Appendix A
A brief résumé of second quantization

Second quantization provides an economic representation of quantum mechanics which includes automatically the statistics fulfilled by the particles composing the system. This appendix summarizes some of the basic results for fermions and bosons.

A.1 Fermions

Let us consider a system of n identical fermions and let $\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n)$ denote the exact wavefunction of the system. Let us introduce the state $\Phi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n)$, a member of a complete set of n-particle wavefunctions. It is constructed as a properly symmetrized product of one-particle wavefunctions $\varphi_\nu(\vec{r})$, which form a complete orthonormal set

$$\int \varphi_\nu^*(\vec{r})\, \varphi_{\nu'}(\vec{r})\, \mathrm{d}^3 r = \delta(\nu, \nu'), \tag{A.1}$$

$$\sum_\nu \varphi_\nu^*(\vec{r}\,')\, \varphi_\nu(\vec{r}) = \delta(\vec{r} - \vec{r}\,'). \tag{A.2}$$

The function $\Phi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n)$, in the case of fermions, is given by the determinant of the single-particle wavefunctions

$$\Phi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_n) = \frac{\det}{\sqrt{n!}}(\varphi_{\nu_1}(\vec{r}_1)\varphi_{\nu_2}(\vec{r}_2)\cdots\varphi_{\nu_n}(\vec{r}_n)). \tag{A.3}$$

The function Ψ is thus a linear combination of determinants.

We now introduce the creation and annihilation fermion operators $a_\nu^\dagger$ and a_ν respectively, acting on the fermion vacuum state $|0\rangle_\mathrm{F}$. These operators satisfy the anticommutation relations

$$\{a_\nu, a_{\nu'}^\dagger\} = a_\nu a_{\nu'}^\dagger + a_{\nu'}^\dagger a_\nu = \delta(\nu, \nu') \tag{A.4}$$

and

$$\{a_\nu, a_{\nu'}\} = \{a_\nu^\dagger, a_{\nu'}^\dagger\} = 0. \tag{A.5}$$

https://doi.org/10.1017/9781009401920.013 Published online by Cambridge University Press

This choice restricts the occupation number of the states ν to 0 or 1 as required by Fermi statistics and to antisymmetric normalized states. Acting with the creation operator $a_j^\dagger$ on the vacuum one creates a single-particle state

$$a_j^\dagger |0\rangle_{\mathrm{F}} = |j\rangle, \tag{A.6}$$

where the r-representation coincides with the single-particle wavefunction

$$\langle \vec{r}\,|\, j\rangle = \varphi_j(\vec{r}).$$

The orthonormalization condition

$$\begin{aligned}\langle j\,|\, j'\rangle &= {}_{\mathrm{F}}\langle 0|a_j a_{j'}^\dagger|0\rangle_{\mathrm{F}} = {}_{\mathrm{F}}\langle 0|\delta(j, j') - a_{j'}^\dagger a_j|0\rangle_{\mathrm{F}} \\ &= \delta(j, j') \equiv {}_{\mathrm{F}}\langle 0|\overbrace{a_j a_{j'}^\dagger}|0\rangle_{\mathrm{F}}\,,\end{aligned} \tag{A.7}$$

where the relation given by equation (A.4) has been used together with

$$a_j|0\rangle_{\mathrm{F}} = 0, \tag{A.8}$$

and

$${}_{\mathrm{F}}\langle 0|0\rangle_{\mathrm{F}} = 1. \tag{A.9}$$

The symbol in the last term of equation (A.7) denotes a contraction. According to Wick's theorem, to calculate overlaps or matrix elements involving $a^\dagger$ and a, one should carry out all possible contractions between creation and annihilation operators, introducing a minus sign each time that in the contraction one jumps over an odd number of operators, and a plus sign otherwise.

A two-particle state in this representation reads

$$a_j^\dagger a_{j'}^\dagger|0\rangle_{\mathrm{F}} = |j, j'\rangle. \tag{A.10}$$

Making use of the anticommutation relation (A.5) one can show that

$$|j, j'\rangle = -|j', j\rangle, \tag{A.11}$$

i.e. the two-particle state is antisymmetric. Consequently,

$$|j, j\rangle = 0, \tag{A.12}$$

i.e. no two fermions can occupy the same quantal state, as required by the Pauli principle.

The orthonormalization condition of the state $|j, j'\rangle$ is given by the relation

$$\langle j_1, j_2|j_1', j_2'\rangle = {}_{\mathrm{F}}\langle 0|\overbrace{a_{j_2}\overbrace{a_{j_1}a_{j_1'}^\dagger}a_{j_2'}^\dagger}|0\rangle_{\mathrm{F}} \tag{A.13}$$

$$= \delta(j_2, j_2')\,\delta(j_1, j_1') - \delta(j_1, j_2')\,\delta(j_1', j_2). \tag{A.14}$$

This result can also be obtained directly without using Wick's theorem by making repeated use of the anticommutation relation given in equation (A.4). Equations (A.11),

https://doi.org/10.1017/9781009401920.013 Published online by Cambridge University Press

(A.12) and (A.14) indicate that

$$\langle \vec{r}, \vec{r}\,' | j_1\, j_2 \rangle = \frac{1}{\sqrt{2}} \begin{vmatrix} \varphi_{j_1}(\vec{r}) & \varphi_{j_2}(\vec{r}) \\ \varphi_{j_1}(\vec{r}\,') & \varphi_{j_2}(\vec{r}\,') \end{vmatrix}. \tag{A.15}$$

Let us now calculate the matrix element of a two-body interaction

$$\begin{aligned} \langle j_1 j_2 | v | j_1' j_2' \rangle_a &= \frac{1}{2} \int \mathrm{d}^3 r\, \mathrm{d}^3 r' \begin{vmatrix} \varphi_{j_1}(\vec{r}) & \varphi_{j_2}(\vec{r}) \\ \varphi_{j_1}(\vec{r}\,') & \varphi_{j_2}(\vec{r}\,') \end{vmatrix}^* v(|\vec{r} - \vec{r}\,'|) \begin{vmatrix} \varphi_{j_1'}(\vec{r}) & \varphi_{j_2'}(\vec{r}) \\ \varphi_{j_1'}(\vec{r}\,') & \varphi_{j_2'}(\vec{r}\,') \end{vmatrix} \\ &= \int \mathrm{d}^3 r\, \mathrm{d}^3 r' \varphi^*_{j_1}(\vec{r})\, \varphi^*_{j_2}(\vec{r}\,') v(|\vec{r} - \vec{r}\,'|) \varphi_{j_1'}(\vec{r})\, \varphi_{j_2'}(\vec{r}\,') \\ &\quad - \int \mathrm{d}^3 r\, \mathrm{d}^3 r' \varphi^*_{j_1}(\vec{r})\, \varphi^*_{j_2}(\vec{r}\,') v(|\vec{r} - \vec{r}\,'|)\, \varphi_{j_2'}(\vec{r})\, \varphi_{j_1'}(\vec{r}\,'). \end{aligned} \tag{A.16}$$

Note that this matrix element changes sign each time two particles are exchanged either in the initial or in the final states. For example,

$$\begin{aligned} \langle j_2 j_1 | v | j_1' j_2' \rangle_a &= \int \mathrm{d}^3 r \mathrm{d}^3 r' \varphi^*_{j_2}(\vec{r}) \varphi^*_{j_1}(\vec{r}\,') v(|\vec{r} - \vec{r}\,'|) \varphi_{j_1'}(\vec{r}) \varphi_{j_2'}(\vec{r}\,') \\ &\quad - \int \mathrm{d}^3 r \mathrm{d}^3 r' \varphi^*_{j_2}(\vec{r}) \varphi^*_{j_1}(\vec{r}\,') v(|\vec{r} - \vec{r}\,'|) \varphi_{j_2'}(\vec{r}) \varphi_{j_1'}(\vec{r}\,') \\ &= \int \mathrm{d}^3 r \mathrm{d}^3 r' \varphi^*_{j_1}(\vec{r}) \varphi^*_{j_2}(\vec{r}\,') v(|\vec{r} - \vec{r}\,'|) \varphi_{j_2'}(\vec{r}) \varphi_{j_1'}(\vec{r}\,') \\ &\quad - \int \mathrm{d}^3 r \mathrm{d}^3 r' \varphi^*_{j_1}(\vec{r}) \varphi^*_{j_2}(\vec{r}\,') v(|\vec{r} - \vec{r}\,'|) \varphi_{j_1'}(\vec{r}) \varphi_{j_2'}(\vec{r}\,') \\ &= -\langle j_1 j_2 | v | j_1' j_2' \rangle_a, \end{aligned}$$

where in going from the first to the second expression one has exchanged $\vec{r}$ to $\vec{r}\,'$. Consequently,

$$\begin{aligned} \langle j_1 j_2 | v | j_1' j_2' \rangle_a &= -\langle j_1 j_2 | v | j_2' j_1' \rangle_a \\ &= -\langle j_2 j_1 | v | j_1' j_2' \rangle_a = \langle j_2 j_1 | v | j_2' j_1' \rangle_a. \end{aligned} \tag{A.17}$$

We now proceed to express operators in second quantization. Because a one-body operator can change, at most, the state of motion of a single particle it must be bilinear in the creation and destruction operators. Similarly, a two-body interaction which can change the state of motion of two particles simultaneously must be a quartic function of the creation and annihilation operators. In particular the Hamiltonian, sum of a kinetic term and a two-body interaction can be written in second quantization as

$$H = \sum_{j_1\, j_2} \langle j_1 | T | j_2 \rangle a^\dagger_{j_1} a_{j_2} + \frac{1}{4} \sum_{\substack{j_1\, j_2 \\ j_3\, j_4}} \langle j_1\, j_2 | v | j_3\, j_4 \rangle_a a^\dagger_{j_2} a^\dagger_{j_1} a_{j_3} a_{j_4}. \tag{A.18}$$

In Fig. A.1 we schematically display the action of the second term on a pair of particles. The matrix element $\langle j_1\, j_2 | v | j_3\, j_4 \rangle_a$ has been defined in equation (A.16).

We now proceed to derive the Hartree–Fock equation associated with H, which means to extract the one-body Hartree–Fock Hamiltonian. For this purpose we have to carry

https://doi.org/10.1017/9781009401920.013 Published online by Cambridge University Press

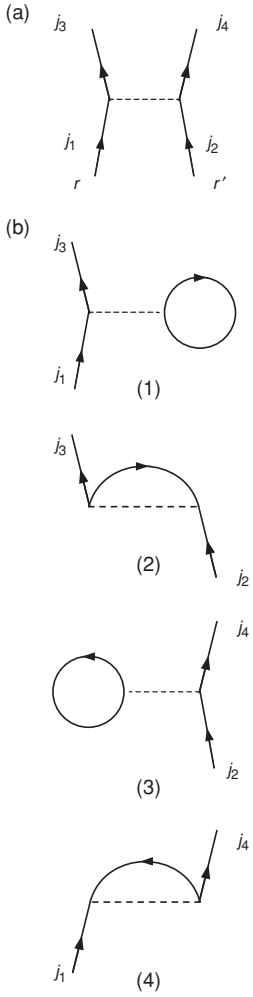

Figure A.1. (a) Scattering of two nucleons through the bare NN interaction. (b) (1) and (3): contributions to the (direct) Hartree potential (see equations (A.20) and (A.22) as well as (A.28)). (2) and (4): contributions to the (exchange) Fock potential (see equations (A.21), (A.23) and (A.30)).

out single contractions in the second term of H. The first term is already bilinear in the creation and annihilation operators. The four possible contractions are

$$\overset{\textcircled{2}}{\overset{\textcircled{1}}{a^\dagger_{j_2} a^\dagger_{j_1} a_{j_3} a_{j_4}}}, \qquad \overset{\textcircled{3}}{\textcircled{4}} \tag{A.19}$$

https://doi.org/10.1017/9781009401920.013 Published online by Cambridge University Press

leading to the four contributions (see Fig. A.1)

$$①= \frac{1}{4}\sum_{j_1\, j_3}\sum_{\substack{i\\(\varepsilon_i \le \varepsilon_F)}} \langle j_1\, i\,|v|\, j_3\, i\rangle_a\, a^\dagger_{j_1}\, a_{j_3}, \tag{A.20}$$

$$②= -\frac{1}{4}\sum_{j_1\, j_4}\sum_{\substack{i\\(\varepsilon_i \le \varepsilon_F)}} \langle j_1 i\,|v|\, i j_4\rangle_a\, a^\dagger_{j_1}\, a_{j_4}, \tag{A.21}$$

$$③= \frac{1}{4}\sum_{j_2\, j_4}\sum_{\substack{i\\(\varepsilon_i \le \varepsilon_F)}} \langle i j_2|v|\, i j_4\rangle_a\, a^\dagger_{j_2}\, a_{j_4}, \tag{A.22}$$

$$④= -\frac{1}{4}\sum_{j_2\, j_3}\sum_{\substack{i\\(\varepsilon_i \le \varepsilon_F)}} \langle i j_2|v|\, j_3 i\rangle_a\, a^\dagger_{j_2}\, a_{j_3}. \tag{A.23}$$

Making use of the relations given in equation (A.17), one notes that all the contributions are equal, their sum being

$$\sum_{j_1\, j_2}\sum_{\substack{i\\(\varepsilon_i \le \varepsilon_F)}} \langle j_1\, i\,|v|\, j_2\, i\rangle_a\, a^\dagger_{j_1} a_{j_2}\ . \tag{A.24}$$

Note that i runs only over occupied states, i.e. $\varepsilon_i \le \varepsilon_F$. This is because to annihilate a particle (e.g. in the contraction ① that is the state j_3) the corresponding quantal state should be occupied.

Equating the sum of the kinetic energy term (see equation in terms of (A.18)) and of the potential term (equation (A.24)) to a diagonal, single-particle energy, provides the mean-field Schrödinger equation

$$\sum_{j_1\, j_2}\left(\langle j_1|T|j_2\rangle + \sum_{\substack{i\\(\varepsilon_i \le \varepsilon_F)}} \langle j_1\, i\,|v|\, j_2\, i\rangle_a\right) a^\dagger_{j_1} a_{j_2} = \sum_{j_1\, j_2} \varepsilon_{j_1} a^\dagger_{j_1}\, a_{j_2}\delta(j_1, j_2), \tag{A.25}$$

that is

$$\begin{aligned}
&\int \mathrm{d}^3 r''\varphi^*_{j'}(\vec{r}\,'')T\varphi_j(\vec{r}\,'') \\
&\qquad + \sum_{\substack{i\\(\varepsilon_i \le \varepsilon_F)}} \int \mathrm{d}^3 r'\mathrm{d}^3 r''\varphi^*_{j'}(\vec{r}\,'')\varphi^*_i(\vec{r}\,')v(|\vec{r}\,'' - \vec{r}\,'|)\varphi_j(\vec{r}\,'')\varphi_i(\vec{r}\,') \\
&\qquad - \sum_{\substack{i\\(\varepsilon_i \le \varepsilon_F)}} \int \mathrm{d}^3 r'\mathrm{d}^3 r''\varphi^*_{j'}(\vec{r}\,'')\varphi^*_i(\vec{r}\,')v(|\vec{r}\,'' - \vec{r}\,'|)\varphi_j(\vec{r}\,')\varphi_i(\vec{r}\,'') \\
&\qquad = \varepsilon_j\delta(j, j')
\end{aligned} \tag{A.26}$$

https://doi.org/10.1017/9781009401920.013 Published online by Cambridge University Press

Multiplying from the left by $\Sigma_{j'}\varphi_{j'}(\vec{r})$, one obtains the Hartree–Fock equation in the r-representation,

$$\Big(T + U(r)\Big)\varphi_j(\vec{r}) + \int \mathrm{d}^3 r'\, U_x(|\vec{r} - \vec{r}\,'|)\varphi_j(\vec{r}\,') = \varepsilon_j \varphi_j(\vec{r}), \tag{A.27}$$

where

$$U(r) = \int \mathrm{d}^3 r'\, \rho(r)\, v(|\vec{r} - \vec{r}\,'|) \tag{A.28}$$

is the Hartree potential associated with processes depicted in graphs (1) and (3) of Fig. A.1 (see also equations (A.20) and (A.22)). In this expression

$$\rho(r) = \sum_{\substack{i \\ (\varepsilon_i \le \varepsilon_\mathrm{F})}} |\varphi_i(\vec{r})|^2, \tag{A.29}$$

is the density of the system. The term

$$U_x = - \sum_{\substack{i \\ (\varepsilon_i \le \varepsilon_\mathrm{F})}} \varphi_i^*(\vec{r}\,')\, v(|\vec{r} - \vec{r}\,'|)\, \varphi_i(\vec{r}) \tag{A.30}$$

is the Fock (exchange) potential and has its origin on the Pauli principle (graphs (2) and (4) of Fig. A.1 and equations (A.21) and (A.23)). This term eliminates contributions to the mean field arising from the interaction of a fermion with itself. To see this let us neglect for a moment the exchange potential. Then equation (A.26) can be written as

$$-\frac{\hbar^2}{2m}\varphi_j(\vec{r}) + \sum_{\substack{i \\ (\varepsilon_i \le \varepsilon_\mathrm{F})}} \int \mathrm{d}^3 r'\, \varphi_i^*(\vec{r}\,') v(|\vec{r} - \vec{r}\,'|)\, \varphi_i(\vec{r}\,')\, \varphi_j(\vec{r}) = \varepsilon_j\, \varphi_j(\vec{r}). \tag{A.31}$$

However, because we are dealing with fermions, the product wavefunction $\varphi_i(\vec{r}\,')\,\varphi_j(\vec{r})$ has to be replaced by $\varphi_i(\vec{r}\,')\,\varphi_j(\vec{r}) - \varphi_i(\vec{r}\,')\,\varphi_j(\vec{r})$, thus leading to equation (A.27). Consequently, all contributions to the mean field from terms with $j = i$ vanish.

Once diagonalized, the Hartree–Fock Hamiltonian can be written in second quantization as

$$H_\mathrm{sp} = \sum_{\nu'} \varepsilon_{\nu'}\, a_{\nu'}^\dagger\, a_{\nu'}. \tag{A.32}$$

where

$$N_\nu = a_\nu^\dagger a_\nu \tag{A.33}$$

When applied to the state

$$|\nu\rangle = a_\nu^\dagger |0\rangle_\mathrm{F}, \tag{A.34}$$

https://doi.org/10.1017/9781009401920.013 Published online by Cambridge University Press

one obtains

$$H_{\rm sp}|\nu\rangle = \sum_{\nu'} \varepsilon_{\nu'}\, a^{\dagger}_{\nu'}\, a_{\nu'}\, a^{\dagger}_{\nu}\, |0\rangle_{\rm F} = \sum_{\nu'} \varepsilon_{\nu'}\, a^{\dagger}_{\nu'} \left(\delta(\nu, \nu') - a^{\dagger}_{\nu}\, a_{\nu'}\right)|0\rangle_{\rm F}$$
$$= \varepsilon_{\nu}\, a^{\dagger}_{\nu}\, |0\rangle_{\rm F} = \varepsilon_{\nu}\, |\nu\rangle, \tag{A.35}$$

making use of the fact that

$$a_{\nu'}\, |0\rangle_{\rm F} = 0. \tag{A.36}$$

A.2 Particles and holes

The ground (vacuum) state of Hartree–Fock theory can be written, in second quantization, as

$$|0\rangle_{\rm HF} = \prod_{\substack{i \\ (\varepsilon_i \le \varepsilon_{\rm F})}} a^{\dagger}_i |0\rangle_{\rm F} \quad \left(\sum_{\substack{i \\ (\varepsilon_i \le \varepsilon_{\rm F})}} 1 = A\right), \tag{A.37}$$

where i runs over the quantum numbers of all the occupied states. Assuming the state $|0\rangle_{\rm HF}$ to have an even number of particles, in particular to correspond to a closed-shell system, the total magnetic quantum number is

$$M_{\rm F} = \sum_i m_i = 0. \tag{A.38}$$

If one annihilates a particle in the state i with magnetic quantum number m_i, the resulting hole state

$$a_i |0\rangle_{\rm HF} \tag{A.39}$$

has projection

$$M_i = \sum_{i' \neq i} m_{i'} = -m_i. \tag{A.40}$$

This is because adding a particle with projection m_i to this state, one obtains a state with zero projection, as expressed by the relation given in equation (A.40). Because the angular momentum projection of the hole state (A.39) is opposite to that of the angular momentum of the corresponding particle state and because the third component of the angular momentum changes sign under time reversal it is possible to relate the creation operator of a hole in a given quantal state to the annihilation operator of a particle in the corresponding time-reversal state.

To be more explicit, the time reversal operator τ acting on a single-particle state $|jm\rangle$ with angular momentum quantum numbers (j, m) changes the sign of the projection of the angular momentum leading to

$$\tau\, |jm\rangle = (-1)^{p-m}\, |j\, -m\rangle\, .$$

The m-dependence of the phase is necessary to maintain the correct angular momentum transformation properties but the phase p can be chosen in various ways. Bohr and

https://doi.org/10.1017/9781009401920.013 Published online by Cambridge University Press

Mottelson (1969) choose $p = j$ but other choices are possible. The operation

$$b^{\dagger}_{jm}|0\rangle_{\rm HF} = (-1)^{j-m}\, a_{j-m}|0\rangle_{\rm HF}$$

creates a hole state with angular momentum quantum numbers (j, m).

More generally, one can define the creation operator of a hole as

$$b^{\dagger}_{i} = a_{\tilde{\imath}}, \tag{A.41}$$

where $|\tilde{\imath}\rangle = \tau\,|i\rangle$ is the time reverse of the state $|i\rangle$. The associate hole state is

$$|i^{-1}\rangle = b^{\dagger}_{i}|0\rangle_{\rm HF} = a_{\tilde{\imath}}|0\rangle_{\rm HF} \quad (\varepsilon_i \le \varepsilon_{\rm F})\,. \tag{A.42}$$

Implicit in equations (A.41) and (A.42) is the requirement that the same phase factors should be used in the definition of the hole creation operator as for the time-reversal operator. Note that

$$b^{\dagger}_{\tilde{\nu}} = a_{\tilde{\tilde{\nu}}} = -a_{\nu} \tag{A.43}$$

because $\tau^2 = -1$.

The economy associated with the concepts of particles and holes is evident. Instead of having to explicitly describe the motion of all the $i' \neq i$ particles present in the Hartree–Fock ground states, one needs to concentrate on the degrees of freedom of the single one which is missing in describing the behaviour of the hole state $|i^{-1}\rangle$. Although not mentioned explicitly, this approach has already been used in dealing with particle states. In fact, in describing the state

$$|k\rangle = a^{\dagger}_{k}|0\rangle_{\rm HF} \quad (\varepsilon_k > \varepsilon_{\rm F}), \tag{A.44}$$

one does not talk about all the $A + 1$ nucleons participating in this state (A are packed in $|0\rangle_{\rm HF}$) but only about the single-particle state k.

Let us now write the single-particle operator $\hat{F}$ in terms of creation and annihilation operators of particles and of holes, i.e.

$$\begin{aligned}\hat{F} &= \sum_{\nu_1\nu_2}\langle\nu_1|F|\nu_2\rangle a^{\dagger}_{\nu_1}a_{\nu_2} \\ &= \sum_{\nu_1\nu_2>\nu_F}\langle\nu_1|F|\nu_2\rangle a^{\dagger}_{\nu_1}a_{\nu_2} + \sum_{\nu_1\nu_2\le\nu_F}\langle\nu_1|F|\nu_2\rangle(-b_{\tilde{\nu}_1})(-b^{\dagger}_{\tilde{\nu}_2}) + \cdots\,,\end{aligned} \tag{A.45}$$

where the relation (A.42) has been used. The sum $\nu_1\nu_2 > \nu_{\rm F}$ is over single-particle states with energies larger than $\varepsilon_{\rm F}$, while $\nu_1\nu_2 \le \nu_{\rm F}$ implies states lying below or at $\varepsilon_{\rm F}$. One can then write

$$\hat{F} = \sum_{\nu_1\nu_2>\nu_{\rm F}}\langle\nu_1|F|\nu_2\rangle a^{\dagger}_{\nu_1}a_{\nu_2} - \sum_{\nu_1\nu_2\le\nu_{\rm F}}\langle\tilde{\nu}_1|F|\tilde{\nu}_2\rangle b^{\dagger}_{\nu_2}b_{\nu_1} + \cdots\,. \tag{A.46}$$

The dots in equations (A.45) and (A.46) refer to terms which create or annihilate particle–hole states.

Consequently

$$\langle\nu_1|\hat{F}|\nu_2\rangle = \langle\nu_1|F|\nu_2\rangle = \int {\rm d}^3r\;\varphi^{*}_{\nu_1}(\vec{r})\,F(\vec{r})\,\varphi_{\nu_2}(\vec{r}), \tag{A.47}$$

https://doi.org/10.1017/9781009401920.013 Published online by Cambridge University Press

while

$$\langle \nu_1^{-1}|\hat{F}|\nu_2^{-1}\rangle = -\langle \tilde{\nu}_2|F|\tilde{\nu}_1\rangle = -\langle \nu_2|\tau^{-1}F\tau|\nu_1\rangle = -\langle \nu_1|(\tau^{-1}F\tau)^\dagger|\nu_2\rangle. \tag{A.48}$$

Many single-particle operators have the time-reversal transformation property (Bohr and Mottelson (1969), Section 3-1b)

$$(\tau^{-1}F\tau)^\dagger = -cF, \tag{A.49}$$

where $c = \pm 1$. For example, time-even operators like the coordinate operator $\hat{\mathbf{r}}$ transform according to equation (A.49) with $c = -1$ while time-odd operators like the momentum $\hat{\mathbf{p}}$ and angular momentum $\hat{\mathbf{l}}$ have $c = 1$ (see Bortignon *et al*. (1983)). If an operator has the time-reversal transformation property (A.49) then the hole and particle state matrix elements are related by

$$\langle \nu_1^{-1}|\hat{F}|\nu_2^{-1}\rangle = c\langle \nu_1|F|\nu_2\rangle. \tag{A.50}$$

As explained earlier, this result depends on a consistent definition of the phases in the time-reversal transformation and particle–hole conjugation (see discussions following equations (3.90) and (8.71)).

A.3 Bosons

In the case of particles fulfilling Bose–Einstein statistics we introduce the boson operators $\Gamma_\alpha^\dagger$, Γ_α which create and annihilate a boson in a state α, and respect the commutation relations

$$[\Gamma_\alpha, \Gamma_{\alpha'}^\dagger] = \Gamma_\alpha\Gamma_{\alpha'}^\dagger - \Gamma_{\alpha'}^\dagger\Gamma_\alpha = \delta(\alpha, \alpha') \tag{A.51}$$

and

$$[\Gamma_\alpha, \Gamma_{\alpha'}] = [\Gamma_\alpha^\dagger, \Gamma_{\alpha'}^\dagger] = 0. \tag{A.52}$$

Calling $|0\rangle_{\mathrm{B}}$ the normalized boson vacuum state, i.e.

$${}_{\mathrm{B}}\langle 0|0\rangle_{\mathrm{B}} = 1, \tag{A.53}$$

one obtains, by definition,

$$\Gamma_\alpha|0\rangle_{\mathrm{B}} = 0. \tag{A.54}$$

The one-phonon state is defined as

$$\Gamma_\alpha^\dagger|0\rangle_{\mathrm{B}} = |n_\alpha = 1\rangle, \tag{A.55}$$

where n_α indicates the number of phonons in the quantal state α. This state is normalized. In fact

$$\begin{aligned}\langle n_\alpha = 1|n_{\alpha'} = 1\rangle &= {}_{\mathrm{B}}\langle 0|\Gamma_\alpha\Gamma_{\alpha'}^\dagger|0\rangle_{\mathrm{B}} \\ &= {}_{\mathrm{B}}\langle 0|\big(\delta(\alpha, \alpha') + \Gamma_{\alpha'}^\dagger\Gamma_\alpha\big)|0\rangle_{\mathrm{B}} = {}_{\mathrm{B}}\langle 0|\underbrace{\Gamma_\alpha\Gamma_{\alpha'}^\dagger}|0\rangle = \delta(\alpha, \alpha').\end{aligned} \tag{A.56}$$

https://doi.org/10.1017/9781009401920.013 Published online by Cambridge University Press

The last step in equation (A.56) contains a contraction between the boson creation and annihilation operators. It is the analogue of the contraction between fermion operators in equation (A.7). There is the Wick theorem for bosons which is the same as the one for fermions except that there are no sign changes when operators are interchanged. The commutation relation given in equation (A.51) implies that

$$\Gamma_\alpha^\dagger \Gamma_\alpha^\dagger |0\rangle_{\mathrm{B}} \neq 0, \tag{A.57}$$

i.e. bosons can occupy the same quantal state. Let us now work out the orthonormalization of this two-phonon state by carrying out all contractions

$${}_{\mathrm{B}}\langle 0|\Gamma_{\alpha'}\Gamma_{\alpha'}\Gamma_\alpha^\dagger\Gamma_\alpha^\dagger|0\rangle_{\mathrm{B}} = \delta(\alpha,\alpha')\,\delta(\alpha,\alpha') + \delta(\alpha,\alpha')\,\delta(\alpha,\alpha') = 2\delta(\alpha,\alpha'). \tag{A.58}$$

Consequently, the two-boson state

$$|n_\alpha = 2\rangle = \frac{1}{\sqrt{2}}\Gamma_\alpha^\dagger\Gamma_\alpha^\dagger|0\rangle_{\mathrm{B}} \tag{A.59}$$

is a normalized state. Note that

$$\Gamma_\alpha^\dagger|n=1\rangle = \Gamma_\alpha^\dagger\Gamma_\alpha^\dagger|0\rangle_{\mathrm{B}} = \sqrt{2}\,|n_\alpha = 1\rangle \tag{A.60}$$

and, in general,

$$\Gamma_\alpha^\dagger|n_\alpha = N\rangle = \sqrt{N+1}\,|n_\alpha = N+1\rangle. \tag{A.61}$$

We will now write the harmonic oscillator Hamiltonian in second quantization as originally done by Dirac (1935),

$$H = \sum_{\alpha'} \hbar\omega_{\alpha'}\left(\Gamma_{\alpha'}^\dagger\Gamma_{\alpha'} + \tfrac{1}{2}\right). \tag{A.62}$$

The energy of the ground state (vacuum state) is

$$H|0\rangle_{\mathrm{B}} = E_0, \tag{A.63}$$

where

$$E_0 = \frac{1}{2}\sum_{\alpha'}\hbar\omega_{\alpha'}. \tag{A.64}$$

It receives a $\frac{1}{2}\hbar\omega_\alpha$ contribution (zero-point fluctuation) for each degree of freedom of the system.

The one-phonon state has an energy

$$\begin{aligned} H|n_\alpha = 1\rangle &= \sum_{\alpha'}\hbar\omega_{\alpha'}\left(\Gamma_{\alpha'}^\dagger\Gamma_{\alpha'} + \frac{1}{2}\right)\Gamma_\alpha^\dagger|0\rangle_{\mathrm{B}} = \sum_{\alpha}\hbar\omega_{\alpha'}\Gamma_{\alpha'}^\dagger\Gamma_{\alpha'}\Gamma_\alpha^\dagger\ |0\rangle_{\mathrm{B}} + E_0\Gamma_\alpha^\dagger|0\rangle_{\mathrm{B}} \\ &= \left(\hbar\omega_\alpha + E_0\right)|n_\alpha = 1\rangle. \end{aligned} \tag{A.65}$$

https://doi.org/10.1017/9781009401920.013 Published online by Cambridge University Press

We will now calculate the commutator

$$[H, \Gamma^\dagger_\alpha] = \sum_\alpha \hbar\omega_{\alpha'}[\Gamma^\dagger_{\alpha'}\Gamma_{\alpha'}, \Gamma^\dagger_\alpha]. \tag{A.66}$$

Making use of the relation

$$[AB, C] = A[B, C] + [A, C]B, \tag{A.67}$$

one obtains

$$[H, \Gamma^\dagger_\alpha] = \sum_{\alpha'} \hbar\omega_{\alpha'}\left(\Gamma^\dagger_{\alpha'}[\Gamma_{\alpha'}, \Gamma^\dagger_\alpha] + [\Gamma^\dagger_{\alpha'}, \Gamma^\dagger_\alpha]\Gamma_{\alpha'}\right) = \sum_{\alpha'} \hbar\omega_{\alpha'}\Gamma^\dagger_{\alpha'}\delta(\alpha, \alpha') = \hbar\omega_\alpha\Gamma^\dagger_\alpha. \tag{A.68}$$

That is, this expression provides a relation to determine the eigenvalues of a Hamiltonian H in the harmonic approximation. Of course this approximation becomes exact if H is the Hamiltonian describing a harmonic oscillator.

A.4 Quasi-bosons

Making use of the relations given in equation (A.67) and those relating commutators to anticommutators,

$$[A, BC] = -B\{A, C\} + \{A, B\}C, \tag{A.69}$$

one can calculate

$$\begin{aligned}
[a_{\bar\nu}a_\nu, a^\dagger_{\nu'}a^\dagger_{\bar\nu'}] &= a_{\bar\nu}[a_\nu, a^\dagger_{\nu'}a^\dagger_{\bar\nu'}] + [a_{\bar\nu}, a^\dagger_{\nu'}a^\dagger_{\bar\nu'}]a_\nu \\
&= a_{\bar\nu}\Big(-a^\dagger_{\nu'}\{a_\nu, a^\dagger_{\bar\nu'}\} + \{a_\nu, a^\dagger_{\nu'}\}a^\dagger_{\bar\nu'} \\
&\qquad -a^\dagger_{\nu'}\{a_{\bar\nu}, a^\dagger_{\bar\nu'}\} + \{a_{\bar\nu}, a^\dagger_{\nu'}\}a^\dagger_{\bar\nu'}\Big)a_\nu \\
&= a_{\bar\nu}\Big(\delta(\nu, \nu')a^\dagger_{\bar\nu} - a^\dagger_\nu\delta(\nu, \nu')\Big)a_\nu \\
&= \delta(\nu, \nu')\,(1 - N_\nu - N_{\bar\nu})\,,
\end{aligned} \tag{A.70}$$

where $N_\nu = a^\dagger_\nu a_\nu$, and where it has been assumed that ν and $\bar\nu\,'$ are two different quantal states, one of the class with positive angular momentum projection and the other with negative m-value. If this commutator is applied to the vacuum state one obtains

$$[a_{\bar\nu}a_\nu, a^\dagger_{\nu'}a^\dagger_{\bar\nu'}]|0\rangle = \delta(\nu, \nu')|0\rangle. \tag{A.71}$$

Consequently, under certain circumstances, a couple of fermions behave like a (quasi-) boson (see equation (5.12)). Making use of (A.70) one obtains

$$[P, P^\dagger] = \delta(\nu, \nu')\Omega\left(1 - \frac{\hat N}{\Omega}\right), \tag{A.72}$$

https://doi.org/10.1017/9781009401920.013 Published online by Cambridge University Press

where

$$P = \sum_{\nu>0} a_\nu^\dagger a_{\bar{\nu}}^\dagger,$$

2Ω is the number of degenerate single fermion states and $\hat{N} = \sum_\nu a_\nu^\dagger a_\nu = \sum_{\nu>0} \left(a_\nu' a_\nu + a_{\bar{\nu}}^\dagger a_{\bar{\nu}} \right)$ is the operator number of particles. It is then clear that the last factor in equation (A.72) arises from the Pauli principle acting between fermions.

https://doi.org/10.1017/9781009401920.013 Published online by Cambridge University Press