Appendix G Pairing mean-field solution

G.1 Solution of the pairing Hamiltonian

This appendix gives an alternative derivation of the pairing mean-field Hamiltonian and the BCS wavefunction to that provided in the text.

Let us start with the Hamiltonian

$$H=H_{\rm sp}+H_{\rm p},$$

which is the sum of a single-particle Hamiltonian

$$H_{\rm sp} = \sum_{\nu>0} (\varepsilon_{\nu} - \lambda) (a_{\nu}^{\dagger} a_{\nu} + a_{\bar{\nu}}^{\dagger} a_{\bar{\nu}})$$

and a pairing interaction with constant matrix elements

$$H_{\rm p} = -G \sum_{\substack{\nu > 0 \\ \nu' > 0}} a_{\nu}^{\dagger} a_{\bar{\nu}'}^{\dagger} a_{\bar{\nu}'} a_{\nu'}.$$
 (G.1)

In what follows we shall solve H in the mean-field approximation. For this purpose we introduce the pair-creation operator,

$$P^{\dagger} = \sum_{\nu > 0} a^{\dagger}_{\nu} a^{\dagger}_{\overline{\nu}} = \alpha_0 + (P^{\dagger} - \alpha_0)$$

and add and subtract from it the mean-field value

$$\alpha_0 = \langle \text{BCS} | P^{\dagger} | \text{BCS} \rangle = \langle \text{BCS} | P | \text{BCS} \rangle$$

of the pair transfer operator in the, still unknown, mean-field ground state. This state is called the $|BCS\rangle$ state, because this solution was first proposed by Bardeen, Cooper and Schrieffer. Note that $\langle BCS|BCS\rangle = 1$. We can now write

$$H_{\rm p} = -G(\alpha_0 + (P^{\dagger} - \alpha_0))(\alpha_0 + (P - \alpha_0))$$

= $-G(\alpha_0^2 + \alpha_0(P^{\dagger} + P - 2\alpha_0) + (P^{\dagger} - \alpha_0)(P - \alpha_0))$

Assuming that the matrix elements of the operators $(P^{\dagger} - \alpha_0)$ and $(P - \alpha_0)$ in the states near to the ground state are much smaller than α_0 , one obtains the pairing field

$$V_{\rm p} = -\Delta (P^{\dagger} + P) + \frac{\Delta^2}{G}, \qquad \Delta = G\alpha_0 .$$
 (G.2)

The mean-field Hamiltonian then becomes

$$\begin{split} H_{\rm MF} &= H_{\rm sp} + V_{\rm p} \\ &= \sum_{\nu>0} (\varepsilon_{\nu} - \lambda) (a_{\nu}^{\dagger} a_{\nu} + a_{\overline{\nu}}^{\dagger} a_{\overline{\nu}}) - \Delta \sum_{\nu>0} (a_{\nu}^{\dagger} a_{\overline{\nu}}^{\dagger} + a_{\overline{\nu}} a_{\nu}) + \frac{\Delta^2}{G} \; . \end{split}$$

This is a bilinear expression in the creation and annihilation operators. Consequently, it can be diagonalized by a rotation in (a^{\dagger}, a) -space. This can be accomplished through the Bogoliubov–Valatin transformation

$$\alpha_{\nu}^{\dagger} = U_{\nu}a_{\nu}^{\dagger} - V_{\nu}a_{\bar{\nu}}.$$

From this definition one can anticipate that the BCS solution does not change the energies ε_{ν} of the single-particle levels or the associated wavefunction $\varphi_{\nu}(\vec{r})$, but the occupation probabilities for levels around the Fermi energy within an energy range 2Δ , a quantity much smaller than the Fermi energy $\varepsilon_{\rm F}$. What is also changed is the mechanism by which the system can be excited, which implies, for nucleons moving around the Fermi energy, the breaking of Cooper pairs.

The creation operator of a quasiparticle α_{ν}^{\dagger} creates a particle in the single-particle state ν with probability U_{ν}^2 , while it creates a hole (annihilates a particle) with probability V_{ν}^2 . To be able to create a particle, the state ν should be empty, while to create a hole it has to be filled, so U_{ν}^2 and V_{ν}^2 are the probabilities that the state ν is empty and is occupied respectively.

Expressing the creation and annihilation operators $(a_{\nu}^{\dagger}, a_{\nu})$ in terms of the quasiparticle operators $(\alpha_{\nu}^{\dagger}, \alpha_{\nu})$, and expressing $H_{\rm MF}$ in terms of quasiparticles, one has the parameters U_{ν} and V_{ν} for each level ν to make this Hamiltonian diagonal (in fact one, see equation (G.3)).

Making use of the anticommutation relations

$$\begin{aligned} \{a_{\nu}, a_{\nu'}^{\dagger}\} &= \delta(\nu, \nu') \\ \{a_{\nu}, a_{\nu'}\} &= \{a_{\nu}^{\dagger}, a_{\nu'}^{\dagger}\} = 0, \end{aligned}$$

one obtains

$$\begin{aligned} \{\alpha_{\nu}, \alpha_{\nu'}^{\dagger}\} &= \{(U_{\nu}a_{\nu} - V_{\nu}a_{\bar{\nu}}^{\dagger}), (U_{\nu'}a_{\nu'}^{\dagger} - V_{\nu'}a_{\bar{\nu}'})\} \\ &= (U_{\nu}U_{\nu'} + V_{\nu}V_{\nu'})\,\delta(\nu, \nu'). \end{aligned}$$

That is, for the quasiparticle transformation to be unitary, the U_{ν} , V_{ν} occupation factors have to fulfil the relation

$$U_{\nu}^{2} + V_{\nu}^{2} = 1, \tag{G.3}$$

implying also that the one-quasiparticle states are orthonormal. In particular

$$\langle \nu | \nu \rangle = 1 = \langle \text{BCS} | \alpha_{\nu} \alpha_{\nu}^{\dagger} | \text{BCS} \rangle = \langle \text{BCS} | \{ \alpha_{\nu}, \alpha_{\nu}^{\dagger} \} | \text{BCS} \rangle$$

= $U_{\nu}^{2} + V_{\nu}^{2}$

implies that the state

$$|\nu\rangle = \alpha_{\nu}^{\dagger}|\text{BCS}\rangle$$

is normalized.

Note that |BCS> is also the quasiparticle vacuum, i.e.

$$\alpha_{\nu}|\text{BCS}\rangle = 0.$$

Let us now invert the quasiparticle transformation, i.e. express a_{ν}^{\dagger} in terms of α_{ν}^{\dagger} and $\alpha_{\bar{\nu}}$. Multiplying α_{ν}^{\dagger} by U_{ν} and $\alpha_{\bar{\nu}}$ by V_{ν} gives

$$U_{\nu}\alpha_{\nu}^{\dagger} = U_{\nu}^2 a_{\nu}^{\dagger} - U_{\nu} V_{\nu} a_{\bar{\nu}},$$

$$V_{\nu}\alpha_{\bar{\nu}} = U_{\nu} V_{\nu} a_{\bar{\nu}} + V_{\nu}^2 a_{\nu}^{\dagger}.$$

Adding these expressions one obtains

$$a_{\nu}^{\dagger} = U_{\nu} \alpha_{\nu}^{\dagger} + V_{\nu} \alpha_{\bar{\nu}}.$$

We shall now express $a_{\nu}^{\dagger}a_{\nu}$ in terms of quasiparticles, i.e.

$$\begin{aligned} a_{\nu}^{\dagger}a_{\nu} &= (U_{\nu}\alpha_{\nu}^{\dagger} + V_{\nu}\alpha_{\bar{\nu}})(U_{\nu}\alpha_{\nu} + V_{\nu}\alpha_{\bar{\nu}}^{\dagger}) \\ &= U_{\nu}^{2}\alpha_{\nu}^{\dagger}\alpha_{\nu} + U_{\nu}V_{\nu}\alpha_{\nu}^{\dagger}\alpha_{\bar{\nu}}^{\dagger} + U_{\nu}V_{\nu}\alpha_{\bar{\nu}}\alpha_{\nu} + V_{\nu}^{2}\alpha_{\bar{\nu}}\alpha_{\bar{\nu}}^{\dagger} \\ &= U_{\nu}^{2}\alpha_{\nu}^{\dagger}\alpha_{\nu} + U_{\nu}V_{\nu}(\alpha_{\nu}^{\dagger}\alpha_{\bar{\nu}}^{\dagger} + \alpha_{\bar{\nu}}\alpha_{\nu}) - V_{\nu}^{2}\alpha_{\bar{\nu}}^{\dagger}\alpha_{\bar{\nu}} + V_{\nu}^{2}. \end{aligned}$$
(G.4)

The time reversal of this expression reads

$$a_{\bar{\nu}}^{\dagger}a_{\bar{\nu}} = U_{\nu}^{2}\alpha_{\bar{\nu}}^{\dagger}\alpha_{\bar{\nu}} + U_{\nu}V_{\nu}(\alpha_{\nu}^{\dagger}\alpha_{\bar{\nu}}^{\dagger} + \alpha_{\bar{\nu}}\alpha_{\nu}) - V_{\nu}^{2}\alpha_{\nu}^{\dagger}\alpha_{\nu} + V_{\nu}^{2},$$

where the phase relation $|\tilde{\tilde{\nu}}\rangle = \tau^2 |\nu\rangle = -|\nu\rangle$ and thus $a_{\tilde{\tilde{\nu}}}^{\dagger} = -a_{\nu}^{\dagger}$ have been used. One can then write

$$(a_{\nu}^{\dagger}a_{\nu} + a_{\bar{\nu}}^{\dagger}a_{\bar{\nu}}) = (U_{\nu}^{2} - V_{\nu}^{2})(\alpha_{\nu}^{\dagger}\alpha_{\nu} + \alpha_{\bar{\nu}}^{\dagger}\alpha_{\bar{\nu}}) + 2U_{\nu}V_{\nu}(\alpha_{\nu}^{\dagger}\alpha_{\bar{\nu}}^{\dagger} + \alpha_{\bar{\nu}}\alpha_{\nu}) + 2V_{\nu}^{2}.$$
(G.5)

Note that

$$N = \langle \text{BCS} | \hat{N} | \text{BCS} \rangle = \langle \text{BCS} | \sum_{\nu > 0} (a_{\nu}^{\dagger} a_{\nu} + a_{\bar{\nu}}^{\dagger} a_{\bar{\nu}}) | \text{BCS} \rangle = 2 \sum_{\nu > 0} V_{\nu}^{2}$$
(G.6)

is the average number of particles in the pairing mean-field ground state (BCS state).

Let us now express the pair-creation field $a^{\dagger}_{\nu}a^{\dagger}_{\bar{\nu}}$ in terms of quasiparticles

$$a_{\nu}^{\dagger}a_{\bar{\nu}}^{\dagger} = (U_{\nu}\alpha_{\nu}^{\dagger} + V_{\nu}\alpha_{\bar{\nu}})(U_{\nu}\alpha_{\bar{\nu}}^{\dagger} - V_{\nu}\alpha_{\nu})$$

$$= U_{\nu}^{2}\alpha_{\nu}^{\dagger}\alpha_{\bar{\nu}}^{\dagger} - U_{\nu}V_{\nu}\alpha_{\nu}^{\dagger}\alpha_{\nu}$$

$$+ V_{\nu}U_{\nu}\alpha_{\bar{\nu}}^{\dagger}\alpha_{\bar{\nu}} - V_{\nu}^{2}\alpha_{\bar{\nu}}\alpha_{\nu} + U_{\nu}V_{\nu}.$$
 (G.7)

The Hermitian conjugate of this expression is then

$$a_{\bar{\nu}}a_{\nu} = U_{\nu}^{2}\alpha_{\bar{\nu}}\alpha_{\nu} - U_{\nu}V_{\nu}(\alpha_{\nu}^{\dagger}\alpha_{\nu} + \alpha_{\bar{\nu}}^{\dagger}\alpha_{\bar{\nu}}) - V_{\nu}^{2}\alpha_{\nu}^{\dagger}\alpha_{\bar{\nu}}^{\dagger} + U_{\nu}V_{\nu}.$$
 (G.8)

Summing these expressions leads to

$$(a_{\nu}^{\dagger}a_{\bar{\nu}}^{\dagger}+a_{\bar{\nu}}a_{\nu})=(U_{\nu}^{2}-V_{\nu}^{2})(\alpha_{\nu}^{\dagger}\alpha_{\bar{\nu}}^{\dagger}+\alpha_{\bar{\nu}}\alpha_{\nu})-2U_{\nu}V_{\nu}(\alpha_{\nu}^{\dagger}\alpha_{\bar{\nu}}+\alpha_{\bar{\nu}}^{\dagger}\alpha_{\nu})+2U_{\nu}V_{\nu}.$$

Note that

$$\alpha_0 = \langle \text{BCS} | P^{\dagger} | \text{BCS} \rangle = \sum_{\nu > 0} \langle \text{BCS} | a_{\nu}^{\dagger} a_{\bar{\nu}} | \text{BCS} \rangle = \sum_{\nu > 0} U_{\nu} V_{\nu} \tag{G.9}$$

and

$$\Delta = G\alpha_0 = G\sum_{\nu>0} U_{\nu} V_{\nu}.$$
(G.10)

Making use of the relations worked out above one can express $H_{\rm MF}$ in terms of quasiparticles, i.e.

$$H_{\rm MF} = U + H_{11} + H_{20},\tag{G.11}$$

where

$$U = 2 \sum_{\nu>0} (\varepsilon_{\nu} - \lambda) V_{\nu}^{2} - \Delta \sum_{\nu>0} 2U_{\nu}V_{\nu} + \frac{\Delta^{2}}{G},$$

$$H_{11} = \sum_{\nu>0} \left\{ (\varepsilon_{\nu} - \lambda)(U_{\nu}^{2} - V_{\nu}^{2}) + \Delta 2U_{\nu}V_{\nu} \right\} (\alpha_{\nu}^{\dagger}\alpha_{\nu} + \alpha_{\bar{\nu}}^{\dagger}\alpha_{\bar{\nu}}),$$

$$H_{20} = \sum_{\nu>0} \left\{ (\varepsilon_{\nu} - \lambda)2U_{\nu}V_{\nu} - \Delta (U_{\nu}^{2} - V_{\nu}^{2}) \right\} (\alpha_{\nu}^{\dagger}\alpha_{\bar{\nu}}^{\dagger} + \alpha_{\bar{\nu}}\alpha_{\nu}).$$

In other words, the mean-field pairing Hamiltonian expressed in terms of quasiparticles is equal to the sum of three terms: one which is a constant, a second one which is diagonal in the quasiparticle basis, and a third one which, although bilinear in the operators α^{\dagger} and α , is not diagonal. Consequently, imposing the condition $H_{20} = 0$, i.e.

$$(\varepsilon_{\nu} - \lambda)2U_{\nu}V_{\nu} = \Delta(U_{\nu}^2 - V_{\nu}^2), \qquad (G.12)$$

is equivalent to diagonalizing H_{MF} . This relation together with equation (G.3) allows us to calculate the corresponding coefficients U_{ν} and V_{ν} .

We start by taking the square of the above relation,

$$(\varepsilon_{\nu} - \lambda)^2 4 U_{\nu}^2 V_{\nu}^2 = \Delta^2 (U_{\nu}^2 - V_{\nu}^2)^2.$$
 (G.13)

From the normalization relation one can write

$$(U_{\nu}^{2} + V_{\nu}^{2})^{2} = 1 = U_{\nu}^{4} + V_{\nu}^{4} + 2U_{\nu}^{2}V_{\nu}^{2}$$

and

$$U_{\nu}^{4} + V_{\nu}^{4} = 1 - 2U_{\nu}^{2}V_{\nu}^{2}.$$

Consequently,

$$(U_{\nu}^{2} - V_{\nu}^{2})^{2} = U_{\nu}^{4} + U_{\nu}^{4} - 2U_{\nu}^{2}V_{\nu}^{2} = 1 - 4U_{\nu}^{2}V_{\nu}^{2}$$

Inserting this relation in equation (G.13) leads to

$$4U_{\nu}^{2}V_{\nu}^{2}((\varepsilon_{\nu}-\lambda)^{2}+\Delta^{2})=\Delta^{2},$$

a relation which can be rewritten as

$$2U_{\nu}V_{\nu} = \frac{\Delta}{E_{\nu}},\tag{G.14}$$

where the + sign of the square root operation implies the minimization of the ground-state energy U. The quantity E_{ν} is given by

$$E_{\nu} = \sqrt{(\varepsilon_{\nu} - \lambda)^2 + \Delta^2}.$$
 (G.15)

Making use again of the condition $H_{20} = 0$ one can write

$$(\varepsilon_{\nu} - \lambda) \frac{\Delta}{E_{\nu}} = \Delta (U_{\nu}^2 - V_{\nu}^2).$$

i.e.

$$(U_{\nu}^{2} - V_{\nu}^{2}) = \frac{\varepsilon_{\nu} - \lambda}{E_{\nu}},$$

$$(G.16)$$

$$U_{\nu}^{2} - V_{\nu}^{2} = 1 - 2V_{\nu}^{2} = \frac{\varepsilon_{\nu} - \lambda}{E_{\nu}},$$

$$V_{\nu}^{2} = \frac{1}{2} \left(1 - \frac{\varepsilon_{\nu} - \lambda}{E_{\nu}} \right),$$

leading to

$$V_{\nu} = \frac{1}{\sqrt{2}} \left(1 - \frac{\varepsilon_{\nu} - \lambda}{E_{\nu}} \right)^{1/2}, \tag{G.17}$$

$$U_{\nu} = \frac{1}{\sqrt{2}} \left(1 + \frac{\varepsilon_{\nu} - \lambda}{E_{\nu}} \right)^{1/2}.$$
 (G.18)

Let us now substitute these expressions in the relation (G.10). One obtains

$$\Delta = \frac{G}{2} \sum_{\nu > 0} \left(1 - \frac{(\varepsilon_{\nu} - \lambda)^2}{E_{\nu}^2} \right)^{1/2} = \frac{G}{2} \sum_{\nu > 0} \frac{\Delta}{E_{\nu}}.$$

The above equation together with equation (G.6) are the BCS equations, i.e.

$$N = 2 \sum_{\nu > 0} V_{\nu}^{2} \qquad \text{(number equation)}, \tag{G.19}$$

$$\frac{1}{G} = \sum_{\nu>0} \frac{1}{2E_{\nu}} \qquad \text{(gap equation).} \tag{G.20}$$

These equations allow us to calculate the parameters λ and Δ from the knowledge of *G* and ε_{ν} , parameters which completely determine the occupation amplitudes U_{ν} and V_{ν} .

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One can now write U in terms of the parameters λ and Δ , i.e.

$$U = 2\sum_{\nu>0} (\varepsilon_{\nu} - \lambda) V_{\nu}^2 - 2\frac{\Delta^2}{G} + \frac{\Delta^2}{G}$$
$$= 2\sum_{\nu>0} (\varepsilon_{\nu} - \lambda) V_{\nu}^2 - \frac{\Delta^2}{G}.$$

Making use of equations (G.14), (G.15) and (G.18) one can write H_{11} in terms of λ and Δ ,

$$H_{11} = \sum_{\nu>0} \left\{ \frac{(\varepsilon_{\nu} - \lambda)^2}{E_{\nu}} + \frac{\Delta^2}{E_{\nu}} \right\} (\alpha_{\nu}^{\dagger} \alpha_{\nu} + \alpha_{\bar{\nu}}^{\dagger} \alpha_{\bar{\nu}})$$

$$= \sum_{\nu>0} E_{\nu} (\alpha_{\nu}^{\dagger} \alpha_{\nu} + \alpha_{\bar{\nu}}^{\dagger} \alpha_{\bar{\nu}}) = \sum_{\nu} E_{\nu} \alpha_{\nu}^{\dagger} \alpha_{\nu}$$

$$= \sum_{\nu} E_{\nu} \hat{N}_{\nu}, \qquad (G.21)$$

where $\hat{N}_{\nu} = \alpha_{\nu}^{\dagger} \alpha_{\nu}$.

G.2 Two-quasiparticle excitations

In the case of a normal system, within the independent-particle model, the lowest excitations are of particle-hole character, i.e.

$$|ki\rangle = a_k^{\dagger} a_i |0\rangle_{\rm HF},$$

where

$$|0\rangle_{\mathrm{HF}} = \prod_{i=1}^{A} a_{i}^{\dagger} |0\rangle \; ,$$

 $(|0\rangle_{HF}$: Hartree–Fock vacuum, $|0\rangle$: fermion vacuum).

Making use of the single-particle Hamiltonian

$$H_{\rm sp} = \sum_{\nu} \varepsilon_{\nu} a_{\nu}^{\dagger} a_{\nu} = \sum_{\nu} \varepsilon_{\nu} \hat{N}_{\nu}$$

one can calculate the energy of the particle-hole states. Let us start with the calculation of the ground-state energy,

$$H_{\rm sp}|0\rangle_{\rm HF} = \sum_{\nu} \varepsilon_{\nu} N_{\nu} \prod_{i=1}^{A} a_{i}^{\dagger}|0\rangle$$
$$= \sum_{\nu} \varepsilon_{\nu} a_{\nu}^{\dagger} a_{\nu} a_{1}^{\dagger} a_{2}^{\dagger} \cdots a_{A}^{\dagger}|0\rangle$$
$$= (\varepsilon_{\nu_{1}} + \varepsilon_{\nu_{2}} + \cdots + \varepsilon_{\nu_{A}})|0\rangle_{\rm HF} = E_{0}|0\rangle_{\rm HF}.$$

Let us now calculate the energy of the particle-hole excitation referred to this energy, i.e.

$$\begin{split} (H_{\rm sp} - E_0) |ki\rangle &= \sum_{\nu} (\varepsilon_{\nu} \hat{N}_{\nu} - E_0) a_k^{\dagger} a_i |0\rangle_{\rm HF} \\ &= \sum_{\nu} \varepsilon_{\nu} (a_k^{\dagger} \left[\hat{N}_{\nu}, a_i \right] + \left[\hat{N}_{\nu}, a_k^{\dagger} \right] a_i) |0\rangle_{\rm HF}. \end{split}$$

We have now to work out the commutation relations appearing in the above equations. They lead to

$$\begin{bmatrix} \hat{N}_{\nu}, a_i \end{bmatrix} = \begin{bmatrix} a_{\nu}^{\dagger} a_{\nu}, a_i \end{bmatrix} = -\{a_{\nu}^{\dagger}, a_i\}a_{\nu} = -\delta(\nu, i)a_{\nu}, \\ \begin{bmatrix} N_{\nu}, a_k^{\dagger} \end{bmatrix} = \begin{bmatrix} a_{\nu}^{\dagger} a_{\nu}, a_k^{\dagger} \end{bmatrix} = a_{\nu}^{\dagger}\{a_{\nu}, a_k^{\dagger}\} = \delta(\nu, k)a_{\nu}^{\dagger},$$

where use was made of the relations

$$[AB, C] = A [B, C] + [A, C] B = ABC - ACB - ACB + CAB$$

and

$$[AB, C] = A\{B, C\} - \{A, C\}B = ABC + ACB - ACB - CAB.$$

One can then write

$$\begin{aligned} (H_{\rm sp} - E_0)|ki\rangle &= \sum_{\nu} \varepsilon(a_k^{\dagger}(-\delta(\nu, i)a_{\nu} + \delta(\nu, k)a_{\nu}^{\dagger}a_i)|0\rangle_{\rm HF} \\ &= (\varepsilon_k - \varepsilon_i)a_k^{\dagger}a_i|0\rangle_{\rm HF} = (\varepsilon_k - \varepsilon_i)|ki\rangle. \end{aligned}$$

Summing up, the simplest excitation of the $|0\rangle_{HF}$ vacuum is

 $a_k^{\dagger}a_i|0\rangle_{\rm HF},$

i.e. a particle-hole excitation. The lowest of these excitations connects the last occupied and the first empty state.

In the case of quasiparticles

$$\begin{split} H_{\rm sp} &\Rightarrow H_{11} + U; \quad |0\rangle_{\rm HF} \Rightarrow |{\rm BCS}\rangle \\ a_k^{\dagger} a_i &\Rightarrow a_\nu^{\dagger} a_\nu = (U_\nu \alpha_\nu^{\dagger} + V_\nu \alpha_{\bar{\nu}})(U_\nu \alpha_\nu + V_\nu \alpha_{\bar{\nu}}^{\dagger}) \\ &= U_\nu^2 \alpha_\nu^{\dagger} \alpha_\nu + U_\nu V_\nu \alpha_\nu^{\dagger} \alpha_{\bar{\nu}}^{\dagger} + V_\nu U_\nu \alpha_{\bar{\nu}} \alpha_\nu \\ &- V_\nu^2 \alpha_\nu^{\dagger} \alpha_\nu + V_\nu^2 \;, \end{split}$$

leading to

$$a_{k}^{\dagger}a_{i}|0\rangle_{\mathrm{HF}} \rightarrow U_{\nu}V_{\nu}\alpha_{\nu}^{\dagger}\alpha_{\overline{\nu}}^{\dagger}|\mathrm{BCS}\rangle \sim \alpha_{\nu}^{\dagger}\alpha_{\overline{\nu}}^{\dagger}|\mathrm{BCS}\rangle,$$

in that $V_{\nu}^2 |\text{BCS}\rangle$ is not an excitation. Thus, the simplest excitation of the $|\text{BCS}\rangle$ vacuum is

$$\alpha_{\nu}^{\dagger}\alpha_{\tilde{\nu}}^{\dagger}|\mathrm{BCS}\rangle = |\nu\tilde{\nu}\rangle,$$

i.e. a two-quasiparticle state.

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The excitation energy associated with these states is

$$H_{11}|\nu_{1}\nu_{2}\rangle = \sum_{\nu} E_{\nu} \hat{N}_{\nu} \alpha_{\nu_{1}}^{\dagger} \alpha_{\nu_{2}}^{\dagger} |\text{BCS}\rangle$$
$$= \sum_{\nu} E_{\nu} [\hat{N}_{\nu_{1}} \alpha_{\nu_{1}}^{\dagger} \alpha_{\nu_{2}}^{\dagger}] |\text{BCS}\rangle$$

in keeping with the fact that $\hat{N}_{\nu}|BCS\rangle = 0$. We now calculate

$$\begin{split} & [\hat{N}_{\nu}, \alpha_{\nu_{1}}^{\dagger} \alpha_{\nu_{2}}^{\dagger}] = \alpha_{\nu_{1}}^{\dagger} [\hat{N}_{\nu}, \alpha_{\nu_{2}}^{\dagger}] + [\hat{N}_{\nu}, \alpha_{\nu_{1}}^{\dagger}] \alpha_{\alpha_{2}}^{\dagger}, \\ & \left[\hat{N}_{\nu}, \alpha_{\nu_{2}}^{\dagger}\right] = [\alpha_{\nu}^{\dagger} \alpha_{\nu}, \alpha_{\nu_{2}}^{\dagger}] = \alpha_{\nu}^{\dagger} \{\alpha_{\nu}, \alpha_{\nu_{2}}^{\dagger}\} - \{\alpha_{\nu}^{\dagger}, \alpha_{\nu_{2}}^{\dagger}\} \alpha_{\nu} \\ & = \delta(\nu, \nu_{2}) \alpha_{\nu}^{\dagger} \end{split}$$

and

$$\begin{split} \left[\hat{N}_{\nu}, \alpha_{\nu_{1}}^{\dagger}\right] &= \left[\alpha_{\nu}^{\dagger}\alpha_{\nu}, \alpha_{\nu_{1}}^{\dagger}\right] = \alpha_{\nu}^{\dagger}\{\alpha_{\nu}, \alpha_{\nu_{1}}^{\dagger}\} - \{\alpha_{\nu}^{\dagger}, \alpha_{\nu_{1}}^{\dagger}\}\alpha_{\nu} \\ &= \delta(\nu, \nu_{1})\alpha_{\nu}^{\dagger}. \end{split}$$
(G.22)

Consequently

$$\left[\hat{N}_{\nu},\alpha_{\nu_{1}}^{\dagger}\alpha_{\nu_{2}}^{\dagger}\right] = \delta(\nu,\nu_{2})\alpha_{\nu_{1}}^{\dagger}\alpha_{\nu}^{\dagger} + \delta(\nu,\nu_{1})\alpha_{\nu}^{\dagger}\alpha_{\nu_{2}}^{\dagger}.$$

From these relations one can write

$$H_{11}|\nu_{1}\nu_{2}\rangle = \sum_{\nu} E_{\nu} \left(\delta(\nu, \nu_{2}) \alpha_{\nu_{1}}^{\dagger} \alpha_{\nu}^{\dagger} + \delta(\nu, \nu_{1}) \alpha_{\nu}^{\dagger} \alpha_{\nu_{2}} \right) |\text{BCS}\rangle$$

= $(E_{\nu_{1}} + E_{\nu_{2}}) \alpha_{\nu_{1}}^{\dagger} \alpha_{\nu_{2}}^{\dagger} |\text{BCS}\rangle = (E_{\nu_{1}} + E_{\nu_{2}}) |\nu_{1}\nu_{2}\rangle.$

Because $(E_{\nu_1} + E_{\nu_2}) \ge 2\Delta$, the lowest excitation in the pairing correlated system lies at an energy $\ge 2\Delta$, i.e. the energy which it takes to break a pair. In fact, in the paired system, the only excitations possible are those associated with the breaking of pairs of particles moving in time-reversal states, an operation which takes an energy of the order of 2Δ .

G.3 Minimization

Writing the pairing Hamiltonian given in equation (G.1) in terms of quasiparticles one can calculate the average value in the $|BCS\rangle$ ground state, obtaining

$$\langle \text{BCS} | H_{\text{p}} | \text{BCS} \rangle = -G \sum_{\nu > 0} V_{\nu}^{4} - G \sum_{\nu, \nu' > 0} U_{\nu} V_{\nu} U_{\nu'} V_{\nu'}$$

= $-G \left(\sum_{\nu > 0} U_{\nu} V_{\nu} \right)^{2} - G \sum_{\nu > 0} V_{\nu}^{4}$
= $-\frac{\Delta^{2}}{G} - G \sum_{\nu > 0} V_{\nu}^{4}.$

Similarly,

$$\langle \mathrm{BCS} | H_{\mathrm{sp}} | \mathrm{BCS} \rangle = 2 \sum_{\nu > 0} (\varepsilon_{\nu} - \lambda) V_{\nu}^{2}.$$

Consequently

$$\begin{split} E_0 &= \langle \mathrm{BCS} | H | \mathrm{BCS} \rangle = 2 \sum_{\nu>0} (\varepsilon_\nu - \lambda) V_\nu^2 - \frac{\Delta^2}{G} - G \sum_{\nu>0} V_\nu^4 \\ &= 2 \sum_{\nu>0} (\varepsilon_\nu - \lambda) V_\nu^2 - G (\sum_{\nu>0} U_\nu V_\nu)^2 - G \sum_{\nu>0} V_\nu^4 \\ &\approx 2 \sum_{\nu>0} (\varepsilon_\nu - \lambda) V_\nu^2 - G \left(\sum_{\nu>0} U_\nu V_\nu \right)^2, \end{split}$$

where we have neglected the mean-field pairing contribution to the single-particle energy (i.e. $\varepsilon'_{\nu} = \varepsilon_{\nu} - GV_{\nu}^2/2 \approx \varepsilon_{\nu}$), in keeping with the fact that $GV_{\nu}^2/2$ is small ($\approx \frac{G}{4} \approx \frac{6}{A}$ MeV ~ 0.05 MeV, with the ansatz $V_{\nu}^2 \approx \frac{1}{2}$ and for $A \approx 120$).

Let us minimize E_0 with respect to V_{ν}

$$\frac{\partial \langle \mathrm{BCS} | H | \mathrm{BCS} \rangle}{\partial V_{\nu}} = 0,$$

taking into account the normalization condition,

$$\begin{aligned} \frac{\partial U_{\nu}}{\partial V_{\nu}} &= \frac{\partial}{\partial V_{\nu}} (1 - V_{\nu}^2)^{1/2} = \frac{1}{2} (1 - V_{\nu}^2)^{-1/2} (-2V_{\nu}) \\ &= -\frac{V_{\nu}}{U_{\nu}} \,. \end{aligned}$$

One thus obtains

$$\begin{aligned} \frac{\partial \langle \text{BCS} | H | \text{BCS} \rangle}{\partial V_{\nu'}} &= 4(\varepsilon_{\nu'} - \lambda) V_{\nu}' - 2G\left(\sum_{\nu > 0} U_{\nu} V_{\nu})(U_{\nu'} - V_{\nu'} \frac{V_{\nu'}}{U_{\nu'}}\right) \\ &= 4(\varepsilon_{\nu'} - \lambda) V_{\nu'} - 2\frac{\Delta}{U_{\nu'}}(U_{\nu'}^2 - V_{\nu'}^2) = 0, \end{aligned}$$

i.e.

$$2(\varepsilon_{\nu'} - \lambda)U_{\nu'}V_{\nu'} = \Delta(U_{\nu'}^2 - V_{\nu'}^2), \qquad (G.23)$$

which is the condition $H_{20} = 0$ (see (G.12)).

G.4 BCS wavefunction

The state $|BCS\rangle$ is the quasiparticle vacuum, i.e.

$$\alpha_{\nu}|\mathrm{BCS}\rangle = 0.$$

Consequently, it can be written as

$$|\mathrm{BCS}
angle\sim\prod_{
u}lpha_{
u}|0
angle\sim\prod_{
u>0}lpha_{
u}lpha_{\overline{
u}}|0
angle.$$

Let us now calculate $\alpha_{\nu}\alpha_{\overline{\nu}}$, i.e. the product of

$$\alpha_{\nu} = U_{\nu}a_{\nu} - V_{\nu}a_{\overline{\nu}}^{\dagger}$$

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and

$$\alpha_{\overline{\nu}} = U_{\nu}a_{\overline{\nu}} + V_{\nu}a_{\nu}^{\dagger}.$$

It leads to

$$\begin{aligned} \alpha_{\nu}\alpha_{\overline{\nu}} &= U_{\nu}^{2}a_{\nu}a_{\overline{\nu}} + U_{\nu}V_{\nu}a_{\nu}a_{\nu}^{\dagger} - U_{\nu}V_{\nu}a_{\overline{\nu}}^{\dagger}a_{\overline{\nu}} - V_{\nu}^{2}a_{\overline{\nu}}^{\dagger}a_{\nu}^{\dagger} \\ &= U_{\nu}^{2}a_{\nu}a_{\overline{\nu}} + U_{\nu}V_{\nu}(1 - a_{\nu}^{\dagger}a_{\nu}) - U_{\nu}V_{\nu}a_{\overline{\nu}}^{\dagger}a_{\overline{\nu}} + V_{\nu}^{2}a_{\nu}^{\dagger}a_{\overline{\nu}}^{\dagger}. \end{aligned}$$

Consequently

$$\begin{split} |\mathrm{BCS}\rangle &= N \prod_{\nu>0} \left(U_{\nu}^{2} a_{\nu} a_{\overline{\nu}} + U_{\nu} V_{\nu} (1 - a_{\nu}^{\dagger} a_{\nu}) - U_{\nu} V_{\nu} a_{\overline{\nu}}^{\dagger} a_{\overline{\nu}} + V_{\nu}^{2} a_{\nu}^{\dagger} a_{\overline{\nu}}^{\dagger} \right) |0\rangle \\ &= N \prod_{\nu>0} \left(U_{\nu} V_{\nu} + V_{\nu}^{2} a_{\nu}^{\dagger} a_{\overline{\nu}}^{\dagger} \right) |0\rangle \\ &= N \prod_{\nu>0} V_{\nu} \left(U_{\nu} + V_{\nu} a_{\nu}^{\dagger} a_{\overline{\nu}}^{\dagger} \right) |0\rangle, \end{split}$$

where N is a normalization constant, to be determined from the relation

$$1 = \langle \text{BCS} | \text{BCS} \rangle$$

= $N^2 \langle 0 | \prod_{\nu > 0} V_{\nu} \left(U_{\nu} + V_{\nu} a_{\overline{\nu}} a_{\nu} \right) \prod_{\nu' > 0} V_{\nu'} \left(U_{\nu'} + V_{\nu'} a_{\nu'}^{\dagger} a_{\overline{\nu'}}^{\dagger} \right) | 0 \rangle$
= $N^2 \langle 0 | \prod_{\nu > 0} V_{\nu}^2 (U_{\nu}^2 + V_{\nu}^2) | 0 \rangle,$
 $N = \left(\prod_{\nu > 0} V_{\nu}^2 \right)^{-\frac{1}{2}} = \left(\prod_{\nu > 0} V_{\nu} \right)^{-1},$

leading to

$$|\mathrm{BCS}\rangle = \prod_{\nu>0} \left(U_{\nu} + V_{\nu} a_{\nu}^{\dagger} a_{\overline{\nu}}^{\dagger} \right) |0\rangle.$$