Appendix I
Fluctuations and symmetry restoration

This appendix contains some relations on spontaneous symmetry breaking which are used in Chapter 4.

I.1 Conjugate variables

The uncertainty relation

$$\Delta x \Delta p \geq \mathrm{i}\hbar \tag{I.1}$$

specifies the limits within which the particle picture can be applied. Any use of the word ‘position’ with an accuracy exceeding that given by the above equation is just meaningless, because quantum mechanical processes can be described equally well in terms of waves as particles.

Momentum and position are conjugate variables and satisfy commutation relations

$$[x, p] = \mathrm{i}\hbar. \tag{I.2}$$

In the coordinate representation the wavefunctions $\psi(x)$ are functions of position, and the momentum operator can be written as

$$p = -\mathrm{i}\hbar \frac{\partial}{\partial x}. \tag{I.3}$$

The relation

$$x = \mathrm{i}\hbar \frac{\partial}{\partial p} \tag{I.4}$$

is a valid form of the position operator in the momentum representation.

The Heisenberg equation of motion for an operator A which does not depend explicitly on the time is

$$\dot{A} = \frac{\mathrm{i}}{\hbar}[H, A], \tag{I.5}$$

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where H is the Hamiltonian. If $H(p)$ is a function of the momentum of a particle then the velocity

$$\dot{x} = \frac{\mathrm{i}}{\hbar}[H, x] = \frac{\partial H}{\partial p}, \tag{I.6}$$

where the first step follows from the Heisenberg equation and the second from the representation of the position operator. Choosing the special form $H = p^2/2m$ we have $\dot{x} = p/m$ and

$$\frac{\partial \dot{x}}{\partial p} = \frac{\partial^2 H}{\partial p^2} = \frac{1}{m}. \tag{I.7}$$

I.2 Rotation about an axis

The situation is similar for the angle and angular momentum of a rigid body rotating about an axis but there are important differences. This is because the angle is restricted to the range $-\pi < \varphi \leqslant \pi$ and the angular momentum L is quantized. In the angle representation the wavefunctions $\psi(\varphi)$ must be periodic functions with period 2π. The commutation relation $[\varphi, L] = \mathrm{i}\hbar$ must be used with care. The representation of the angular momentum operator

$$L = -\mathrm{i}\hbar \frac{\partial}{\partial \varphi} \tag{I.8}$$

is valid when applied to wavefunctions which have the correct periodicity properties but the representation

$$\varphi = \mathrm{i}\hbar \frac{\partial}{\partial L} \tag{I.9}$$

is correct only in a heuristic or semiclassical sense. This is because L is quantized and the derivative is not defined.

Suppose that the rotor has a Hamiltonian $H(L)$ which is a function of L. Heisenberg's equation of motion gives

$$\omega_{\mathrm{rot}} = \dot{\varphi} = \frac{\mathrm{i}}{\hbar}[H, \varphi] \tag{I.10}$$

where ω_{rot} is the rotational frequency. Making use of the semiclassical relation

$$\frac{\mathrm{i}}{\hbar}[H, \varphi]\,|\,\psi\,\rangle = \frac{\partial H}{\partial L}\,|\,\psi\,\rangle, \tag{I.11}$$

which follows from equation (I.9), we get

$$\hbar\omega_{\mathrm{rot}} = \hbar\frac{\partial H}{\partial L} = \frac{\partial H}{\partial I} = \frac{\hbar^2 I}{\mathcal{I}}. \tag{I.12}$$

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Here we have used $L = \hbar I$ so that L has the dimensions of angular momentum while I is dimensionless. Equation (I.12) defines a moment of inertia $\mathcal{I}$. Consequently

$$\frac{\partial \hbar\omega_{\text{rot}}}{\partial I} = \frac{\hbar^2}{\mathcal{I}} = \frac{\partial^2 H}{\partial I^2}, \tag{I.13}$$

a consequence of the structure of the Hamiltonian. If the moment of inertia is constant then

$$H = \frac{L^2}{2\mathcal{I}} = \frac{\hbar^2 I^2}{2\mathcal{I}}. \tag{I.14}$$

This last relation is the Hamiltonian of a rigid body. Equations (I.13) and (I.14) are used in the analysis the rotational spectra of deformed nuclei. As discussed in Chapter 6, equation (I.13) defines the first moment of inertia and equation (I.13) the second moment of inertia. For an even nucleus $I = 0, 2, 4, \ldots$, the quantities $\hbar\omega_{\text{rot}}$ are related to gamma ray energies and the derivatives are calculated as finite differences.

I.3 Rotations in gauge space

The above discussions concerning rotations about an axis carry over to rotations in gauge space.* In this case the particle number operator $\hat{N}$ plays the role of the angular momentum. The gauge angle ϕ and the particle number operator satisfy the commutation relation $[\phi, \hat{N}] = i$ and in the number representation

$$\phi = \mathrm{i}\frac{\partial}{\partial N}. \tag{I.15}$$

The Hamiltonian for the BCS pairing problem is

$$H = H_0 - \lambda \hat{N}, \tag{I.16}$$

where H_0 includes the kinetic energy of the nucleons and the pairing interaction, $\hat{N}$ is the particle number operator and λ is a Lagrange multiplier which is used to fix the number of nucleons. Physically it is the Fermi energy and is determined by measuring the energy change of the system when adding and subtracting particles. For example the change in energy of the nucleus when an even number δN of nucleons are added is

$$\delta \langle E \rangle = \lambda \delta N. \tag{I.17}$$

The time derivative of the gauge angle is given by Heisenberg's equation of motion

$$\dot{\phi} = \frac{\mathrm{i}}{\hbar}[H, \phi] = \frac{1}{\hbar}\frac{\partial H}{\partial N} = \frac{1}{\hbar}\lambda. \tag{I.18}$$

* The role of conjugate variables becomes very intuitive when viewed in terms of the corresponding unitary transformation leaving invariant the total Hamiltonian: Galilean (translational invariance homogeneity of space) $T = \exp(-\mathrm{i}p_x x)$, Rotation (rotational invariance, space isotropy) $R = \exp(-\mathrm{i}\varphi I)$, Gauge (conservation particle number) $G = \exp(-\mathrm{i}\phi N)$, etc. Nature breaks spontaneously all these symmetries. The fingerprints of the associated deformations are the families of states corresponding to the quantized rotation of the system as a whole (AGN modes).

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Thus the combination

$$2\hbar\dot{\phi} = 2\lambda = \delta \langle E \rangle \tag{I.19}$$

has the physical meaning of the change in energy of the nucleus when a pair ($\delta N = 2$) of nucleons is added to it. Taking the derivative with respect to N

$$\frac{\partial \dot{\phi}}{\partial N} = \frac{1}{\hbar}\frac{\partial \lambda}{\partial N} = \frac{1}{\hbar}\frac{\partial^2 H}{\partial N^2} = \frac{\hbar}{\mathcal{I}}. \tag{I.20}$$

This equation defines the pairing 'moment of inertia' $\mathcal{I}$ describing rotations in gauge space. It is analogous to the moment of inertia for rotations in ordinary space. The 'pairing moment of inertia' can also be written as

$$\frac{\mathcal{I}}{\hbar^2} = \frac{\partial N}{\partial \lambda}. \tag{I.21}$$

This expression is very general and depends only on λ being a Lagrange multiplier in a variational principle for the energy. If $E(N_0)$ is the energy of a nucleus with N_0 nucleons and if the pairing 'moment of inertia' is approximately constant then equation (I.21) can be integrated to give the energy of nearby nuclei with N nucleons

$$E(N) \approx E(N_0) + \lambda(N - N_0) + \frac{\hbar^2}{2\mathcal{I}}(N - N_0)^2 . \tag{I.22}$$

This is the energy dependence of a 'pairing rotational band'. The importance of the quadratic term depends on the value of the moment of inertia. The simplest way to calculate the pairing moment of inertia in the BCS model is to use equation (I.21). The average number of particles is

$$N = 2\sum_{\nu>0} V_\nu^2 = \sum_{\nu>0}\left[1 - \frac{\varepsilon_\nu - \lambda}{E_\nu}\right], \tag{I.23}$$

where E_ν are the quasiparticle energies. Evaluating the derivative with respect to λ gives

$$\frac{\mathcal{I}}{\hbar^2} = \frac{\partial N}{\partial \lambda} = \sum_{\nu>0}\frac{\Delta^2}{E_\nu^3} + \Delta\frac{\mathrm{d}\Delta}{\mathrm{d}\lambda}\sum_{\nu>0}\frac{\varepsilon_\nu - \lambda}{E_\nu^3}. \tag{I.24}$$

The derivative $\mathrm{d}\Delta/\mathrm{d}\lambda$ in the second term can be calculated by differentiating the gap equation. The second term is expected to be small in a situation where the energy level distribution is more or less symmetrical above and below the Fermi level. It is more important near the beginning or end of a shell. Neglecting this term we obtain the cranking formula given in equation (H.17).

I.4 Symmetry restoring fluctuations and pairing rotations

Another method to obtain the pairing moment of inertia is to extract it from the zero frequency mode of the pairing RPA. The Hamiltonian is

$$H = H_{\mathrm{MF}} + H_{\mathrm{p}}'' \tag{I.25}$$

making the approximation of taking only the even part H_p'' of the fluctuating term $H_p' + H_p''$. Solving the RPA equation of motion

$$[H, \Gamma_n{}^\dagger] = W_n'' \Gamma_n{}^\dagger. \tag{I.26}$$

The discussion in Section 4.2.2 showed that equation (I.26) has a zero-frequency solution $\left(W_1'' = 0\right)$ related to the gauge invariance of the original Hamiltonian. The corresponding creation operator was related to the number operator by

$$\Gamma_1^\dagger = \frac{\Lambda_1''}{2\Delta}\left(\hat{N} - N_0\right), \tag{I.27}$$

where N_0 is the average number of nucleons in the BCS state, which is the eigenstate of the mean-field Hamiltonian H_{MF} and the normalization constant

$$\Lambda_1'' = \frac{1}{2}\left[\sum_{\nu>0} \frac{2E_\nu W_1''}{((2E_\nu)^2 - W_1''^2)^2}\right]^{-1/2}. \tag{I.28}$$

The normalization constant Λ_1'' (particle–vibration coupling) diverges for the zero-frequency mode, but for the moment we assume that $W_1'' > 0$ and then take the limit $W_n'' \to 0$ later in the calculation.

Now we make a comparison with an oscillator with Hamiltonian

$$H = \frac{p^2}{2D_1''} + \frac{1}{2} D_1'' \omega_1''^2 q^2, \tag{I.29}$$

and identify the momentum with the number operator, the coordinate with the gauge angle and the frequency with the RPA energy:

$$p = \hbar\left(\hat{N} - N_0\right), \qquad q = \phi, \qquad \hbar\omega_1'' = W_1''. \tag{I.30}$$

The phonon creation operator for the oscillator is

$$\Gamma^\dagger = \sqrt{\frac{\hbar^2}{2D_1''W_1''}}\left(\hat{N} - N_0\right) + \mathrm{i}\phi\sqrt{\frac{D_1''W_1''}{2\hbar^2}}. \tag{I.31}$$

Comparing the coefficients of $\left(\hat{N} - N_0\right)$ in equations (I.27) and (I.31) and noting that the coefficient of ϕ in equation (I.31) vanishes in the limit $W_1'' \to 0$, we get an expression for the mass parameter

$$\frac{\hbar^2}{2D_1''W_1''} = \left(\frac{\Lambda_1''}{2\Delta}\right)^2 \quad \text{or} \quad \frac{D_1''}{\hbar^2} = \frac{4\Delta^2}{2W_1''\Lambda_1''^2}. \tag{I.32}$$

Taking the limit $W_1'' \to 0$ we have

$$\frac{1}{W_1''\Lambda_1''^2} = \frac{4}{W_1''}\left[\sum_{\nu>0} \frac{2E_\nu W_1''}{((2E_\nu)^2 - W_1''^2)^2}\right] = \sum_\nu \frac{1}{2E_\nu^3} \tag{I.33}$$

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and the mass parameter reduces to

$$\frac{D_1''}{\hbar^2} = \sum_{\nu>0} \frac{\Delta^2}{E_\nu^3}. \tag{I.34}$$

This agrees with the previous approximate expressions for the pairing moment of inertia (see equations (4.47), (H.17)). A more accurate calculation which includes the effect of the odd part H_p' of the interaction modifies this result and leads to an expression equivalent to (I.24).

Making use of the above result, and the fact that $\lambda = \partial H/\partial N$, the energy of the members of the pairing rotational band can be written as

$$E = \lambda N + \frac{\hbar^2}{2\mathcal{I}} N^2, \tag{I.35}$$

where

$$\frac{\mathcal{I}}{\hbar^2} = \frac{D_1''}{\hbar^2} = \sum_{\nu>0} \frac{4U_\nu^2 V_\nu^2}{E_\nu} = 2\sum_{\nu>0} \frac{\langle \nu\bar{\nu}|\hat{N}|BCS\rangle^2}{2E_\nu}, \tag{I.36}$$

which is the cranking formula of the moment of inertia rotations in gauge space.

I.4.1 Demonstration that $[H_{\mathrm{MF}} + H_p'', \tilde{N}] = 0$

In what follows we demonstrate that

$$[H_{\mathrm{MF}} + H_p'', \tilde{N}] = 0, \tag{I.37}$$

where (see equations (G.11), (G.12) and (G.21))

$$H_{\mathrm{MF}} = U + H_{11}, \tag{I.38}$$

U being a constant and

$$H_{11} = \sum_\nu E_\nu \alpha_\nu^\dagger \alpha_\nu. \tag{I.39}$$

We do this within the harmonic approximation (RPA), where two-quasiparticle excitations are described in terms of the (quasi-boson) operators

$$\Gamma_\nu^\dagger = \alpha_\nu^\dagger \alpha_{\bar{\nu}}^\dagger, \quad \Gamma_\nu = \alpha_{\bar{\nu}} \alpha_\nu, \tag{I.40}$$

for which we impose the condition (see equation (A.71))

$$[\Gamma_\nu, \Gamma_{\nu'}^\dagger] = \delta(\nu, \nu'). \tag{I.41}$$

Within this approximation H_{MF} can be written as

$$H_{\mathrm{MF}} = \sum_\nu 2E_\nu \Gamma_\nu^\dagger \Gamma_\nu. \tag{I.42}$$

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Within the same approximation, the relation (G.5) is

$$a_\nu^\dagger a_\nu + a_{\bar\nu}^\dagger a_{\bar\nu} \approx 2U_\nu V_\nu \left(\Gamma_\nu^\dagger + \Gamma_\nu\right) + 2V_\nu^2,$$

and the operator number of particles is

$$\tilde N = \Delta \sum_{\nu>0} \frac{1}{E_\nu}\left(\Gamma_\nu^\dagger + \Gamma_\nu\right) + N_0. \tag{I.43}$$

Making use of the commutation relations

$$\begin{aligned}\left[\Gamma_\nu^\dagger \Gamma_\nu, \left(\Gamma_{\nu'}^\dagger + \Gamma_{\nu'}\right)\right] &= \Gamma_\nu \left[\Gamma_\nu, \left(\Gamma_{\nu'}^\dagger + \Gamma_{\nu'}\right)\right] + \left[\Gamma_\nu^\dagger, \left(\Gamma_{\nu'}^\dagger + \Gamma_{\nu'}\right)\right]\Gamma_\nu \\ &= \delta(\nu,\nu')\left(\Gamma_\nu^\dagger - \Gamma_{\nu'}\right)\end{aligned}$$

and

$$\left[\left(\Gamma_\nu^\dagger - \Gamma_{\nu'}\right), \left(\Gamma_{\nu'}^\dagger + \Gamma_{\nu'}\right)\right] = -2\delta(\nu,\nu'),$$

one obtains

$$\begin{aligned}[H_{\mathrm{MF}}, \tilde N] &= \sum_{\nu>0} 2E_\nu \sum_{\nu'>0} \frac{\Delta}{E_{\nu'}}\left[\Gamma_\nu^\dagger\Gamma_\nu, \left(\Gamma_{\nu'}^\dagger + \Gamma_\nu\right)\right] \\ &= 2\Delta \sum_{\nu>0}\left(\Gamma_\nu^\dagger - \Gamma_\nu\right)\end{aligned} \tag{I.44}$$

and

$$\begin{aligned}[H_{\mathrm{p}}'', \tilde N] &= \frac{G}{4}\sum_{\nu'>0}\frac{\Delta}{E_{\nu'}}\left[\sum_{\nu>0}\left(\Gamma_\nu^\dagger - \Gamma_\nu\right)^2, \left(\Gamma_\nu^\dagger + \Gamma_{\nu'}\right)\right] \\ &= \frac{G}{4}\sum_{\nu'>0}\frac{\Delta}{E_{\nu'}} 2\left(\sum_{\nu>0}\left(\Gamma_\nu^\dagger - \Gamma_\nu\right)\right)\left[\sum_{\nu''}\left(\Gamma_{\nu''}^\dagger - \Gamma_{\nu''}\right)\left(\Gamma_{\nu'}^\dagger + \Gamma_{\nu'}\right)\right] \\ &= -G\sum_{\nu'>0}\frac{\Delta}{E_{\nu'}}\sum_{\nu>0}\left(\Gamma_\nu^\dagger - \Gamma_\nu\right) \\ &= -2\Delta\sum_{\nu>0}\left(\Gamma_\nu^\dagger - \Gamma_\nu\right),\end{aligned} \tag{I.45}$$

where in the last step use was made of the BCS gap equation.

From equations (I.44) and (I.45) one obtains

$$[H_{\mathrm{MF}} + H_{\mathrm{p}}'', \tilde N] = 0. \tag{I.46}$$

Because

$$\begin{aligned}\left[\left(\Gamma_\nu^\dagger + \Gamma_\nu\right), \left(\Gamma_{\nu'}^\dagger + \Gamma_{\nu'}\right)\right] &= -\delta(\nu,\nu') + \delta(\nu,\nu') = 0, \\ [H_{\mathrm{p}}', \tilde N] &= 0.\end{aligned} \tag{I.47}$$

Consequently, H_{p}'' is the term of the residual interaction among the quasiparticles which, within the quasi-boson approximation, restores gauge invariance to the symmetry-breaking BCS Hamiltonian H_{MF}.

We now show the quasi-boson approximation is a good approximation provided the number of quasiparticles excited in the system is small. In fact,

$$\begin{aligned}[\alpha_{\bar{\nu}}\alpha_\nu, \alpha^\dagger_{\nu'}\alpha^\dagger_{\bar{\nu}'}] &= \alpha_{\bar{\nu}}[\alpha_\nu, \alpha^\dagger_{\nu'}\alpha^\dagger_{\bar{\nu}'}] + [\alpha_{\bar{\nu}}, \alpha^\dagger_{\nu'}\alpha_{\bar{\nu}'}]\alpha_\nu \\ &= \alpha_{\bar{\nu}}\left\{\alpha_\nu, \alpha^\dagger_{\nu'}\right\}\alpha^\dagger_{\bar{\nu}'} - \alpha^\dagger_{\nu'}\left\{\alpha_{\bar{\nu}}, \alpha^\dagger_{\bar{\nu}'}\right\}\alpha_\nu \\ &= \delta(\nu, \nu')(1 - N_\nu - N_{\bar{\nu}}),\end{aligned} \tag{I.48}$$

where

$$N_\nu = \alpha^\dagger_\nu \alpha_\nu. \tag{I.49}$$

Consequently, the last two terms in the parentheses in equation (I.48) are connected with the Pauli principle. Furthermore,

$$[\alpha_{\bar{\nu}}\alpha_\nu, \alpha^\dagger_{\nu'}\alpha^\dagger_{\bar{\nu}'}]|\mathrm{BCS}\rangle = \delta(\nu, \nu')|\mathrm{BCS}\rangle \tag{I.50}$$

Let us end this technical section with a physical image. Restoration of gauge symmetry arises, within the picture of deformation in gauge space developed in Chapter 4 (see Fig. 4.1), in terms of fluctuations in the orientation of the body-fixed system $\mathcal{K}'$ defining a privileged direction in gauge space. In the present case, this is also the orientation defined by the symmetry axis of the (static) deformation of the system.

In keeping with the analogies carried out in Section I.1 (Euler angle $\varphi \leftrightarrow$ gauge angle ϕ, rotational frequency $\omega_{\mathrm{rot}} \leftrightarrow$ Fermi energy in units of Planck's constant $\lambda/\hbar$, angular momentum $I \leftrightarrow$ number of particles N), and the fact that quantum mechanically a spherical system cannot rotate, one can view the pairing gap Δ as the deformation in gauge space (or equivalently α_0, see equation (G.2)) corresponding to the static quadrupole moment Q_0 of a deformed nucleus in normal space (axial symmetry has been assumed for simplicity).

Let us now use this deformed system, which is easy to visualize, to develop the line of reasoning. For a fixed orientation this system violates rotational invariance. To restore this symmetry, the privileged orientation has to be averaged out. That is, the system has to rotate at given frequencies ($\omega_{\mathrm{rot}} = \hbar I/\mathcal{I}$), tantamount to saying that it has to be in a state of definite angular momentum I.

Summing up, starting from a rotational invariant Hamiltonian the (mean-field) state of lowest energy describes a deformed system and thus a privileged orientation in space. A part of the residual interaction (corresponding to H''_{p} in gauge space) gives rise to a vibrational mode which, in the harmonic approximation, has zero frequency (i.e. its associated restoring force vanishes) and divergent zero-point fluctuations. Making an analogy with deformations in three-dimensional space: an axially symmetric quadrupole vibration defines dynamically a privileged orientation which, changing direction with time, is averaged out leaving the system in a state of angular momentum $L = 2$ (surface wave). As the restoring constant C tends to zero, the time in which a privileged direction in space is well defined increases. In the limit in which $C = 0$, one has a deformed system which rotates as a whole, the resulting lowest energy state having zero angular momentum.