1
Introduction

1.1
Second-Quantized Representation for Electrons

The use of a Schrödinger equation to describe one or more electrons already treats the electron quantum mechanically and is sometimes referred to as first quantization. As long as electrons are neither created nor destroyed, such a description is complete. However, an electron that is transferred from state n to state m is often described as the destruction of an electron in state n and creation in state m by an operator obeying an algebra of the form $c_m^\dagger c_n$. It is convenient therefore to further refine the algebra of such operators analogous to the operators $b_q^\dagger$ and b_q that create and destroy phonons of wave-vector $\boldsymbol{q}$. However, electrons are fermions rather than bosons and the state occupancy number $c_n^\dagger c_n$ should only be permitted to take the values zero or one. This aim is achieved by using anti-commutation rules {described by braces} or by square brackets with a + subscript, that is, $[\cdots]_+$, instead of commutation rules described by brackets or square brackets with a − subscript, that is, $[\cdots]_-$.

In this book, we will be primarily concerned with low-dimensional systems such as quantum wells, dots and wires. A typical band structure of the valence and conduction bands for a heterostructure like GaAs/AlGaAs is shown in Figure 1.1. However, the formulation in this chapter and in some of the others is independent of dimensionality.

The phrase "second quantization" is descriptive of the notion that the Schrödinger wave function $\Psi(\boldsymbol{r})$ is to be quantized, that is, treated as an operator. In terms of any complete set of states $\phi_k(\boldsymbol{r})$, we can write:

$$\Psi(\boldsymbol{r}) = \sum_k c_k \phi_k(\boldsymbol{r}) \ , \quad \int d^3\boldsymbol{r}\,\phi_k^*(\boldsymbol{r})\,\phi_{k'}(\boldsymbol{r}) = \delta_{kk'} \ , \tag{1.1}$$

where the anti-commutation rules are given by

$$\left[c_k, c_{k'}^\dagger\right]_+ = \delta_{kk'} \ , \tag{1.2}$$

and

$$[c_k, c_{k'}]_+ = \left[c_k^\dagger, c_{k'}^\dagger\right]_+ = 0 \ . \tag{1.3}$$
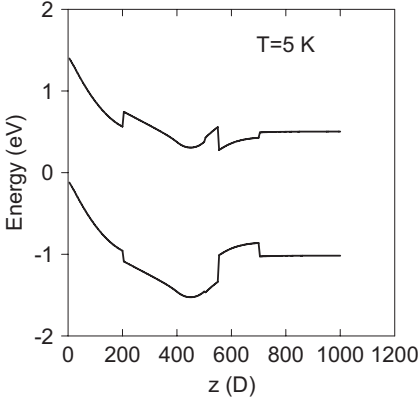
Figure 1.1 Valence (lower curve) and conduction (upper curve) bands of electrons in a semi-conductor heterostructure.

For a single state, we can omit the subscripts and examine the consequences. Equation (1.3) implies that

$$c^2 = 0, \quad \left(c^\dagger\right)^2 = 0. \tag{1.4}$$

Let $N = c^\dagger c$, then

$$\begin{aligned} N^2 = \left(c^\dagger c\right)^2 &= c^\dagger c c^\dagger c = c^\dagger \left(1 - c^\dagger c\right) c \\ &= c^\dagger c - \left(c^\dagger\right)^2 c^2 = c^\dagger c - 0 = N. \end{aligned} \tag{1.5}$$

Thus, $N = 1$ or 0.

Consider the two eigenstates of N:

$$N\Psi_0 = 0\Psi_0, \quad \text{and} \quad N\Psi_1 = 1\Psi_1. \tag{1.6}$$

Then, is $c^\dagger \Psi_0$ also an eigenstate of N?

$$\begin{aligned} \left(c^\dagger c\right) c^\dagger \Psi_0 &= c^\dagger \left(1 - c^\dagger c\right) \Psi_0 \\ &= c^\dagger \Psi_0 - \left(c^\dagger\right)^2 c \Psi_0 = c^\dagger \Psi_0. \end{aligned} \tag{1.7}$$

Therefore,

$$N\left(c^\dagger \Psi_0\right) = 1\left(c^\dagger \Psi_0\right), \tag{1.8}$$

that is, $c^\dagger \Psi_0$ is proportional to Ψ_1. Evaluate the normalization:

$$\begin{aligned} \int d^3r \left(c^\dagger \Psi_0\right)^* \left(c^\dagger \Psi_0\right) &= \int d^3r \, \Psi_0^* c c^\dagger \Psi_0 \\ &= \int d^3r \, \Psi_0^* \left(1 - c^\dagger c \Psi_0\right) = 1. \end{aligned} \tag{1.9}$$

Therefore, $c^\dagger \Psi_0$ is normalized and we can simply choose

$$c^\dagger \Psi_0 = \Psi_1 \ . \tag{1.10}$$

Similarly,

$$cc^\dagger \left(c \Psi_1\right) = c \left(1 - cc^\dagger\right) \Psi_1 = c \Psi_1 \ . \tag{1.11}$$

Therefore, $c \Psi_1$ is an eigenvector of $cc^\dagger = 1 - c^\dagger c$ with eigenvalue 1 or eigenvector of $c^\dagger c$ with eigenvector 0. By a similar procedure to Eq. (1.9), $c \Psi_1$ is normalized and we can write

$$c \Psi_1 = \Psi_0 \ . \tag{1.12}$$

Note that

$$c \Psi_0 = c^2 \Psi_1 = 0 \ , \tag{1.13}$$
$$c^\dagger \Psi_1 = \left(c^\dagger\right)^2 \Psi_0 = 0 \ . \tag{1.14}$$

We begin by rewriting the Schrödinger equation in second quantized form. In most cases, the Hamiltonian has the form

$$H = \sum_{i=1}^{N} T \left(x_i\right) + \frac{1}{2} \sum_{i \neq j=1}^{N} V \left(x_i, x_j\right) \ , \tag{1.15}$$

where T is the kinetic energy and V is the potential energy of interaction of the particles. Here, $x_i = (x_i, t_i, s_i)$ is the space-time-spin point. The potential energy term represents the interaction between every pair of particles counted once, precisely why we have the factor of 1/2. We will not give the details for reformulating Eq. (1.15) in second quantized form since it can be found in many textbooks on quantum mechanics and will simply quote the results along with some others. For the Hamiltonian in Eq. (1.15), we have

$$\begin{aligned}
\hat{H} = &\int d^3x, \hat{\Psi}^\dagger \left(x\right) T \left(x\right) \hat{\Psi} \left(x\right) \\
&+ \frac{1}{2} \int d^3x \int d^3x' \hat{\Psi}^\dagger \left(x\right) \hat{\Psi}^\dagger \left(x'\right) V \left(x, x'\right) \hat{\Psi} \left(x'\right) \hat{\Psi} \left(x\right) \ .
\end{aligned} \tag{1.16}$$

The single-particle operator

$$J = \sum_{i=1}^{N} J \left(x_i\right) \tag{1.17}$$

in second quantized form becomes

$$\hat{J} = \int d^3x \hat{\Psi}^\dagger \left(x\right) J \left(x\right) \hat{\Psi} \left(x\right) \ , \tag{1.18}$$

and, in particular, the number density $n(x) = \sum_{i=1}^{N} \delta(x - x_i)$ is given by

$$\hat{n} \left(x\right) = \hat{\Psi}^\dagger \left(x\right) \hat{\Psi} \left(x\right) \ , \tag{1.19}$$

where $\hat{\Psi}^\dagger(x)$ and $\hat{\Psi}(x)$ are creation and annihilation operators, respectively.

1.2
Second Quantization and Fock States

For a system in which the number of particles is variable, it is essential to introduce creation and destruction operators. However, it is also possible to do so when the number of particles is conserved. In that case, of course, the perturbation operators will contain an equal number of creation and destruction operators. In that case, it is customary to describe the procedure as "second quantization". First quantization replaces classical mechanical equations of motion, and second quantization replaces a Hamiltonian containing one-body forces, two-body forces, and so on by a Hamiltonian that is bilinear in creation and destruction operators, quadratic in creation and destruction operators, and so on. Nothing new is added, but the commutation rules of the creation and destruction operators make the bookkeeping of the states simpler than using permanents or determinants for the Schrödinger wave functions. For Bose particles, second quantization was developed by Dirac [1], and extended to Fermi particles by Wigner and Jordan [2]. A more detailed discussion is given by Fock [3] and by Landau and Lifshitz [4].

1.3
The Boson Case

It is simplest to describe the relation between the Schrödinger description and the second quantized description by assuming that we have a set of N non-interacting particles that can occupy any one of a set of orthonormal states $\phi_n(x_i)$. Besides, if the particles do not interact, the wave function can be a product of the ϕ_n that are occupied. In addition, (for Boson statistics) the wave function must be symmetric with respect to exchange of any two particles. If there are N_1 particles in state ϕ_1, N_2 in ϕ_2 for a total $N = \sum_i N_i$ of particles, the wave function can be written in the form

$$\Psi(N_1, N_2, \cdots) = \sqrt{\frac{N_1! N_2! \cdots}{N!}} \sum \phi_{p_1}(x_1) \phi_{p_2}(x_2) \cdots \phi_{p_N}(x_N) , \qquad (1.20)$$

where $p_1, p_2, \ldots, p_N$ is any set of occupied states (such as $p_1 = 1$, $p_2 = 3$, $p_3 = 4$, etc.). These indices must not all be different since some states can be multiply occupied. However, where they are distinct, the sum must be taken over all permutations of the distinct indices. Since the number of ways of placing N_1 particles (out of N) in one box, N_2 in a second and so on is given by $N!/(N_1! N_2! \cdots)$. The prefactor in Eq. (1.20) is added to preserve normalization. We can refer to $\Psi(N_1, N_2, \cdots)$ as a Fock state with N_1 particles in $\phi_1(x)$, N_2 in $\phi_2(x)$, and so on.

We then introduce creation and destruction operators $B_i^\dagger$ and B_j defined by

$$B_i^\dagger \Psi(N_1, \cdots, N_i, \cdots) = \sqrt{N_i + 1}\, \Psi(N_1, \cdots, N_i + 1, \cdots) , \qquad (1.21)$$

and

$$B_j \Psi(N_1, \cdots, N_j, \cdots) = \sqrt{N_j}\, \Psi(N_1, \cdots, N_j - 1, \cdots) . \qquad (1.22)$$

The principal simplification of second quantization is that a one-body operator

$$V = \sum_a V(\mathbf{r}_a) \; , \tag{1.23}$$

which can take $\Psi(N_i - 1, N_k)$ into $\Psi(N_i, N_k - 1)$ by "destroying" a particle in state k and creating one in state i in the Schrödinger permanent wave functions can be much more easily calculated when the operator

$$\hat{V} = V_{ik} B_i^\dagger B_k \tag{1.24}$$

acts on the Fock states. In particular, the matrix element

$$\int d^3\mathbf{r}\, \Psi^*(N_i, N_k - 1) \, \hat{V} \, \Psi(N_i - 1, N_k)$$
$$= \int d^3\mathbf{r}\, \Psi^*(N_i, N_k - 1) \, V_{ik} B_i^\dagger B_k \, \Psi(N_i - 1, N_k)$$
$$= \sqrt{N_i N_k}\, V_{ik} \; , \tag{1.25}$$

where the first integral is over the Schrödinger space $dx_l\, dx_2 \cdots dx_N$. The second one is thought of in terms of creation and destruction operators in a space described by the number set $\{N_j\}$, and the matrix element

$$V_{ik} = \int d^3\mathbf{r}\, \phi_i^*(\mathbf{r}) \, V(\mathbf{r}) \, \phi_k(\mathbf{r}) \tag{1.26}$$

is the usual one-body matrix element in the Schrödinger representation.

Landau and Lifshitz [4] do not derive this result. They merely state that "The calculation of these matrix elements is, in principle, very simple, it is easier to do it oneself than to follow an account of it." It would be unfair to leave the matter there: Landau knows how to do it; let it be an exercise for the reader.

We can make the answer plausible by showing that the right-hand side of Eq. (1.25) is a product of four factors:

$$P \equiv \left[\frac{(N_i - 1)!\, N_k!}{(N_i + N_k - 1)!} \right]^{1/2} \left[\frac{N_i!\, (N_k - 1)!}{(N_i + N_k - 1)!} \right]^{1/2} V_{ik}\, M \; . \tag{1.27}$$

The first factor comes from the normalization factor of the initial state, and the second from the normalization of the final state. Factors involving N_j for $j \neq i$ or k are ignored since they merely contribute to the normalization of the remaining states. A single product of ϕs for the initial state, a product for the final state and one $V(\mathbf{r}_a)$ give rise to a term V_{ik} or zero. The factor M is simply the number of such non-vanishing terms. Since each $V(\mathbf{r}_a)$ for $a = 1, 2, \ldots, N$ makes the same contribution, M contains a factor $N = (N_i - 1) + N_k = N_i + (N_k - 1)$, the total number of particles in these two states (in either the final or the initial states). For a given $V(\mathbf{r}_a)$, the factor $\int d^3\mathbf{r}_a \phi_i^*(\mathbf{r}_a) V(\mathbf{r}_a) \phi_k(\mathbf{r}_a)$ appears and one particle is used up. The remaining $N - 1 = N_i + N_k - 2$ particles must now be distributed with $N_i - 1$ in the ith state and $N_k - 1$ in the kth state. Thus,

$$M = N \frac{(N - 1)!}{(N_i - 1)!\, (N_k - 1)!} \; , \tag{1.28}$$

where the first factor, $N = N_i + N_k - 1$, is the number of terms in the sum $\sum_a V(\mathbf{r}_a)$ and the second factor is the number of ways of distributing $N - 1$ particles in two states with $N_i - 1$ in the first state and $N_k - 1$ in the second state. Finally,

$$P = \sqrt{N_i N_k} \frac{(N_i - 1)! \, (N_k - 1)!}{(N_i + N_k - 1)!} V_{ik} \frac{(N_i + N_k - 1)!}{(N_i - 1)! \, (N_k - 1)!}$$

$$= \sqrt{N_i N_k} \, V_{ik} \, . \tag{1.29}$$

The matrix elements in Eqs. (1.21) and (1.22) are such as to insure the commutations rules

$$[B_i, B_j]_- = [B_i^\dagger, B_j^\dagger]_- = 0 \, , \quad [B_i, B_j^\dagger]_- = \delta_{ij} \, . \tag{1.30}$$

A natural generalization of Eq. (1.25) to two-body operators implies the replacement:

$$\sum_{a>b} W(\mathbf{r}_a, \mathbf{r}_b) \rightarrow \sum W_{lm}^{ik} B_i^\dagger B_k^\dagger B_l B_m \, . \tag{1.31}$$

A compact statement of these commutation rules in Eq. (1.30) can be obtained by introducing an operator $\psi(\mathbf{r})$ in the form

$$\psi(\mathbf{r}) = \sum_i B_i \phi_i(\mathbf{r}) \, , \quad \psi^\dagger(\mathbf{r}) = \sum_i B_i^\dagger \phi_i^*(\mathbf{r}) \, . \tag{1.32}$$

Then, the "Schrödinger operators", $\psi(\mathbf{r})$ and $\psi^\dagger(\mathbf{r}')$, obey the commutation rules

$$\left[\psi(\mathbf{r}), \psi(\mathbf{r}')\right]_- = \left[\psi^\dagger(\mathbf{r}), \psi^\dagger(\mathbf{r}')\right]_- = 0 \, , \tag{1.33}$$

$$\left[\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}')\right]_- = \sum_{i,j} \phi_i(\mathbf{r}) \, \phi_j^*(\mathbf{r}') \, \delta_{ij} = \delta(\mathbf{r} - \mathbf{r}') \, , \tag{1.34}$$

where the δ_{ij} arises from Eq. (1.30) and the Dirac delta function follows from the completeness.

The second quantized Hamiltonian of a boson system with one and two-body forces can be written in the form

$$\hat{H} = \int d^3 r \left[\frac{\hbar^2}{2m} \nabla \psi^\dagger(\mathbf{r}) \cdot \nabla \psi(\mathbf{r}) + V(\mathbf{r}) \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}) \right]$$

$$+ \frac{1}{2} \int d^3 r \int d^3 r' \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') W(\mathbf{r}, \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}) \, . \tag{1.35}$$

In addition to the correspondence

$$\sum_a V(\mathbf{r}_a) \rightarrow \sum_{i,k} V_{ik} B_i^\dagger B_k \tag{1.36}$$

for one-body forces, we have a similar correspondence for two-body forces:

$$\sum_{a>b} W(\mathbf{r}_a, \mathbf{r}_b) \rightarrow \sum_{i,k;l,m} W_{lm}^{ik} B_i^\dagger B_k^\dagger B_l B_m \, , \tag{1.37}$$

where

$$W_{lm}^{ik} = \int d^3 r \int d^3 r' \phi_i^*(r) \phi_k^*(r') W(r, r') \phi_l(r) \phi_m(r') .$$ (1.38)

We note that the commutation rules, Eqs. (1.30), (1.33), and (1.34) for bosons are the same as the ones we are familiar with for harmonic oscillators and phonons, which are of course bosons.

1.4
The Fermion Case

In the fermion case, the Pauli principle requires that the wave function be antisymmetric. The simplest example of a set of independent fermions is then described by a determinant

$$\Psi(N_1, N_2, \cdots) = \begin{vmatrix} \phi_{p_1}(r_1) & \phi_{p_1}(r_2) & \cdots \phi_{p_1}(r_N) \\ \phi_{p_2}(r_1) & \phi_{p_2}(r_2) & \cdots \phi_{p_2}(r_N) \\ \cdots & \cdots & \cdots\cdots \\ \phi_{p_N}(r_1) & \phi_{p_N}(r_2) & \cdots \phi_{p_N}(r_N) \end{vmatrix}$$ (1.39)

in terms of the set of functions $\phi_i(r)$. The latter are usually taken as members of a complete set of eigen-functions of the one-body Hamiltonian. Here, N is the total number of eigen-functions appearing in the determinant, that is, the total number of occupied states. The set of numbers $p_1, p_2, \cdots, p_N$ are some chosen ordering of the set $\{i\}$. To make the sign of the determinant unique, a fixed order must be chosen. It is conventional to choose the ordering

$$p_1 < p_2 < p_3 < \cdots < p_N .$$ (1.40)

This is not necessary, but a fixed choice must be maintained in the ensuing discussion.

The result of second quantization for fermions will look similar to that for bosons in the sense that Eq. (1.32) is replaced by

$$\psi(r) = \sum_i F_i \phi_i(r) , \quad \psi^\dagger(r) = \sum_i F_i^\dagger \phi_i^*(r) ,$$ (1.41)

where the boson operators B_i have been replaced by the fermion operators F_i. With this change, Eqs. (1.35)–(1.38) remain valid. However, fermion states can have occupancies only of $N_i = 0$ or $N_i = 1$. This is accomplished by the use of anticommutation rules

$$\left[F_i, F_j^\dagger\right]_+ = \delta_{ij} , \quad \left[F_i, F_j\right]_+ = 0 , \quad \left[F_i^\dagger, F_j^\dagger\right]_+ = 0$$ (1.42)

rather than the commutation rules used in the boson case. In particular, Eqs. (1.33) and (1.34) are replaced by

$$[\psi(r), \psi(r')]_+ = [\psi^\dagger(r), \psi^\dagger(r')]_+ = 0 ,$$ (1.43)

$$[\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}')]_+ = \delta(\mathbf{r} - \mathbf{r}') , \tag{1.44}$$

which follows directly from Eq. (1.42).

To see that the anti-commutation rules, Eq. (1.42), accomplish the desired objectives, we first consider a single state $\phi_i(\mathbf{r})$ with operators F_i and $F_i^\dagger$, and omit the index i.

$$F^2 = 0 , \quad \left(F^\dagger\right)^2 = 0 . \tag{1.45}$$

Let $N = F^\dagger F$. Then,

$$N^2 = \left(F^\dagger F\right)^2 = F^\dagger F F^\dagger F = F^\dagger \left(1 - F^\dagger F\right) F$$
$$= F^\dagger F - \left(F^\dagger\right)^2 F^2 = F^\dagger F - 0 = N \tag{1.46}$$

so that

$$N = 1 \quad \text{or} \quad N = 0 . \tag{1.47}$$

Consider the eigenstates of N:

$$N\Psi_0 = 0\Psi_0 \quad \text{or} \quad N\Psi_1 = \Psi_1 . \tag{1.48}$$

Then, is $F^\dagger \Psi_0$ also an eigenstate of N?

$$\left(F^\dagger F\right) F^\dagger \Psi_0 = F^\dagger \left(1 - F^\dagger F\right) \Psi_0$$
$$= F^\dagger \Psi_0 - \left(F^\dagger\right)^2 F \Psi_0 . \tag{1.49}$$

Therefore,

$$N F^\dagger \Psi_0 = 1 \left(F^\dagger \Psi_0\right) , \tag{1.50}$$

that is, $F^\dagger \Psi_0$ is proportional to Ψ_1. Evaluate the normalization:

$$\int d^3\mathbf{r} \left(F^\dagger \Psi_0\right)^* \left(F^\dagger \Psi_0\right) = \int d^3\mathbf{r}, \Psi_0^* F F^\dagger \Psi_0$$
$$= \int d^3\mathbf{r} \Psi_0^* \left(1 - F^\dagger F\right) \Psi_0 = 1 . \tag{1.51}$$

Therefore, $F^\dagger \Psi_0$ is normalized and we can choose

$$F^\dagger \Psi_0 = \Psi_1 . \tag{1.52}$$

Similarly,

$$F F^\dagger \left(F \Psi_1\right) = F \left(1 - F F^\dagger\right) \Psi_1 = F \Psi_1 . \tag{1.53}$$

Therefore, $F \Psi_1$ is an eigenvector of $F F^\dagger = 1 - F^\dagger F$ with eigenvalue one or eigenvector of $F^\dagger F$ with eigenvector zero. By a similar procedure to Eq. (1.28), $F \Psi_1$ is normalized and we choose

$$F \Psi_1 = \Psi_0 . \tag{1.54}$$

Note that

$$F \Psi_0 = F^2 \Psi_1 = 0 \, , \tag{1.55}$$

$$F^\dagger \Psi_1 = \left(F^\dagger\right)^2 \Psi_0 = 0 \, . \tag{1.56}$$

The above discussion has established that the anti-commutation rules generate a set of states with occupancies zero and one. The full correspondence between first and second quantization requires that we establish the analogue of Eq. (1.36):

$$V = \sum_a V\left(\mathbf{r}_a\right) \rightarrow \sum_{ik} V_{i,k} F_i^\dagger F_k \, . \tag{1.57}$$

This involves the matrix element of the one-body operator V between two determinantal states. In effect, a transition in which a fermion in state k is destroyed and one in state i is created was found to have the matrix element

$$\int d^3r \, \Psi^* \left(N_i, N_k - 1\right) V \Psi \left(N_i - 1, N_k\right) = V_{ik} \tag{1.58}$$

between determinantal states.

[4, Eq. (61.3)] allege (without proof) that the result in Eq. (1.58) should instead be

$$\int d^3r \, \Psi^* \left(N_i, N_k - 1\right) V \Psi \left(N_i - 1, N_k\right) = V_{ik}(-1)^\Sigma \, , \tag{1.59}$$

where the symbol

$$\Sigma = \sum_{j=i+1}^{k-1} N_j \, . \tag{1.60}$$

This discrepancy can be resolved as follows. In our calculation, we obtained the final wave function (before anti-symmetrization) from the initial wave function simply by replacing $\phi_k(\mathbf{r}_a)$ with $\phi_i(\mathbf{r}_b)$. However, this procedure does not preserve the chosen ordering, Eq. (1.40). To restore the chosen ordering, one must interchange row i and k in the final determinant. These gain a factor $(-1)^\Sigma$ where Σ is the number of occupied states between i and k.

To maintain the validity of Eq. (1.57), the operator F_k takes the state $N_k = 1$ into $N_k = 0$ with an extra factor

$$F_k \Psi \left(N_k = 1\right) = \eta_k \Psi \left(N_k = 0\right) \, , \tag{1.61}$$

and

$$F_k^\dagger \Psi \left(N_k = 0\right) = \eta_k^* \Psi \left(N_k = 1\right) \, . \tag{1.62}$$

The anti-commutator $[F_k, F_k^\dagger]_+$ is unchanged as long as $|\eta_k|^2 = 1$. If we define

$$\eta_k = \prod_{j=1}^{k-1} (-1)^{N_j} \, , \tag{1.63}$$

then $F_i^\dagger F_k$ acquires just the extra factor $(-1)^{\sum(i+1,k-1)}$ demanded by Eq. (1.59). Moreover, it is easy to see why

$$F_m F_n = -F_n F_m \tag{1.64}$$

because one of m, n (say m) is higher in the sequence of states. Then, the matrix for F_m in $F_m F_n$ is reversed in sign because F_n has acted and eliminated the state n below m. In the reverse order, $F_n F_m$, F_n is unaffected by the elimination of state m above it. Hence, the two orders differ by a factor -1 to yield the desired anti-commutation rule. These remarks are stated clearly in [5].

1.5
The Hamiltonian of Electrons

We first consider the case of a single electron, or of a set of non-interacting electrons. The Hamiltonian can be written in the form:

$$H = \int d^3r \, \psi^\dagger(r) \, U(r) \, \psi(r) \ . \tag{1.65}$$

Here, $\psi(r)$ and $\psi^\dagger(r)$ are regarded as operators that can be expanded in an arbitrary orthonormal set $\phi_n(r)$:

$$\psi(r) = \sum_n c_n \phi_n(r) \ , \tag{1.66}$$

$$\psi^\dagger(r) = \sum_m c_m^\dagger \phi_m^*(r) \ . \tag{1.67}$$

The Hamiltonian then takes the form

$$\begin{aligned} H &= \sum_{m,n} c_m^\dagger \int d^3r \, \phi_m^*(r) \, U(r) \, \phi_n(r) \, c_n \\ &= \sum_{m,n} c_m^\dagger \langle m|U|n\rangle c_n \ , \end{aligned} \tag{1.68}$$

where $\langle m|U|n\rangle$ represents the matrix for destruction of electrons in n and its creation in m. If the original Schrödinger equation is

$$\left[-\frac{\hbar^2}{2m^*}\nabla^2 + V(r)\right]\phi = E\phi \ , \tag{1.69}$$

where m^* represents the mass of an electron, then U is the operator defined by

$$U = -\frac{\hbar^2}{2m}\nabla^2 + V(r) \ , \tag{1.70}$$

whose matrix element is

$$\langle m|U|n\rangle = \int d^3r \, \phi_m^*(r) \left[-\frac{\hbar^2}{2m^*}\nabla^2 + V(r)\right]\phi_n(r) = U_{mn} \ . \tag{1.71}$$

To best understand the eigenstates of the operator

$$H = \sum_{m,n} U_{mn} c_m^\dagger c_n \,, \tag{1.72}$$

we can choose the ϕ_n to be the eigenstates of U with eigenvalues E_n. Then,

$$U_{mn} = E_m \delta_{mn} \,, \tag{1.73}$$

$$H = \sum_n E_n c_n^\dagger c_n \,. \tag{1.74}$$

The Hilbert vector Ψ that is an eigenvector of H will then simply be described by a set of occupancies zero or one of each $N = c_n^\dagger c_n$, for example, $|0,1,0,0,1,1,0,1,\ldots\rangle$. To solve the Schrödinger equation $H\Psi = E\Psi$, we can write

$$\sum_{m,n} \left(c_m^\dagger c_n U_{mn} \right) \Psi = E\Psi \,. \tag{1.75}$$

1.6
Electron–Phonon Interaction

Following Callaway [6] the Hamiltonian is written as an electron energy, plus a phonon energy, plus an electron–phonon interaction:

$$H = \sum_{k,\sigma} E_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_q \hbar\omega_q a_q^\dagger a_q$$
$$+ \sum_{k,q,\sigma} \left[D(q) c_{k+q,\sigma}^\dagger c_{k\sigma} a_q + D(-q) c_{k-q,\sigma}^\dagger c_{k\sigma} a_q^\dagger \right] \,. \tag{1.76}$$

Quasi-momentum conservation is built into the above expression and σ is the index for electron spin. The original form for phonon absorption was

$$V_{k'k} \delta_{k',k+q} c_{k'\sigma}^\dagger c_{k\sigma} a_q \,. \tag{1.77}$$

We assume that the potential is local so that $V_{k'k} = V_{k'-k}$. There are also screened Coulomb electron–electron terms that we ignore here. These have the form

$$\int d^3 r_1 \cdots \int d^3 r_n \Psi^* (r_1, \cdots, r_n) \frac{1}{2} \sum_{i \neq j=1}^n W\left(r_i - r_j \right) \Psi (r_1, \cdots, r_n) \,, \tag{1.78}$$

corresponding to the many-body wave-function energy. If we insert $\psi(r) = \sum_j c_j \phi_j(r)$ which expresses the operators $\psi(r)$ in terms of the c_j operators, we get

$$H_{\text{two-body}} = \frac{1}{2} \sum_{i,k:l,m} c_i^\dagger c_k^\dagger \langle kl| W |ml\rangle c_l c_m \,, \tag{1.79}$$

which is a representation of two-body interactions in second quantized form.

1.7
Effective Electron–Electron Interaction

In an electromagnetic field, the charge-1 acts on the field and the field acts on charge-2. If we can eliminate the field, we obtain a direct interaction between charge-1 and charge-2. Here, the field is the phonon field. After we eliminate the electron–phonon interaction, we should obtain an effective electron–electron interaction.

Let

$$H = H_0 + H_1 \,, \tag{1.80}$$

where H_1 is the interaction Hamiltonian. The transformed Hamiltonian

$$
\begin{aligned}
H_{\mathrm{T}} &= e^{-iS} H e^{iS} \\
&= H + i[H, S] - \frac{1}{2}[[H, S], S] + \cdots \\
&= H_0 + H_1 + i[H_0, S] + i[H_1, S] - \frac{1}{2}[[H_0, S], S] + \cdots
\end{aligned} \tag{1.81}
$$

to second order of S. To dispose of H_1 to lowest order, we set

$$H_1 + i[H_0, S] = 0 \,, \quad \text{i.e.,} \quad [H_0, S] = i H_1 \,. \tag{1.82}$$

Then,

$$H_{\mathrm{T}} = H_0 + i[H_1, S] - \frac{i}{2}[H_1, S] = H_0 + \frac{i}{2}[H_1, S] \,. \tag{1.83}$$

Let $|m\rangle$ and $|n\rangle$ be energy eigenstates of the complete system of electrons and phonons. Then, we get

$$
\begin{aligned}
\langle m|[H_0, S]|n\rangle &= i\langle m|H_1|n\rangle \,, \quad \text{and} \quad \langle m|H_1|m\rangle = 0 \,, \\
(E_m - E_n) S_{mn} &= i\langle m|H_1|n\rangle \,, \\
S_{mn} &= \frac{\langle m|H_1|n\rangle}{E_m - E_n} \,, \quad \text{for} \quad m \neq n \,.
\end{aligned} \tag{1.84}
$$

However,

$$\langle n_q - 1|a_q|n_q\rangle = n_q^{1/2} \,, \quad \langle n_q + 1|a_q^\dagger|n_q\rangle = (n_q + 1)^{1/2} \,. \tag{1.85}$$

Writing S as operators cs (electronic part) and as a matrix in the vibrational part, we obtain

$$\langle n_q - 1|S|n_q\rangle = i \sum_{k,\sigma} \frac{D(q) c_{k+q,\sigma}^\dagger c_{k\sigma} n_q^{1/2}}{E(k + q) - E(k) - \hbar\omega_q} \,. \tag{1.86}$$

Here, a phonon of wave vector q is absorbed and an electron is scattered from k to $k + q$ at the same time, that is,

$$\langle n_q + 1|S|n_q \rangle = i \sum_{k,\sigma} \frac{D(-q)c^\dagger_{k-q,\sigma}c_{k\sigma}\left(n_q + 1\right)^{1/2}}{E\left(k - q\right) - E(k) - \hbar\omega_q}. \tag{1.87}$$

In Eq. (1.87), a phonon of wave vector q is created and an electron is scattered from k to $k - q$ at the same time.

We are concerned with the effective second-order interaction

$$\frac{i}{2}[H_1, S]$$

and by this we mean the part diagonal in the phonon numbers. (The off-diagonal elements can be transformed away to give still higher-order interactions). We can write

$$\langle n_q|\frac{i}{2}[H_1, S]|n_q \rangle = \frac{i}{2} \sum \{\langle n_q|H_1|n_q \pm 1\rangle\langle n_q \pm 1|S|n_q\rangle$$
$$- \langle n_q|S|n_q \pm 1\rangle\langle n_q \pm 1|H_1|n_q\rangle\}, \tag{1.88}$$

where the intermediate states $|n_q \pm 1\rangle$ are summed over. We write out one term explicitly:

$$\frac{i}{2}\langle n_q|H_1|n_q - 1\rangle\langle n_q - 1|S|n_q\rangle$$

$$= \frac{i}{2} \sum_{k',\sigma'} D(-q)n_q^{1/2}c^\dagger_{k'-q\sigma'}c_{k'\sigma'} \sum_{k,\sigma} \frac{i\,D(q)c^\dagger_{k+q,\sigma}c_{k\sigma}n_q^{1/2}}{E(k + q) - E(k) - \hbar\omega_q}$$

$$= -\frac{1}{2} \sum_{k,k';\sigma,\sigma'} \frac{|D(q)|^2 c^\dagger_{k'-q,\sigma'}c_{k'\sigma'}c^\dagger_{k+q\sigma}c_{k\sigma}}{E(k + q) - E(k) - \hbar\omega_q}, \tag{1.89}$$

where $D(-q) = D^*(q)$. Callaway's Eq. (7.8.5) [6] states that the four terms combine to give

$$H_1 = \sum_{k,k',q;\sigma,\sigma'} \frac{|D(q)|^2\hbar\omega_q}{[E(k) - E(k - q)]^2 - \left(\hbar\omega_q\right)^2}$$
$$\times c^\dagger_{k-q\sigma}c^\dagger_{k'+q\sigma'}c_{k'\sigma'}c_{k\sigma}. \tag{1.90}$$

With the replacement $k \to k + q$, we get

$$H_1 = \sum_{k,k',q;\sigma,\sigma'} \frac{|D(q)|^2\hbar\omega_q}{[E(k + q) - E(k)]^2 - (\hbar\omega_q)^2}$$
$$\times c^\dagger_{k\sigma}c^\dagger_{k'+q\sigma'}c_{k'\sigma'}c_{k+q\sigma}. \tag{1.91}$$

Note that the effective Hamiltonian is independent of temperature. For $E(k) - E(k - q) < \hbar\omega_q$, the interaction becomes attractive.

An alternate derivation of the above H_1 is obtained in a semiclassical way by Rickayzen [7, p. 117–121], by considering an electron fluid and an ion fluid and retarded interactions between the two components.

We will be dealing with systems of many interacting particles and, as a result, we need to include the inter-particle potential in the Schrödinger equation. This problem is the basis of the present book. The *N*-particle wave function in configuration space contains all the possible information. However, a direct solution of the Schrödinger equation is not practical. We therefore need other techniques which involve (a) second quantization, (b) quantum field theory, and (c) Green's functions.

Second quantization describes the creation and annihilation of particles and quantum statistics as well as simplifying the problem of many interacting particles. This approach reformulates the Schrödinger equation. The advantage it has is that we avoid the awkward use of symmetrized and anti-symmetrized product of single-particle wave functions. With the method of quantum field theory, we avoid dealing with the wave functions and thus the coordinates of all the particles – bosons and fermions.

Green's functions can be used to calculate many physical quantities such as (1) the ground state energy, (2) thermodynamic functions, (3) the energy and lifetime of excited states, and (4) linear response to external perturbations. The exact Green's functions are also difficult to calculate which means we must use perturbation theory. This is presented with the use of Feynman diagrams. This approach allows us to calculate physical quantities to any order of perturbation theory. We use functional derivative techniques in the perturbation expansion of the Green's function determined by the Dyson equation and show that only linked diagrams contribute. Wick's theorem which forms all possible pairs of the field operators is not used in this approach.

1.8
Degenerate Electron Gases

We now illustrate the usefulness of the second quantization representation by applying it to obtain some qualitative results for a metal. The simple model we use is that of an interacting electron gas with a uniform positive background so that the total system is neutral. We ignore the motion of the ions/positive charge. We do not consider any surface effects by restricting our attention to the bulk medium. We insert the system into a large box of side L and apply periodic boundary conditions; this ensures invariance under spatial translations of all physical quantities. The single-particle states are plane waves

$$\varphi_{k,\lambda}\left(x\right) = \frac{1}{L^{3/2}} e^{i k \cdot x} \eta_\lambda , \quad \eta\!\uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \eta\!\downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{1.92}$$

where $k_i = 2\pi n_i/L$, $n_i = 0, \pm 1, \pm 2, \ldots$ The total Hamiltonian is

$$H = H_e + H_{e-b} + H_b , \tag{1.93}$$

where

$$H_e = \sum_{i=1}^{N} \frac{p_i^2}{2m^*} + \frac{e^2}{2} \sum_{\substack{i \neq j=1}}^{N} \frac{e^{-\kappa|x_i - x_j|}}{|x_i - x_j|} \,, \tag{1.94}$$

$$H_b = \frac{e^2}{2} \int d^3x \int d^3x' \frac{n(x)\, n(x')}{|x - x'|} e^{-\kappa|x - x'|} \,, \tag{1.95}$$

$$H_{e-b} = -e^2 \sum_{i=1}^{N} \int d^3x\, n(x) \frac{e^{-\kappa|x - x_i|}}{|x - x_i|} \,. \tag{1.96}$$

Here, κ is the inverse screening length required for convergence of the integrals. Individual integrals diverge in the thermodynamic limit $N \to \infty$, $\mathcal{V} \to \infty$ but $n = N/\mathcal{V}$ is a constant. The sum of the three terms must however remain meaningful in this limit. For a uniform positive background $n(x) = N/\mathcal{V}$, we have

$$\begin{aligned}
H_b &= \frac{e^2}{2} \left(\frac{N}{\mathcal{V}}\right)^2 \int d^3x \int d^3x' \frac{e^{-\kappa|x - x'|}}{|x - x'|} \\
&= \frac{e^2}{2} \left(\frac{N}{\mathcal{V}}\right)^2 \int d^3x \int d^3x'' \frac{e^{-\kappa x''}}{x''} \\
&= \frac{e^2}{2} \frac{N^2}{\mathcal{V}} \frac{4\pi}{\kappa^2} \,,
\end{aligned} \tag{1.97}$$

$$\begin{aligned}
H_{e-b} &= -e^2 \sum_{i=1}^{N} \left(\frac{N}{\mathcal{V}}\right) \int d^3x \frac{e^{-\kappa|x - x_i|}}{|x - x_i|} \\
&= -e^2 \sum_{i=1}^{N} \left(\frac{N}{\mathcal{V}}\right) \int d^3x \int d^3x'' \frac{e^{-\kappa x''}}{x''} \\
&= -e^2 \frac{N^2}{\mathcal{V}} \frac{4\pi}{\kappa^2} \,.
\end{aligned} \tag{1.98}$$

Therefore, the total Hamiltonian is

$$H = \underbrace{-\frac{e^2}{2} \frac{N^2}{\mathcal{V}} \frac{4\pi}{\kappa^2}}_{\text{a C-number}} + H_e \,. \tag{1.99}$$

Forming a linear combination of the creation and destruction operators as

$$\hat{\psi}(x) = \sum_{k,\lambda} \varphi_{k,\lambda}(x)\, \hat{a}_{k,\lambda} \,, \quad \hat{\psi}^\dagger(x) = \sum_{k,\lambda} \varphi^*_{k,\lambda}(x)\, \hat{a}^\dagger_{k,\lambda} \,, \tag{1.100}$$

we rewrite H_e in second quantized form and the total Hamiltonian is

$$\begin{aligned}
H = {}&-\frac{e^2}{2} \frac{N^2}{\mathcal{V}} \frac{4\pi}{\kappa^2} + \sum_{k,\lambda} \frac{\hbar^2 k^2}{2m^*} \hat{a}^\dagger_{k,\lambda} \hat{a}_{k,\lambda} \\
&+ \frac{e^2}{2\mathcal{V}} \sum_{k_1,\lambda_1} \sum_{k_2,\lambda_2} \sum_{k_3,\lambda_3} \sum_{k_4,\lambda_4} \delta_{\lambda_1,\lambda_3} \delta_{\lambda_2,\lambda_4} \delta_{k_1+k_2,k_3+k_4} \\
&\times \frac{4\pi}{|k_1 - k_3|^2 + \kappa^2} \hat{a}^\dagger_{k_1,\lambda_1} \hat{a}^\dagger_{k_2,\lambda_2} \hat{a}_{k_4,\lambda_4} \hat{a}_{k_3,\lambda_3} \,.
\end{aligned} \tag{1.101}$$

By changing variables in the potential energy term to k, p and q, where $k_1 = k + q$, $k_2 = p - q$, $k_3 = k$ and $k_4 = p$, it becomes

$$
\begin{aligned}
\text{P.E.} &= \frac{e^2}{2\mathcal{V}} \sum_{k,p,q} \sum_{\lambda_1,\lambda_2} \frac{4\pi}{q^2 + \kappa^2} \hat{a}^\dagger_{k+q,\lambda_1} \hat{a}^\dagger_{p-q,\lambda_2} \hat{a}_{p,\lambda_2} \hat{a}_{k,\lambda_1} \\
&= \frac{e^2}{2\mathcal{V}} \sum_{k,p,q \neq 0} \sum_{\lambda_1,\lambda_2} \frac{4\pi}{q^2 + \kappa^2} \hat{a}^\dagger_{k+q,\lambda_1} \hat{a}^\dagger_{p-q,\lambda_2} \hat{a}_{p,\lambda_2} \hat{a}_{k,\lambda_1} \\
&\quad + \underbrace{\frac{e^2}{2\mathcal{V}} \sum_{k,p} \sum_{\lambda_1,\lambda_2} \frac{4\pi}{\kappa^2} \hat{a}^\dagger_{k,\lambda_1} \hat{a}^\dagger_{p,\lambda_2} \hat{a}_{p,\lambda_2} \hat{a}_{k,\lambda_1}}_{\frac{e^2}{2\mathcal{V}} \frac{4\pi}{\kappa^2} \sum_{k,\lambda_1} \sum_{p,\lambda_2} \hat{a}^\dagger_{k,\lambda_1} \hat{a}_{k,\lambda_1} \left(\hat{a}^\dagger_{p,\lambda_2} \hat{a}_{p,\lambda_2} - \delta_{kp} \delta_{\lambda_1 \lambda_2} \right)} \quad ,
\end{aligned}
\tag{1.102}
$$

where we separated the potential energy term into two terms corresponding to $q = 0$ and $q \neq 0$. The $q = 0$ term can be further simplified as

$$
\frac{e^2}{2\mathcal{V}} \frac{4\pi}{\kappa^2} \left(\hat{N}^2 - \hat{N} \right) \, ,
\tag{1.103}
$$

where $\hat{N}$ is the number operator. The ground state expectation value of Eq. (1.103) is

$$
\frac{e^2}{2} \frac{N^2}{\mathcal{V}} \frac{4\pi}{\kappa^2} - \frac{e^2}{2} \frac{N}{\mathcal{V}} \frac{4\pi}{\kappa^2} \, ,
\tag{1.104}
$$

where the first term in Eq. (1.104) cancels the first term of the Hamiltonian in Eq. (1.99) and the second term in Eq. (1.104) gives $-(e^2/2)(4\pi/\mathcal{V}\kappa^2)$ as an energy per particle. This second term vanishes when the thermodynamic limit is taken first. Therefore, the Hamiltonian for a bulk electron gas in a uniform positive background is

$$
H = \sum_{k,\lambda} \frac{\hbar^2 k^2}{2m^*} \hat{a}^\dagger_{k,\lambda} \hat{a}_{k,\lambda} + \frac{2\pi e^2}{\mathcal{V}} \sum_{k,p,q = \neq 0} \sum_{\lambda_1,\lambda_2} \frac{1}{q^2} \hat{a}^\dagger_{k+q,\lambda_1} \hat{a}^\dagger_{p-q,\lambda_2} \hat{a}_{p,\lambda_2} \hat{a}_{k,\lambda_1} \, ,
\tag{1.105}
$$

where we have now safely set $\kappa = 0$.

1.9
Ground-State Energy in the High Density Limit

Let us denote the Bohr radius by $a_0 = \hbar^2/m^* e^2$ and the inter-particle spacing by r_0 so that $4/3\pi r_0^3 = \mathcal{V}/N$. Also, set $r_s = r_0/a_0$ so that $r_s \to 0$ in the high density limit.

Setting $\bar{V} = V/r_0^3$ ($\bar{V}$ is fixed for given N) and $\bar{k} = kr_0$, we rewrite Eq. (1.105) as

$$H = \frac{e^2}{a_0 r_s^2} \left\{ \frac{1}{2} \sum_{\bar{k},\lambda} \bar{k}^2 \hat{a}_{\bar{k},\lambda}^\dagger \hat{a}_{\bar{k},\lambda} \right.$$

$$\left. + \frac{2\pi r_s}{\bar{V}} \sum_{\bar{k},\bar{p},\bar{q} \neq 0} \sum_{\lambda_1,\lambda_2} \frac{1}{q^2} \hat{a}_{\bar{k}+\bar{q},\lambda_1}^\dagger \hat{a}_{\bar{p}-\bar{q},\lambda_2}^\dagger \hat{a}_{\bar{p},\lambda_2} \hat{a}_{\bar{k},\lambda_1} \right\}. \qquad (1.106)$$

Therefore,

1. The potential energy is a small perturbation of the kinetic energy in the high density limit, that is, $r_s \to 0$, of an electron gas.
2. The leading term of the interaction energy of a high density electron gas can be obtained using first order perturbation theory even though the potential is not weak or short-ranged.
3. The ground state energy is given by

$$E_{GS} = \frac{e^2}{a_0 r_s^2} \left\{ a + br_s + cr_s^2 \ln r_s + dr_s^2 + \cdots \right\}, \qquad (1.107)$$

where a, b and c are numerical constants. As a matter of fact, the "a" term corresponds to the ground state energy $E^{(0)}$ of a free Fermi gas, the "b" term gives the first-order energy shift $E^{(1)}$.

It is fairly straightforward to obtain $E^{(0)}$ and $E^{(1)}$, though we need advanced techniques to obtain the coefficients c and d. Denote the Fermi wave vector by $k_F = (3\pi^2 N/V)^{1/3} = (9\pi/4)^{1/3} r_s^{-1}$ so that

$$E^{(0)} = \frac{\hbar^2}{2m^*} \sum_{k,\lambda} k^2 \theta \left(k_F - k \right) = \frac{\hbar^2}{2m^*} \cdot 2 \cdot \frac{V}{(2\pi)^3} \int d^3k \, k^2 \theta \left(k_F - k \right)$$

$$= \frac{e^2}{2a_0} \frac{N}{r_s^2} \frac{3}{5} \left(\frac{9\pi}{4} \right)^{2/3},$$

$$(1.108)$$

where $\theta(x)$ is the unit step function. Thus, for a free Fermi gas, the ground state energy per particle is $E^{(0)}/N = 2.21/r_s^2$ Ry where $e^2/2a_0 = 13.6$ eV is 1 Ry. We now calculate the first-order correction to $E^{(0)}$, that is,

$$E^{(1)} = \frac{2\pi e^2}{V} \sum_{k,p,q \neq 0} \sum_{\lambda_1,\lambda_2} \frac{1}{q^2} \langle g | \hat{a}_{k+q,\lambda_1}^\dagger \hat{a}_{p-q,\lambda_2}^\dagger \hat{a}_{p,\lambda_2} \hat{a}_{k,\lambda_1} | g \rangle, \qquad (1.109)$$

where $|g\rangle$ is the ground state for non-interacting electrons. The states (k, λ_1) and (p, λ_2) must be occupied, and the states $(k + q, \lambda_1)$ and $(p - q, \lambda_2)$ must also be occupied. Therefore, we must have either

$$\text{either (a)} \begin{cases} (k + q, \lambda_1) = (k, \lambda_1) \\ (p - q, \lambda_2) = (p, \lambda_2) \end{cases} \text{or (b)} \begin{cases} (k + q, \lambda_1) = (p, \lambda_2) \\ (p - q, \lambda_2) = (k, \lambda_1) \end{cases}. \qquad (1.110)$$

The choice given as (a) is forbidden since $q \neq 0$ and the matrix element in Eq. (1.109) is

$$
\begin{aligned}
\langle g | \cdots | g \rangle &= \delta_{p,k+q} \delta_{\lambda_1 \lambda_2} \langle g | \hat{a}^\dagger_{k+q,\lambda_1} \hat{a}^\dagger_{k,\lambda_1} \hat{a}_{k+q,\lambda_1} \hat{a}_{k,\lambda_1} | g \rangle \\
&= -\delta_{p,k+q} \delta_{\lambda_1 \lambda_2} \langle g | \hat{n}_{k+q,\lambda_1} \hat{n}_{k,\lambda_1} | g \rangle \\
&= -\delta_{p,k+q} \delta_{\lambda_1 \lambda_2} \theta \left(k_F - k \right) \theta \left(k_F - |k + q| \right),
\end{aligned} \tag{1.111}
$$

so that

$$
\begin{aligned}
E^{(1)} &= -\frac{2 \pi e^2}{\mathcal{V}} \sum_\lambda \sum_{k,q \neq 0} \frac{1}{q^2} \theta \left(k_F - k \right) \theta \left(k_F - |k + q| \right) \\
&= -\frac{e^2}{2 a_0} \frac{N}{r_s} \frac{3}{2 \pi} \left(\frac{9 \pi}{4} \right)^{1/3}.
\end{aligned} \tag{1.112}
$$

Thus, by combining the results for $E^{(0)}$ and $E^{(1)}$, we obtain the energy per particle in the limit as $r_s \to 0$ to be given by

$$
\lim_{r_s \to 0} \frac{E_{GS}}{N} \approx \frac{e^2}{2 a_0} \left\{ \frac{2.21}{r_s^2} - \frac{0.916}{r_s} + \cdots \right\}. \tag{1.113}
$$

The first term is the kinetic energy of the Fermi gas of electrons and dominates in the high density limit. The second term is the exchange energy term. It is negative and arises from the antisymmetry of the wave function. The direct part arises from the $q = 0$ part of the Hamiltonian and cancels the $H_b + H_{e-b}$ terms as a result of charge neutrality.

The exchange term is not the total that arises from the electron–electron interaction. All that is left out is called the correlation energy. The leading contribution to the correlation energy of the degenerate electron gas will be obtained using Feynman graph techniques. However, we note that E_{GS}/N has a minimum at a negative value of the energy, that is, the system is bound, as shown in Figure 1.2. The Rayleigh–Ritz variational principle tells us that the exact ground state energy of a quantum mechanical system always has a lower energy than that evaluated using a normalized state for the expectation value of the Hamiltonian. The exact solution must also be that for a bound system with energy below our approximate solution and the binding energy is that of vaporization for metals.

1.10
Wigner Solid

The energy of the Fermi gas can be lowered if the electrons crystallize into a Wigner solid. The range of values of r_s for metals is $1.8 \lesssim r_s \lesssim 6.0$. At low densities, Wigner suggested that the electrons will become localized and form a regular lattice. This lattice could be a closed packed structure such as bcc, fcc or hcp. The electrons would vibrate around their equilibrium positions and the positive charge
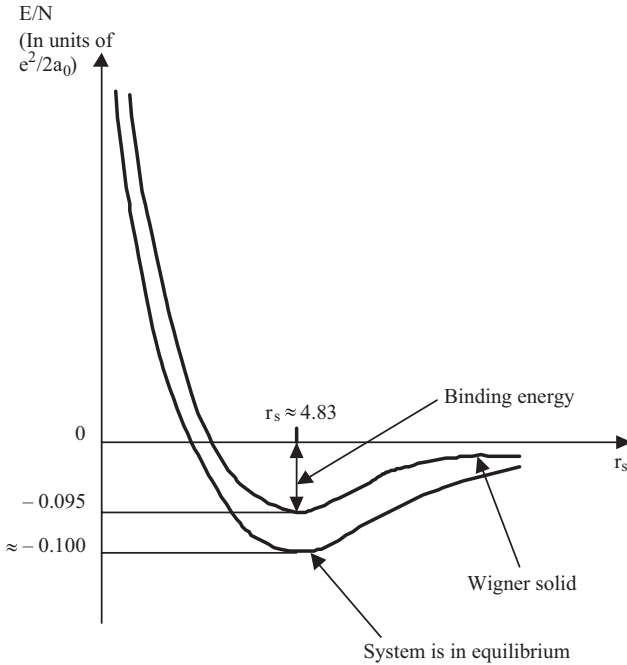
E/N
(In units of
$e^2/2a_0$)

$r_s \approx 4.83$

Binding energy

0

-0.095

≈ -0.100

r_s

Wigner solid

System is in equilibrium

Figure 1.2 The energy per particle as a function of a dimensionless density parameter r_s, where $r_s \to 0$ corresponds to the high density limit, while $r_s \to \infty$ corresponds to the low density limit.

is still spread out in the system. The vibrational modes of the electrons would be at the plasmon frequency. For large r_s, the potential energy is much larger than the kinetic energy and there could be localization. In our discussion, the unit cell is taken as a sphere of radius $r_s a_0$ with the electron at the center. The total charge within the sphere is zero. Outside each sphere, the electric field is zero and consequently the spheres do not exert any electric fields on each other.

The potential energy between the electron and the uniform positive background is

$$E_{e-b} = n \int d^3\mathbf{r} \left(\frac{-e^2}{r} \right) = -\frac{3e^2}{r_s^3 a_0^3} \int\limits_0^{r_s a_0} r\, dr = -\frac{3}{r_s} \left(\frac{e^2}{2a_0} \right). \tag{1.114}$$

The potential energy due to the interaction of the positive charge with itself is obtained as follows. Let $V(r)$ be the potential energy from the positive charge at distance r from the center. The electric field is $E(r)$ where

$$e\, E(r) = -\frac{\partial V(r)}{\partial r} = \frac{e^2}{r^2} n \left(\frac{4}{3}\pi r^3 \right) = \left(\frac{e^2}{r_s^3 a_0^3} \right) r. \tag{1.115}$$

Integrating to obtain $V(r)$ gives a constant of integration. This is obtained by observing that the total potential from the electron and positive charge must vanish

on the surface of the sphere and we obtain

$$V(r) = \frac{1}{r_s}\left[3 - \left(\frac{r}{r_s a_0}\right)^2\right]\frac{e^2}{2 a_0} \, . \tag{1.116}$$

The interaction of the positive charge with itself is found by using

$$E_{b-b} = \frac{n}{2}\int d^3 r\, V(r) = \frac{6}{5 r_s}\left(\frac{e^2}{2 a_0}\right). \tag{1.117}$$

Therefore, the total potential energy for the Wigner lattice in the Wigner–Seitz approximation is

$$E_{e-b} + E_{b-b} = -\frac{1.8}{r_s}\left(\frac{e^2}{2 a_0}\right) \, . \tag{1.118}$$

This is larger than the exchange contribution for the free particle system. This system has gained energy by the localization of the electrons. Stroll has calculated the actual energy for several lattices. His results, expressed as $-A/r_s$, in unit of $(e^2/2 a_0)$ are given as follows:

Lattice	A
sc	1.76
fcc	1.79175
bcc	1.79186
hcp	1.79168

1.11
The Chemical Potential of an Ideal Bose Gas and Bose–Einstein Condensation

For non-interacting bosons of energy $\varepsilon_k = \hbar^2 k^2/2 m^*$, the total number at temperature T ($\beta = 1/(k_B T)$) is

$$\frac{N}{V} = \frac{g}{(2\pi)^3}\int\limits_0^\infty dk\, 4\pi k^2 \frac{1}{e^{\beta(\varepsilon_k - \mu)} - 1}$$

$$= \frac{g}{4\pi^2}\left(\frac{2 m^*}{\hbar^2}\right)^{3/2}\int\limits_0^\infty d\varepsilon \frac{\varepsilon^{1/2}}{e^{\beta(\varepsilon - \mu)} - 1} \, , \tag{1.119}$$

where g is the degeneracy and μ is the chemical potential. We must have $\varepsilon - \mu \geq 0$ since the mean occupation number must be positive for all energies. However, since we can have $\varepsilon = 0$, then $\mu \leq 0$. If a classical limit is taken with

$$\frac{\mu}{k_B T} \to -\infty \, , \tag{1.120}$$

then we get

$$\frac{N}{\mathcal{V}} \to \frac{g}{4\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{3/2} \int\limits_0^\infty d\varepsilon\, \varepsilon^{1/2} e^{\beta(\mu-\varepsilon)}$$

$$= g e^{\beta\mu} \left(\frac{m^* k_B T}{2\pi\hbar^2} \right)^{3/2}, \tag{1.121}$$

which is the result of the Boltzmann distribution, where $\int_0^\infty dx\, x^2 e^{-x^2} = \sqrt{\pi}/4$ is used. Solving this equation for μ, we obtain

$$\frac{\mu}{k_B T} = \ln\left[\frac{N}{g\mathcal{V}} \left(\frac{2\pi\hbar^2}{m^* k_B T} \right)^{3/2} \right]. \tag{1.122}$$

A plot of this classical result is shown in Figure 1.3.

If T_0 is the temperature where $\mu = 0$, then Eq. (1.119) gives

$$\frac{N}{\mathcal{V}} = \frac{g}{4\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{3/2} \int\limits_0^\infty d\varepsilon \frac{\varepsilon^{1/2}}{e^{\varepsilon/(k_B T_0)} - 1}. \tag{1.123}$$

The question which we now answer is what is the value of μ for $T < T_0$. If $\mu = 0$ for $T < T_0$, the integral in Eq. (1.119) is less than $N/\mathcal{V}$ in Eq. (1.123) because the value of the denominator is increased relative to its value at T_0 and the full value of $N/\mathcal{V}$ will not be reproduced. This can be rectified if we treat the system as follows. Below T_0, the system consists of two components: (1) particles occupying the zero momentum state with a mean occupation number N_0, and (2) particles occupying the excited state. This leads to

$$\frac{N}{\mathcal{V}} = \frac{N_0}{\mathcal{V}} + \frac{g}{4\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{3/2} \int\limits_{0+}^\infty d\varepsilon \frac{\varepsilon^{1/2}}{e^{\varepsilon/k_B T} - 1}, \tag{1.124}$$

which gives $N_0/\mathcal{V} = (N/\mathcal{V})[1 - (T/T_0)^{3/2}]$ for $T < T_0$. Experimentally, it has been found that liquid He^4 has a phase transition at 2.2 K. Below that temperature, it acts
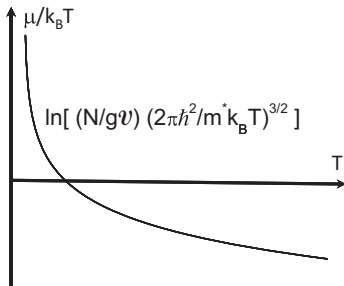

Figure 1.3 $\mu/(k_B T) = \ln[(N/g\mathcal{V})(2\pi\hbar^2/(m^* k_B T))^{3/2}]$ of a Bose gas as a function of T for fixed $N/\mathcal{V}$ in the classical limit.

like a mixture of superfluid and normal fluid. This discussion illustrates the Bose–Einstein condensation of the ideal Bose gas and thus gives a qualitative description of He^4. Inter-particle interactions play a key role in the properties of quantum fluids such as liquid He^4.

1.12
Problems

1. Show that

    $$\left[\psi\left(x\right), \psi^{\dagger}\left(x'\right)\psi\left(x''\right)\right] = \delta\left(x - x'\right)\psi\left(x''\right)$$
    $$\left[\psi^{\dagger}(x), \psi^{\dagger}\left(x'\right)\psi\left(x''\right)\right] = -\delta\left(x - x''\right)\psi^{\dagger}\left(x'\right),$$

    where $\psi\left(x\right)$ is a Boson field or a fermion field.

2. Show that for a fermion field

    $$\left[\psi\left(x\right), \psi^{\dagger}\left(x'\right)\psi^{\dagger}\left(x''\right)\psi\left(x'''\right)\psi\left(x''''\right)\right]$$
    $$= \delta\left(x - x'\right)\psi^{\dagger}\left(x''\right)\psi\left(x'''\right)\psi\left(x''''\right)$$
    $$\quad - \delta\left(x - x''\right)\psi^{\dagger}\left(x'\right)\psi\left(x'''\right)\psi\left(x''''\right)$$

    and

    $$\left[\psi^{\dagger}(x), \psi^{\dagger}\left(x'\right)\psi^{\dagger}\left(x''\right)\psi\left(x'''\right)\psi\left(x''''\right)\right]$$
    $$= \delta\left(x - x'''\right)\psi^{\dagger}\left(x'\right)\psi^{\dagger}\left(x''\right)\psi\left(x''''\right)$$
    $$\quad - \delta\left(x - x''''\right)\psi^{\dagger}\left(x'\right)\psi^{\dagger}\left(x''\right)\psi\left(x'''\right).$$

3. Show that for fermions

    $$[a_{k'}a_{k''}, a^{\dagger}_{k'''}a_{k''''}]_{-} = \delta\left(k'' - k'''\right)a_{k'}a_{k''''} - \delta\left(k' - k'''\right)a_{k''}a_{k''''}.$$

4. a) Starting with the commutation relation $[a, a^{\dagger}] = 1$ for bosonic creation $a^{\dagger}$ and annihilation a operators, show that

    $$\left[a^{\dagger}a, a\right] = -a, \quad \left[a^{\dagger}a, a^{\dagger}\right] = a^{\dagger}.$$

    Using this result, show that if $|\alpha\rangle$ represents an eigenstate of the operator $a^{\dagger}a$ with eigenvalue α, $a|\alpha\rangle$ is also an eigenstate with eigenvalue $\alpha - 1$ (unless $a|\alpha\rangle = 0$).

    b) If $|\alpha\rangle$ represents a normalized eigenstate of the operator $a^{\dagger}a$ with eigenvalue α for all $\alpha \geq 0$, show that

    $$a|\alpha\rangle = \sqrt{\alpha}|\alpha - 1\rangle, \quad a^{\dagger}|\alpha\rangle = \sqrt{\alpha + 1}|\alpha + 1\rangle.$$

    Defining the normalized vacuum state $|\Omega\rangle$ as the normalized state that is annihilated by the operator a, show that $|n\rangle = (1/\sqrt{n!})(a^{\dagger})^{n}|\Omega\rangle$ is a normalized eigenstate of $a^{\dagger}a$ with eigenvalue n.

c) Assuming the operators a and $a^\dagger$ obey Fermionic anti-commutation relations, repeat parts (a) and (b).

5. Starting from first principles, show that the second quantized representation of the one-body kinetic energy operator is given by

$$\hat{T} = \int_0^L dx\, a^\dagger(x) \frac{p^2}{2m^*} a(x) \,.$$

Hint: Remember that the representation is most easily obtained from the basis in which the operator is diagonal.

6. Transforming to the Fourier basis, diagonalize the non-interacting three-dimensional cubic lattice tight-binding Hamiltonian

$$\hat{\mathcal{H}}^{(0)} = -\sum_{(m,n)} t_{mn,\sigma} c^\dagger_{m\sigma} c_{n\sigma} \,,$$

where the matrix elements t_{mn} take the positive real value t between neighboring sites and zero otherwise. Comment on how this result compares with the spectrum of the Heisenberg ferromagnet.

7. Making use of the Pauli matrix identity $\sigma_{\alpha\beta} \cdot \sigma_{\gamma\delta} = 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta}$, where "·" denotes the scalar or dot product, prove that

$$\hat{S}_m \cdot \hat{S}_n = -\frac{1}{2} \sum_{\alpha,\beta} c^\dagger_{m\alpha} c^\dagger_{n\beta} c_{m\beta} c_{n\alpha} - \frac{1}{4} \hat{n}_m \hat{n}_n \,,$$

where $\hat{S}_m = 1/2 \sum_{\alpha,\beta} c^\dagger_{m\alpha} \sigma_{\alpha\beta} c_{m\beta}$ denotes the spin operator and $\hat{n}_m = \sum_\alpha c^\dagger_{m\alpha} c_{m\beta}$ represents the total number operator on site m. (Here, assume that lattice sites m and n are distinct.)

8. Starting with the definition

$$\hat{S}^- = (2S)^{1/2} a^\dagger \left(1 - \frac{a^\dagger a}{2S}\right)^{1/2} \,,$$

confirm the validity of the Holstein–Primakoff transformation by explicitly checking the commutation relations of spin raising and lowering operators.

9. **Frustration**: On a bipartite lattice (i.e., one in which the neighbors of one sublattice belong to the other sublattice), the ground state (known as a Néel state) of a classical antiferromagnet can adopt a staggered spin configuration in which the exchange energy is maximized. Lattices which cannot be classified in this way are said to be frustrated – the maximal exchange energy associated with each bond cannot be recovered. Using only symmetry arguments, specify one of the possible ground states of a classical three-site triangular lattice antiferromagnet. (Note that the invariance of the Hamiltonian under a global

rotation of the spins means that there is a manifold of continuous degeneracy in the ground state.) Using the result, construct one of the classical ground states of the infinite triangular lattice.

10. Confirm that the bosonic commutation relations of the operators a and $a^\dagger$ are preserved by the Bogoliubov transformation,

$$\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} = \begin{pmatrix} \cosh\theta & \sinh\theta \\ \sinh\theta & \cosh\theta \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix}.$$

11. a) Making use of the spin commutation relation, $[S_i^\alpha, S_j^\beta] = i\delta_{ij}\varepsilon^{\alpha\beta\gamma}S_i^\gamma$, apply the identity to express the equation of motion of a spin in a nearest-neighbor spin S one-dimensional Heisenberg ferromagnet as a difference equation.

    b) Interpreting the spins as classical vectors and taking the continuum limit, show that the equation of motion of the *hydrodynamic modes* takes the form

    $$\hbar\dot{S} = Ja^2 S \times \partial^2 S,$$

    where a denotes the lattice spacing. (Hint: Going to the continuum limit, apply a Taylor expansion to the spins, i.e., $S_{i+1} = S_i + a\partial S_i + a^2\partial^2 S_i/2 + \cdots$)

    c) Parameterizing the spin as

    $$S = \left(C\cos(kx - \omega t), C\sin(kx - \omega t), \sqrt{S^2 - C^2} \right),$$

    solve the equation. Sketch a "snapshot" configuration of the spins in a spin chain.

12. **Valence bond solid**: Starting with the spin-1/2 Majumdar–Ghosh Hamiltonian

    $$\hat{H}_{\mathrm{MG}} = \frac{4|J|}{3} \sum_{n=1}^{N} \left(\hat{S}_n \cdot \hat{S}_{n+1} + \frac{1}{2}\hat{S}_n \cdot \hat{S}_{n+2} \right) + \frac{N}{2},$$

    where the total number of states N is even and $\hat{S}_{N+1} = \hat{S}_1$, show that the two-dimer or valence bond states

    $$|0_+\rangle = \prod_{n=1}^{N/2} \frac{1}{\sqrt{2}} \left(|\uparrow_{2n}\rangle \otimes |\downarrow_{2n\pm1}\rangle - |\downarrow_{2n}\rangle \otimes |\uparrow_{2n\pm1}\rangle \right)$$

    are exact eigenstates. (Hint: Try to recast the Hamiltonian in terms of the total spin of a triad $\hat{J}_n = \hat{S}_{n+1} + \hat{S}_n + \hat{S}_{n-1}$ and consider what this representation implies.) In fact, these states represent the ground states of the Hamiltonian. Suggest what would happen if the total number of states was odd.

13. **Su–Schrieffer–Heeger model** of conducting polymers: Polyacetylene consists of bonded CH groups forming an isomeric long chain polymer. According to molecular orbital theory, the carbon atoms are expected to be sp^2 hybridized

suggesting a planar configuration of the molecule. An unpaired electron is expected to occupy a single *p*-orbital which points out of the plane. The weak overlap of the *p*-orbitals delocalizes the electrons into a π-conduction band. Therefore, according to the nearly-free electron theory, one might expect the half-filled conduction band of a polyacetylene chain to be metallic. However, the energy of a half-filled band of a one-dimensional system can always be lowered by applying a periodic lattice distortion known as the *Peierls instability*. One can think of an enhanced probability of finding the π electron on the short bond where the orbital overlap is stronger than the "the double bond". The aim of this problem is to explore the instability.

a) At its simplest level, the conduction band of polyacetylene can be modeled by a simple Hamiltonian, due to Su, Schrieffer and Heeger, in which the hopping matrix elements of the electrons are modulated by the lattice distortion of the atoms. Taking the displacement of the atomic sites from the equilibrium from the equilibrium separation $a \equiv 1$ to be unity, and treating their dynamics as classical, the effective Hamiltonian takes the form

$$\hat{H} = -t \sum_{n=1}^{N} \sum_{\sigma} (1 + u_n) \left[c_{n\sigma}^{\dagger} c_{n+1\sigma} + \text{h.c.} \right] + \sum_{n=1}^{N} \frac{k_s}{2} (u_{n+1} - u_n)^2 \,,$$

where, for simplicity, the boundary conditions are taken to be periodic. The first term describes the hopping of electrons between neighboring sites with a matrix element modulated by the periodic distortion of the bond length, while the last term represents the associated increase in the elastic energy. Taking the lattice distortion to be periodic, $u_n = (-1)^n \alpha$, and the number of sites to be even, diagonalize the Hamiltonian. (Hint: The lattice distortion lowers the symmetry of the lattice. The Hamiltonian is most easily diagonalized by distinguishing the two sites of the sublattice, i.e., doubling the size of the elementary unit cell, and transforming to the Fourier representation.) Show that the Peierls distortion of the lattice opens a gap in the spectrum at the Fermi level of the half-filled system.

b) By estimating the total electronic and elastic energy of the half-filled band, that is, an average of one electron per lattice site, show that the one-dimensional system is always unstable towards the Peierls distortion. To do this calculation, you will need the approximate formula for the elliptic integral,

$$\int_{-\pi/2}^{\pi/2} dk \sqrt{1 - (1 - \alpha^2) \sin^2 k} \approx 2 + \left(a_1 - b_1 \ln \alpha^2 \right) \alpha^2 \,,$$

where a_1 and b_1 are unspecified numerical constants.

c) For an even number of sites, the Peierls instability has two degenerate configurations – ABABAB$\cdots$ and BABABA$\cdots$ Comment on the qualitative form of the ground state lattice configuration if the number of sites is odd. Explain why such configurations give rise to mid-gap states.

14. In the Schwinger boson representation, the quantum mechanical spin is expressed in terms of two bosonic operators a and b in the form

$$\hat{S}^+ = a^\dagger b , \quad \hat{S}^- = \left(\hat{S}^+\right)^\dagger , \quad \hat{S}^z = \frac{1}{2}\left(a^\dagger a - b^\dagger b\right) .$$

   a) Show that this definition is consistent with the commutation relations for spin: $[\hat{S}^+, \hat{S}^-] = 2\hat{S}^z$.

   b) Using the bosonic commutation relations, show that

$$|S, m\rangle = \frac{\left(a^\dagger\right)^{S+m}}{\sqrt{(S+m)!}} \frac{\left(b^\dagger\right)^{S-m}}{\sqrt{(S-m)!}}|\Omega\rangle$$

   is compatible with the definition of an eigenstate of the total spin operator S^2 and S^z. Here, $|\Omega\rangle$ denotes the vacuum of the Schwinger bosons, and the total spin S defines the physical subspace

$$\{|n_a, n_b\rangle : n_a + n_b = 2S\} .$$

15. **The Jordan–Wigner transformation**: So far, we have shown how the algebra of quantum mechanical spin can be expressed using boson operators, c.f., the Holstein–Primakoff transformation and the Schwinger representation. In this problem, we show that a representation for spin 1/2 can be obtained in terms of Fermion operators. Specifically, let us formally represent an up-spin as a particle and a down-spin as the vacuum $|0\rangle$, namely,

$$|\uparrow\rangle \equiv |1\rangle = f^\dagger(0) ,$$
$$|\downarrow\rangle \equiv |0\rangle = f(1) .$$

   In this representation, the spin raising and lowering operators are expressed in the form $\hat{S}^+ = f^\dagger$ and $\hat{S}^- = f$, while $\hat{S}^z = f^\dagger f - 1/2$.

   a) With this definition, confirm that the spins obey the algebra $[\hat{S}^+, \hat{S}^-] = 2\hat{S}^z$. However, there is a problem, that is, spins on different sites commute while fermion operators anticommute, for example,

$$\hat{S}_i^+ \hat{S}_j^+ = \hat{S}_j^+ \hat{S}_i^+ , \quad \text{but} \quad f_i^\dagger f_j^\dagger = -f_j^\dagger f_i^\dagger .$$

   To obtain a faithful spin representation, it is necessary to cancel this unwanted sign. Although a general procedure is hard to formulate in one dimension, this can be achieved by a nonlinear transformation, that is,

$$\hat{S}_l^+ = f_l^\dagger e^{i\pi \sum_{j<l} \hat{n}_j} , \quad \hat{S}_l^- = e^{-i\pi \sum_{j<l} \hat{n}_j} f_l , \quad \hat{S}_l^z = f_l^\dagger f_l - \frac{1}{2} .$$

   Operationally, this seemingly complicated transformation is straightforward; in one dimension, the particles can be ordered on the line. By counting the number of particles "to the left", we can assign an overall phase of $+1$ or -1 to a given configuration and thereby transmute the particles into fermions. (Put differently, the exchange to two fermions induces a sign change which is compensated by the factor arising from the phase – the "Jordan–Wigner string".)

b) Using the Jordan–Wigner representation, show that

$$\hat{S}_m^+ \, \hat{S}_{m+1}^- = f_m^\dagger \, f_{m+1} \, .$$

c) For the spin 1/2 anisotropic quantum Heisenberg spin chain, the spin Hamiltonian assumes the form

$$\hat{H} = -\sum_n \left[J_z \hat{S}_n^z \hat{S}_{n+1}^z + \frac{J_\perp}{2} \left(\hat{S}_n^+ \hat{S}_{n+1}^- + \hat{S}_n^- \hat{S}_{n+1}^+ \right) \right].$$

Turning to the Jordan–Wigner representation, show that the Hamiltonian can be cast in the form

$$\hat{H} = \sum_n \left[\frac{J_\perp}{2} \left(f_n^\dagger f_{n+1} + \text{h.c.} \right) + J_z \left(\frac{1}{4} - f_n^\dagger f_n + f_n^\dagger f_n f_{n+1}^\dagger f_{n+1} \right) \right].$$

d) The mapping above shows that the one-dimensional quantum spin-1/2 XY-model, that is, $J_z = 0$, can be diagonalized as a non-interacting theory of spinless fermions. In this case, show that the spectrum assumes the form

$$\epsilon(k) = -J_\perp \cos(k a) \, .$$

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