{g}\left(\boldsymbol{r}_s\right)$ at the points $\boldsymbol{r}_s$ of the surface is given by (see (A.11) and keep in mind that $\boldsymbol{M} = \boldsymbol{H} = \boldsymbol{B}/\mu_o$)

$$\boldsymbol{g}\left(\boldsymbol{r}_s\right) = \frac{1}{\mu_o}\boldsymbol{n} \times \mathbf{B}\left(\boldsymbol{r}_s\right). \tag{5}$$

For a spherical superconductor, the most general solution of ϕ_{ind}which vanishes as $r \to \infty$ is the sum $\sum_{\ell=1}^{\infty} c_\ell Y_\ell\left(\theta\right) r^{-\ell-1}$. Only the $\ell = 1$ spherical harmonic has a $\cos\theta$ dependence identical to that of the $\phi_0 = -B_0 r\cos\theta$ as to satisfy (3). Hence

$$\phi(\boldsymbol{r}) = -\left(B_0 r + \frac{c_1}{r^2}\right)\cos\theta, \tag{6}$$

where, because of (3), $c_1 = \frac{1}{2}B_0 a^3$. From (1), we have

$$\begin{aligned}\boldsymbol{B}(\boldsymbol{r}) &= \boldsymbol{B}_o - B_0\left[\boldsymbol{\theta}_0\frac{a^3}{2r^3}\sin\theta + \boldsymbol{r}_o\frac{a^3}{r^3}\cos\theta\right]\\ &= B_0\left[\boldsymbol{r}_0\left(1 - \frac{a^3}{r^3}\right)\cos\theta - \boldsymbol{\theta}_o\left(1 + \frac{a^3}{2r^3}\right)\sin\theta\right],\end{aligned}$$

and, according to (5), the surface current density is

$$\boldsymbol{g}\left(r = a, \theta, \phi\right) = -\frac{3}{2}\frac{B_0}{\mu_0}\sin\theta\,\boldsymbol{\phi}_o. \tag{7}$$

We can calculate the magnetic moment $\boldsymbol{m}_t$ induced by the surface charge density using (A.7)

$$\begin{aligned}\boldsymbol{m}_{\mathrm{t}} &= \frac{1}{2}\int \boldsymbol{r}\times\ \boldsymbol{g}\,\mathrm{d}S = -\frac{3}{4}\frac{B_0}{\mu_0}\int \mathrm{d}S\sin\theta\, r\,\boldsymbol{r}_0\times\boldsymbol{\phi}_0 = +\,\frac{3}{4}\frac{B_0 a}{\mu_0} \\ &\int a^2\mathrm{d}\phi\,\mathrm{d}\theta\,\sin\theta\,\sin\theta\,\boldsymbol{\theta}_0 = \frac{3}{4}\frac{B_o a^3}{\mu_o}2\pi\int \mathrm{d}\theta\,\sin^2\theta\,\boldsymbol{\theta}_0 = -\,\frac{3\pi}{2}\frac{B_0 a^3}{\mu_0} \\ &\int \mathrm{d}\theta\,\sin^2\theta\,\sin\theta\boldsymbol{z}_0 = -\,2\pi\boldsymbol{H}_0 a^3 = -\frac{3}{2}V\boldsymbol{H}_0. \qquad (8)\end{aligned}$$

which could have been obtained from the very beginning by using the general formula

$$\boldsymbol{m}_{\mathrm{t}} = -\frac{V\boldsymbol{H}_0}{1-n^{(z)}}, \qquad (9)$$

where $n^{(z)}$ is the depolarization coefficient along the axis z (Notice that in general for the principal axes $n^{(x)}+n^{(y)}+n^{(z)}=1$ and for a sphere $n^{(x)}=n^{(y)}=n^{(z)}=1/3$).

Problem 22.2s

Differentiating (22.11) with respect to the temperature under constant pressure and omitting the small term $\partial V_{so}/\partial T$ we have the entropy difference

$$S_N - S_S = -\mu_0 V_{s0} H_c \partial H_{\mathrm{c}}/\partial T, \quad T\le T_{\mathrm{c}}, \qquad (1)$$

which shows that for $T<T_c$, $S_N>S_S$, since $\partial H_{\mathrm{c}}/\partial T$ is negative; at $T=T_{\mathrm{c}}$, $S_N=S_S$, since $H_{\mathrm{c}}=0$ there. Differentiating once more with respect to T and then multiplying by T we obtain the difference in the specific heats

$$C_S - C_N = \mu_0 V_{s0} T\left(\frac{\partial H_c}{\partial T}\right)^2 + \mu_0 V_{s0} T\, H_c\frac{\partial^2 H_c}{\partial T^2}, \quad T\le T_{\mathrm{c}}. \qquad (2)$$

At $T=T_{\mathrm{c}}$, $H_{\mathrm{c}}=0$ and $(\partial H_{\mathrm{c}}/\partial T)^2 = 4H_{\mathrm{c}}^2(0)/T_{\mathrm{c}}^2$ according to (22.1). Actually the BCS theory (to be presented in the next chapter) shows that $(\partial H_{\mathrm{c}}/\partial T)^2 = 3.02H_{\mathrm{c}}^2(0)/T_{\mathrm{c}}^2$. Hence, using this improved value, we have

$$C_s - C_N = 3.02\mu_o V_{so} H_c^2(0)/T_c = 3.02\rho_{\mathrm{F}}\Delta^2/T_{\mathrm{c}} = 9.41\rho_{\mathrm{F}} k_{\mathrm{B}}^2 T_{\mathrm{c}} = 1.43C_N.$$

To arrive at the last result we employed the BCS relation $2\Delta(0) = 3.53k_B T_c$ (see (23.28) in the next chapter) and the relation $C_N = (2\pi^2/3)\rho_{\mathrm{F}} k_{\mathrm{F}}^2 T_{\mathrm{c}} \simeq 6.58\rho_{\mathrm{F}} k_{\mathrm{F}}^2 T_{\mathrm{c}}$.

Problem 22.5s

Since $\boldsymbol{A}(\boldsymbol{r}')$ is essentially constant over length scales much larger than ξ_{P} we can take it out of the integral. Moreover, if θ is the angle between $\boldsymbol{R}$ and $\boldsymbol{A}$, we will have $\boldsymbol{R}\cdot\boldsymbol{A} = R\,A\cos\theta$. Hence, $\boldsymbol{R}(\boldsymbol{R}\cdot\boldsymbol{A}) = R^2\cos^2\theta\boldsymbol{A}+\boldsymbol{R}_\perp A\,R\cos\theta$. Notice that the component $\boldsymbol{R}_\perp$ (normal to $\boldsymbol{A}$) of $\boldsymbol{R}$ will be integrated to zero because of rotational symmetry around $\boldsymbol{A}$. We change integration variables from $\boldsymbol{r}'$ to $\mathbf{R} = \boldsymbol{r} - \boldsymbol{r}'$ and we have

$$\begin{aligned} \boldsymbol{j} &= -\frac{3}{4\pi\xi_o}\frac{e^2 n_s}{mc}\boldsymbol{A}\,2\pi\int_{-1}^{1}\mathrm{d}(\cos\theta)\cos^2\theta\int_0^\infty \mathrm{d}R\mathrm{e}^{-R/\xi_P} \\ &= -(2\pi)\frac{3}{4\pi\xi_o}\frac{e^2 n_s}{mc}\boldsymbol{A}\frac{2}{3}\xi_P = -\frac{e^2 n_s}{mc}\frac{\xi_P}{\xi_o}\boldsymbol{A}, \end{aligned}$$

which coincides with (22.17), if $\xi_p = \xi_o$.

Chapter 23

Problem 23.1ts

We have the following relations:

$\boldsymbol{P} = \hbar\boldsymbol{K}$, $\boldsymbol{p} = \hbar\boldsymbol{k}$, $\boldsymbol{k}_1 = \frac{1}{2}\boldsymbol{K}+\boldsymbol{k}$, $\boldsymbol{k}_2 = \frac{1}{2}\boldsymbol{K}-\boldsymbol{k}$; $E = (\hbar^2K^2/4m)+(\hbar^2k^2/m)$; $k_1^2 = \frac{1}{4}K^2+k^2+K\,k\cos\theta$, $k_2^2 = \frac{1}{4}K^2+k^2-K\,k\cos\theta$. Since both k_1^2 and k_2^2 are equal to or larger than k_F^2 we have the inequalities:

$$-t_1 \le \cos\theta \le t_1 \equiv \left(\frac{1}{4}K^2+k^2-k_\mathrm{F}^2\right)/K\,k.$$

t_1 can be written as follows: $t_1 = \sqrt{m}(E-2E_\mathrm{F})/P[E-(P^2/4m)]^{1/2}$. Of course, $|\cos\theta|$ must be smaller than or equal to one. Thus,

$$-\,t \le \cos\theta < t; \quad t = \min[1,\, t_1]. \tag{1}$$

Inequalities (1) imply both $k_1 \ge k_\mathrm{F}$, $k_2 \ge k_\mathrm{F}$ as well as the obvious fact that $\cos\theta$ cannot be larger than 1. According to (23.10) and (1) we have

$$\begin{aligned} \rho_0(E) &= \frac{2\pi}{(2\pi)^3}\int_{-t}^{t}\mathrm{d}(\cos\theta)\int_0^\infty \mathrm{d}\,k\,k^2\delta(E-(\hbar^2K^2/4m)-\big(\hbar^2k^2/m\big)) \\ \text{or } \rho_0(E) &= \frac{t}{(2\pi)^2}\left(\frac{m}{\hbar^2}\right)^{3/2}\left[E-\frac{\hbar^2K^2}{4m}\right]^{1/2},\ E \ge \max\left[2E_\mathrm{F},\,\frac{P^2}{4m}\right]. \end{aligned} \tag{2}$$

When $P = \hbar K = 0$, $t = 1$ according to (23.12), and $\rho_0(2E_\mathrm{F}) = \frac{1}{2}\rho_\mathrm{FV}$. On the other hand, if $P \ne 0$ with $2E_\mathrm{F} > P^2/4m$, then $t \to 0$, as $E \to 2E_\mathrm{F}$ and

$$\rho_0(E) \to \frac{m^2}{(2\pi)^2\hbar^3}\frac{E-2E_\mathrm{F}}{P},\ E \to 2E_\mathrm{F}.$$

Problem 23.8ts

Because $\tanh \frac{x}{2} = 1 - 2(e^x + 1)^{-1}$, (23.58) can be written as follows

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_\mathrm{D}} \frac{\mathrm{d}\varepsilon}{(\varepsilon^2 + \Delta^2)^{1/2}} - \int_0^{\hbar\omega_\mathrm{D}} \frac{\mathrm{d}\varepsilon}{(\varepsilon^2 + \Delta^2)^{1/2}} \frac{2}{\exp(\beta\sqrt{\varepsilon^2 + \Delta^2}) + 1}. \tag{1}$$

We notice that the second integral vanishes for $T \to 0$, $\beta \to \infty$. Hence

$$\frac{1}{\lambda} = \int_0^{\hbar\omega_\mathrm{D}} \frac{d\varepsilon}{(\varepsilon^2 + \Delta_0^2)^{1/2}}, \quad T = 0. \tag{2}$$

Subtracting (1) from (2) and taking into account that the integral in (2) (and the similar one in (1)) is $\ln \frac{\hbar\omega_\mathrm{D} + \sqrt{(\hbar\omega_\mathrm{D})^2 + \Delta_0^2}}{\Delta_0}$, we have (by changing variables to $y = \beta\varepsilon$)

$$\ln \frac{\Delta}{\Delta_o} = -\int_0^{\beta\hbar\omega_D} \frac{dy}{(y^2 + \gamma^2)^{1/2}} \frac{2}{e^{\sqrt{y^2+\gamma^2}} + 1}, \qquad \gamma = \beta\Delta, \quad \textit{and} \quad \beta\hbar\omega_D \gg 1. \tag{3}$$

Equation (3) shows that Δ/Δ_0 is a function only of $\gamma = \Delta/k_\mathrm{B}T$ (since $\beta\hbar\omega_\mathrm{D}$ will be replaced by ∞). This function can be approximated by $\Delta/\Delta_0 = \tanh[T_\mathrm{c}\Delta/T\Delta_0]$ (recall that $\Delta_0/T_\mathrm{c} = 1.7639k_\mathrm{B}$). Taking into account that $\tanh x = x - \frac{1}{3}x^3 + \ldots (x \to 0)$ we have

$$\frac{\Delta^2}{\Delta_0^2} = 3\left(\frac{\beta}{\beta_c} - 1\right)\left(\frac{\beta_\mathrm{c}}{\beta}\right)^3 = 3\left(\frac{T}{T_\mathrm{c}}\right)^3\left(\frac{T_\mathrm{c}}{T} - 1\right), \quad T \to T_\mathrm{c}^-. \tag{4}$$

In the solution of problem 22.2s instead of 3 we have used the more accurate value of 3.02.

Problem 23.9ts

According to (4) of the solution of problem 23.8ts, we have that $\partial\Delta^2/\partial\beta = 3.02\Delta_0^2/\beta_\mathrm{c} = 3.02\Delta_0^2 k_\mathrm{B}T_\mathrm{c}$ in the limit $T \to T_\mathrm{c}$. In the same limit $T \to T_\mathrm{c}^-$, (23.59) becomes

$$C_\mathrm{V} = -\frac{2\rho_\mathrm{F}}{T}\int_{-\infty}^{\infty} \mathrm{d}\varepsilon \left[\varepsilon^2 + \frac{3.02}{2}\Delta_0^2\right] \frac{\partial}{\partial\varepsilon}\left(\frac{1}{e^{\beta\varepsilon} + 1}\right),$$

or, by introducing $x = \beta\varepsilon$ and $\gamma_0 = \beta_c \Delta_0$,

$$\begin{aligned} C_{\mathrm{V}} &= -2\rho_{\mathrm{F}} k_{\mathrm{B}}^2 T \int_{-\infty}^{\infty} \mathrm{d}x \left[x^2 + \tfrac{3.02}{2}\gamma_0^2\right] \tfrac{\mathrm{d}}{\mathrm{d}x}\left(\tfrac{1}{e^x+1}\right) \\ &= 8\rho_{\mathrm{F}} k_{\mathrm{B}}^2 T \int_0^{\infty} \mathrm{d}x x \tfrac{1}{e^x+1} + 3.02\rho_{\mathrm{F}} \tfrac{\Delta_0^2}{T} \\ &= 8\rho_{\mathrm{F}} k_{\mathrm{B}}^2 T \tfrac{\pi^2}{12} + 3.02\rho_{\mathrm{F}} \tfrac{(1.7639)^2 k_{\mathrm{B}}^2 T_{\mathrm{c}}^2}{\mathrm{T}}, \quad T \to T_{\mathrm{c}} \\ &= 15.98\rho_{\mathrm{F}} k_{\mathrm{B}}^2 T_{\mathrm{c}}, \end{aligned}$$

vs. $(2\pi^2/3)\rho_{\mathrm{F}} k_{\mathrm{B}}^2 T$ for the electronic contribution to the specific heat for the normal state. Thus

$$\left.\frac{C_{Vs} - C_{VN}}{C_{VN}}\right|_{T=T_{\mathrm{c}}^-} = \frac{3.02 \times (1.7639)^2}{(2\pi^2/3)} = 1.43.$$

Problem 23.1s

Schrödinger's equation becomes

$$\left(\frac{\hbar^2 k^2}{2\mu} - E\right) c_{\boldsymbol{k}} + \frac{1}{V}\sum_{\boldsymbol{k}'} V_{\boldsymbol{k}-\boldsymbol{k}'} c_{\boldsymbol{k}'} = 0, \quad \mu = m/2,$$

which, taking into account the forms of $c_{\boldsymbol{k}}$ and $V_{\boldsymbol{k}-\boldsymbol{k}'}$, becomes

$$(2\varepsilon - E)a(\varepsilon) = \lambda \int_{E_{\mathrm{F}}}^{E_{\mathrm{F}}+\hbar\omega_{\mathrm{D}}} \mathrm{d}\varepsilon' a(\varepsilon'). \tag{1}$$

Call Δ' the integral in (1) so that $a(\varepsilon) = \lambda\Delta'/(2\varepsilon - E)$ and

$$\Delta' \equiv \int_{E_{\mathrm{F}}}^{E_{\mathrm{F}}+\hbar\omega_{\mathrm{D}}} \mathrm{d}\varepsilon' a(\varepsilon') = \lambda\Delta' \int_{E_{\mathrm{F}}}^{E_{\mathrm{F}}+\hbar\omega_{\mathrm{D}}} \mathrm{d}\varepsilon' \frac{1}{2\varepsilon' - E}$$

or

$$\frac{1}{\lambda} = \frac{1}{2}\ln\left|\frac{2E_{\mathrm{F}} + 2\hbar\omega_{\mathrm{D}} - E}{2E_{\mathrm{F}} - E}\right| \simeq \frac{1}{2}\ln\left|\frac{2\hbar\omega_{\mathrm{D}}}{2E_{\mathrm{F}} - E}\right|,$$

or

$$|2E_{\mathrm{F}} - E| = 2\hbar\omega_{\mathrm{D}} \exp\left(-\frac{2}{\lambda}\right).$$

Problem 23.2s

By implementing the change in variables we have

$$-I = \frac{1}{2}\rho_{\mathrm{VF}} \int_{-\beta\hbar\omega_{\mathrm{D}}}^{\beta\hbar\omega_{\mathrm{D}}} \mathrm{d}x \frac{2}{\beta} \frac{\tanh(x/2)}{(2x/\beta)} = \rho_{\mathrm{VF}} \int_{0}^{\beta\hbar\omega_{\mathrm{D}}} \mathrm{d}x \frac{\tanh(x/2)}{x}.$$

Integrating by parts we obtain

$$-I = \rho_{\mathrm{VF}}(\ln \beta\hbar\omega_{\mathrm{D}}) \tanh \frac{\beta\hbar\omega_{\mathrm{D}}}{2} - \rho_{\mathrm{VF}} \int_{0}^{\beta\hbar\omega_{\mathrm{D}}} \mathrm{d}x \ln x \frac{\mathrm{d}}{\mathrm{d}x} \tanh\left(\frac{x}{2}\right).$$

In the last integral we replace $\beta\hbar\omega_{\mathrm{D}}$ (which is much larger than 1) by ∞ (the resulting error is of the order of $\ln \beta\hbar\omega_{\mathrm{D}} \exp(-\beta\hbar\omega_{\mathrm{D}})$). The integral $\int_0^\infty \mathrm{d}x \ln x\, \mathrm{d}[\tanh(x/2)]/\mathrm{d}x$ is equal to $-\ln(2e^\gamma/\pi)$ (See [D5], p. 580, 4.371.3) Thus

$$I = -\rho_{\mathrm{VF}} \ln\left(\frac{2e^\gamma}{\pi}\beta\hbar\omega_{\mathrm{D}}\right) + \mathcal{O}\left(\ln \beta\hbar\omega_{\mathrm{D}} \mathrm{e}^{-\beta\hbar\omega_{\mathrm{D}}}\right).$$

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