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Umklapp scattering of pairs in BCS superconductivity theory

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Abstract

The BCS theory of superconductivity is extended to recognize pairing of electrons by both normal and umklapp phonon scattering. Application of the variational approach shows that the coexistence of normal and umklapp scattering frustrates superconductivity.

1. Introduction

We wish to call attention to a result which, to our knowledge, has not previously been noticed: in a BCS (Bardeen, Cooper and Schrieffer) superconductor [1] a range of pair end states may be accessed via both normal and umklapp scattering. The situation resembles a double-slit experiment in which electrons have two paths to access the screen and cancel each other periodically in the production of the analogue of Young's fringes.

Umklapp scattering is compatible with the canonical transformation [2] which is the basis of the BCS theory. Discussion about umklapp contributions to superconductivity started almost immediately after the BCS theory was forged [3, 4]. This discussion has gathered renewed momentum since the high T_c superconductors have been discovered [5–10]. It is therefore timely to discuss our new result in some detail.

We show that the trial electron wavefunction in the standard BCS theory is not designed to accommodate states with multiple access paths. We find that, if we allow all the end states of both normal and umklapp scattering to be generated by this wavefunction, then we are not able to normalize it.

We extend the approach of BCS, who already modified their $T = 0$ trial function to accommodate single particles and excited pairs that appear at $T > 0$. We modify the BCS trial function at both $T = 0$ and $T > 0$ to include the occupation of states by both normal and umklapp scattering. We show that the modified trial function is always normalized.

We also show that the effect of umklapp scattering is to cancel the pairing effect of normal electron–phonon scattering. The cancellation is actually the physical foundation for

the average phonon frequency, significantly lower than the Debye frequency, introduced by BCS. We restrict our discussion exclusively to the BCS formalism, based on the principle of variation. We do not discuss for example the Eliashberg formalism [11], which derives from a different principle.

2. Hamiltonian

In the BCS theory the standard procedure of variation is followed. It starts with the reduced Hamiltonian

$$H_{\mathrm{BCS}} = 2\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} - \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} b_{\mathbf{k}'}^{\dagger} b_{\mathbf{k}} \tag{1}$$

where $V_{\mathbf{k},\mathbf{k}'}$ measures the strength of the electron–phonon interaction in second order,

$$b_{\mathbf{k}}^{\dagger} = a_{-\mathbf{k}\downarrow}^{\dagger} a_{\mathbf{k}\uparrow}^{\dagger} \tag{2}$$

generates pairs, $a^{\dagger}$ being the particle generation operator, $\mathbf{k}$ the electron wavevector, and $\uparrow$ and $\downarrow$ spin. In equation (1) $\mathbf{k}$ runs over each and every state of the first electron Brillouin zone exactly once with spin $\uparrow$ (we assume a single band throughout our discussion). Simultaneously $-\mathbf{k}$ runs over the same range with spin $\downarrow$. An alternative approach, which we do not adopt, is to let $\mathbf{k}$ in equation (1) run over half the Brillouin zone and sum the spins. Either way, we may have spin $\uparrow$ and $\downarrow$ for any specific value of $\mathbf{k}$. Consequently the paired particles may be in $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ or $(\mathbf{k}\downarrow, -\mathbf{k}\uparrow)$.

In equation (1) the electron term is in $b_{\mathbf{k}}^{\dagger}$ and $b_{\mathbf{k}}$, which is not entirely equivalent to the standard electron Hamiltonian

$$\sum_{\mathbf{k}} \left(\epsilon_{\mathbf{k}} a_{\mathbf{k}\uparrow}^{\dagger} a_{\mathbf{k}\uparrow} + \epsilon_{\mathbf{k}} a_{\mathbf{k}\downarrow}^{\dagger} a_{\mathbf{k}\downarrow} \right). \tag{3}$$

The electron term in equation (1) will vanish when applied to single particles, but the Hamiltonian in expression (3) will not: equation (1) is designed only for a pair ensemble. Indeed even expression (3) is designed only for electrons in crystals, where we have discrete electron energy $\epsilon_{\mathbf{k}}$, which is produced automatically by the Hamiltonian when an electron is detected by the particle destruction operator $a_{\mathbf{k}\uparrow}$ or $a_{\mathbf{k}\downarrow}$.

3. Trial function

Next is introduced the trial wavefunction for quasi-particles. At $T = 0$ this function is of the following form in the BCS theory [1]:

$$|\Psi\rangle = \prod_{\mathbf{k}} \left(\sqrt{1 - h_{\mathbf{k}}} + \sqrt{h_{\mathbf{k}}} b_{\mathbf{k}}^{\dagger} \right) |0\rangle \tag{4}$$

where $h_{\mathbf{k}}$ is the pair occupation probability and $|0\rangle$ the pair vacuum. Here we seek the equilibrium configuration of the particle ensemble under the influence of the electron–phonon interaction. The trial function must accommodate all the initial and end states of the paired quasi-particles, which are indicated by $\mathbf{k}$ and $\mathbf{k}'$ in equation (1), with occupancy probabilities $h_{\mathbf{k}}$ to be determined for both the initial and end states in a single step of the process of variation.

Now in equation (4) the product over $\mathbf{k}$ also runs over the first electron Brillouin zone, i.e. the number of orbits in equation (4) equals the number of Bloch states. However, this does not mean that we cannot add further orbits to equation (4). The growth of the superconductive energy gap can be compared with the splitting of the spectral line of, for example, the hydrogen atom, where the electron has several configurations, with different patterns of particle location

probability and/or spin but the same energy. This energy degeneracy splits to reveal further structure in the presence of, for example, an external magnetic field. Similarly, a particle pair has two configurations, generated by

$$\sqrt{1-h_{\mathbf{k}}}+\sqrt{h_{\mathbf{k}}}b_{\mathbf{k}}^{\dagger} \tag{5}$$

and

$$\sqrt{1-h_{\mathbf{k}}}b_{\mathbf{k}}^{\dagger}-\sqrt{h_{\mathbf{k}}} \tag{6}$$

respectively, whose energy splits from the Bloch energy $\epsilon_{\mathbf{k}}$ in the presence of the electron–phonon interaction. The energy of the pair generated by expression (5) shifts downwards to give the energy gap. The energy of the pair generated by expression (6) shifts upwards. Apparently, in addition to the Bloch orbits, we may have two more orbits per primitive cell. Equation (4) does not include all the available orbits, because the paired states there suffice to accommodate the physics: the superconductive current is carried only by the paired quasi-particles with energy shifted downwards under the electron–phonon interaction.

When $T > 0$, equation (4) no longer suffices to accommodate the physics. Indeed, if we continue to employ equation (4) as our trial function, then we have no chance to see what happens when superconductive pairs break into single particles or are excited under the attack of thermal phonons. To cope, BCS modified equation (4) into the following form:

$$|\Psi\rangle_{\mathrm{exc}}=\prod_{\mathbf{k}''(\mathcal{S})}a_{\mathbf{k}''\sigma}^{\dagger}\prod_{\mathbf{k}'(\mathcal{P})}\left(\sqrt{1-h_{\mathbf{k}'}}b_{\mathbf{k}'}^{\dagger}-\sqrt{h_{\mathbf{k}'}}\right)\prod_{\mathbf{k}(\mathcal{G})}\left(\sqrt{1-h_{\mathbf{k}}}+\sqrt{h_{\mathbf{k}}}b_{\mathbf{k}}^{\dagger}\right)|0\rangle \tag{7}$$

where $\mathcal{S}$, $\mathcal{P}$ and $\mathcal{G}$ specify the states occupied by single particles, excited pairs and ground pairs respectively, σ (which could be denoted as $\sigma_{\mathbf{k}}$) stands for either $\uparrow$ or $\downarrow$ depending on the value of $\mathbf{k}$ [1]. It is interesting to note that in equation (7) $\mathbf{k}$, $\mathbf{k}'$ and $\mathbf{k}''$ do not have to be different. Indeed we can check through direct calculation that, when $\mathbf{k}=\mathbf{k}'=\mathbf{k}''$, the wavefunctions of the single particle, the excited pair and the ground pair are orthogonal to each other: the total number of states in equation (7) can be three times as large as that in equation (4).

4. Destination state with multiple access paths

Consider in figure 1 a spherical Fermi surface that does not intersect the boundary of a Brillouin zone: suppose also there is a minimum separation q_0 between adjacent Fermi surfaces. An electron in state $\mathbf{k}$ may be scattered into $\mathbf{k}+\mathbf{q}$ to lie on the adjacent Fermi surface if the phonon momentum q exceeds q_0. Since it makes no physical difference if the reciprocal lattice vector $\mathbf{G}$ (parallel to $\mathbf{k}$ for simplicity) is added to an electron state, we can replace $\mathbf{k}+\mathbf{q}$ with $\mathbf{k}+\mathbf{q}+\mathbf{G}$, which lies on the original Fermi surface. This state is known as the end state of umklapp scattering and, in a non-superconducting metal, cannot be accessed through normal scattering (in the reduced zone scheme), at least for a range of $\mathbf{q}$ values.

In a superconductor one destination state may have multiple access paths. For example, in figure 1 $\mathbf{k}$ and $-\mathbf{k}$ are paired and, correspondingly, $\mathbf{k}+\mathbf{q}+\mathbf{G}$ and $-\mathbf{k}-\mathbf{q}-\mathbf{G}$ are also paired: scattering of the particle pair is synchronized, reminiscent of the synchronized motion of rotating doors. In the umklapp process in figure 1 we have the following possible chains of events concerning state occupation:

$$\mathbf{k}\rightarrow\mathbf{k}+\mathbf{q}\rightarrow\mathbf{k}+\mathbf{q}+\mathbf{G}\rightarrow-\mathbf{k}-\mathbf{q}-\mathbf{G}. \tag{8}$$

The first two arrows represent scattering and umklapp folding. The third arrow denotes synchronized occupation of the state $-\mathbf{k}-\mathbf{q}-\mathbf{G}$ by the particle initially in state $-\mathbf{k}$. These events can be compared with, for example, the passage of an electron through a slit, or reflection of a photon by a mirror, in an interference experiment. It is evident from figure 1 that $-\mathbf{k}-\mathbf{q}-\mathbf{G}$

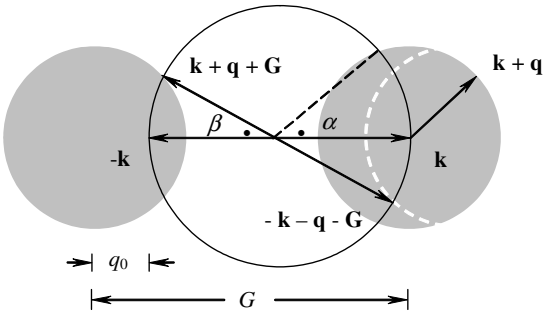

Figure 1. A spherical Fermi surface (open circle) and a pair of electrons in states $\mathbf{k}$ and $-\mathbf{k}$. This pair is scattered into states $\mathbf{k}+\mathbf{q}+\mathbf{G}$ and $-\mathbf{k}-\mathbf{q}-\mathbf{G}$ in the umklapp process, $\mathbf{q}$ being the phonon wavevector, and $\mathbf{G}$ the reciprocal lattice vector. The shaded circles represent two identical spherical phonon zones. We use angles α and β to measure the size of the sections of the Fermi surface being intersected by these phonon zones. We have $\alpha > \beta$ because a larger section of the Fermi surface is intersected by the phonon sphere centred at this surface (the other sphere is centred above the Fermi surface at height q_0). As a result, the electron state $-\mathbf{k}-\mathbf{q}-\mathbf{G}$ must lie inside the phonon sphere centred at $\mathbf{k}$, where all the states are involved in normal scattering. When $\mathbf{k}+\mathbf{q}+\mathbf{G}$ runs over the shaded phonon zone on the left, $-\mathbf{k}-\mathbf{q}-\mathbf{G}$ also runs over a sphere indicated in part by the broken white circle (centred above the Fermi surface at height q_0 to mirror the phonon sphere on the left).

lies inside the phonon sphere centred at $\mathbf{k}$, where all the electron normal-scattering end states lie, and therefore we also have the following normal-scattering event:

$$\mathbf{k} \rightarrow -\mathbf{k}-\mathbf{q}-\mathbf{G}. \tag{9}$$

Apparently the state $-\mathbf{k}-\mathbf{q}-\mathbf{G}$ can be accessed via two different paths.

We use $\mathcal{N}$ and $\mathcal{U}$ to denote collections of all the (single) end states of normal and umklapp scattering, respectively, which form thin layers about the Fermi surface, in which empty states are available to accommodate scattered particles. In figure 2 $\mathcal{N}$ is a section of the Fermi surface intersected by the phonon sphere centred at $\mathbf{k}$, whose radius is q_{D} (Debye momentum) to include all the phonons allowed in the Debye model. This phonon sphere may be transported to the left by a lattice constant G. The transported phonon sphere also intersects a section, $\mathcal{U}$, of the Fermi surface to accommodate particles scattered from $\mathbf{k}$ in the umklapp process. We separate $\mathcal{N}$ into two subsets, $\mathcal{N}_1$ and $\mathcal{N}_2$, where $\mathcal{N}_1$ accommodates particles scattered from $-\mathbf{k}$ in the umklapp process. It is apparent from figure 2 that an extensive range of states in $\mathcal{N}$ can be accessed via both normal and umklapp scattering.

We also use $\mathcal{N}$ and $\mathcal{U}$ to specify paired end states of normal and umklapp scattering (or normal and umklapp pairs for short). In figure 2 the single particle in state $\mathbf{k}$ may have spin $\uparrow$ or $\downarrow$. Consequently the normal or umklapp pair may be in $(\mathbf{k}'\uparrow, -\mathbf{k}'\downarrow)$ or $(\mathbf{k}'\downarrow, -\mathbf{k}'\uparrow)$ after scattering. The shape of $\mathcal{N}$ and $\mathcal{U}$ is the same in both cases.

5. Limitation of BCS trial function

The BCS trial function is not designed to accommodate states with multiple access paths, such as those described in expressions (8) and (9). To appreciate this, we study the example in figure 2, where we illustrate how states are linked by $V_{\mathbf{k},\mathbf{k}'}$ in equation (1) when $\mathbf{k}$ is in the direction of $\mathbf{G}$. We write equation (4) in the following equivalent form:

$$|\Psi\rangle = \prod_{\mathbf{k}'(\mathcal{N}_1)} \prod_{\mathbf{k}'(\mathcal{N}_2)} \prod_{\mathbf{k}'(\mathcal{U})} \left(\sqrt{1-h_{\mathbf{k}'}} + \sqrt{h_{\mathbf{k}'}}\, b^{\dagger}_{\mathbf{k}'}\right)|\Phi\rangle \tag{10}$$

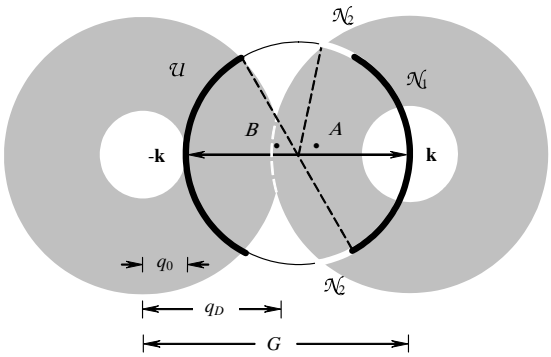

Figure 2. A spherical Fermi surface (open circle) with two phonon spheres of radius q_{D} (Debye momentum). In umklapp scattering the particle in $\mathbf{k}$ is scattered into $\mathcal{U}$, which is a layer about the Fermi surface shown as a thick black arc. In normal scattering the particle in state $\mathbf{k}$ is scattered into $\mathcal{N} = \mathcal{N}_1 + \mathcal{N}_2$, which is also a layer about the Fermi surface shown as a thick arc in black and white, $\mathcal{N}_1$ and $\mathcal{U}$ are symmetric with respect to the centre of the Fermi sphere. The sizes of $\mathcal{N}$ and $\mathcal{U}$ are measured by A and B, which are maximum values of α and β in figure 1. There is a hole in the phonon spheres to indicate that umklapp scattering is not invoked when the phonon momentum is less than q_0.

with

$$|\Phi\rangle = \prod_{\mathbf{k}''(\mathcal{R})} \left(\sqrt{1-h_{\mathbf{k}''}} + \sqrt{h_{\mathbf{k}''}}\, b^{\dagger}_{\mathbf{k}''}\right)|0\rangle \tag{11}$$

where $\mathcal{R}$ specifies states not in $\mathcal{N}_1$, $\mathcal{N}_2$ and $\mathcal{U}$. By definition for each $\mathbf{k}'$ in $\mathcal{U}$ we have $-\mathbf{k}'$ in $\mathcal{N}_1$ and vice versa, so that we can write the product over $\mathbf{k}'(\mathcal{N}_1)$ in equation (10) as

$$\prod_{\mathbf{k}'(\mathcal{U})} \left(\sqrt{1-h_{-\mathbf{k}'}} + \sqrt{h_{-\mathbf{k}'}}\, b^{\dagger}_{-\mathbf{k}'}\right). \tag{12}$$

Combining equations (10) and (12), we find

$$\langle\Psi|\Psi\rangle = \prod_{\mathbf{k}'(\mathcal{U})} \left[1 + 2\sqrt{h_{\mathbf{k}'}(1-h_{\mathbf{k}'})}\sqrt{h_{-\mathbf{k}'}(1-h_{-\mathbf{k}'})}\right]\langle\Phi|\Phi\rangle \tag{13}$$

so that $\langle\Psi|\Psi\rangle > 1$ even when $\langle\Phi|\Phi\rangle = 1$. Obviously the standard BCS theory is not designed to endorse the umklapp process in figure 1.

We cannot attribute the self-contradictory result in equation (13) to counting $\mathbf{k} + \mathbf{q}$ and $\mathbf{k} + \mathbf{q} + \mathbf{G}$ in figure 1 as different states, because the states in equation (10) are all in the first electron Brillouin zone (figure 2). We might like to attribute equation (13) to the proposition that normal and umklapp scattering drive two pairs into the same state, and thus violate the exclusion principle. However, the entity scattered in both the normal and umklapp processes is the same pair in $\mathbf{k}$ and $-\mathbf{k}$ (figures 1, 2): we do not have two pairs to violate that principle. It appears that, in equation (4), the number of orbits is simply not enough to cope with the situation that some areas of the Fermi surface, such as $\mathcal{N}_1$ in figure 2, suffer enhanced high probability of pair bombardment when normal and umklapp scattering coexist. Indeed equation (13) does suggest that the number of pairs landing in $\mathcal{U}$ and $\mathcal{N}_1$ exceeds the limit of its design.

6. Modified trial function

We extend the approach of BCS, who modified the trial function at $T = 0$, equation (4), into the trial function at $T > 0$, equation (7), to accommodate single particles and excited pairs.

We will modify the trial function at both $T = 0$ and $T > 0$ to accommodate umklapp scattering. We will add more orbits to equation (4) to allow umklapp pairs to land in $\mathcal{U}$ and $\mathcal{N}_1$ in figure 2, without self-contradiction as in equation (13). Since expression (5) has already been used to generate normal pairs in equation (4), we have no choice but to use expression (6) to generate umklapp pairs and find

$$|\Psi\rangle = \prod_{\mathbf{k}(\mathcal{U})} \left(\sqrt{1-h_{\mathbf{k}}}b_{\mathbf{k}}^{\dagger} - \sqrt{h_{\mathbf{k}}}\right) \prod_{\mathbf{k}(\mathcal{N})} \left(\sqrt{1-h_{\mathbf{k}}} + \sqrt{h_{\mathbf{k}}}b_{\mathbf{k}}^{\dagger}\right)|0\rangle \tag{14}$$

as our trial electron wavefunction in the presence of umklapp scattering.

According to equation (14) the equilibrium state of the particle ensemble consists of a mixture of normal and umklapp pairs. We find through direct calculation that we always have $\langle\Psi|\Psi\rangle = 1$ if we can prove

$$h_{\mathbf{k}} = h_{-\mathbf{k}} \tag{15}$$

where $\mathbf{k}$ and $-\mathbf{k}$ are specified by $\mathcal{U}$ and $\mathcal{N}$, respectively, in order to avoid a self-contradiction similar to that in equation (13). Equation (15) must be true, because both the Fermi sea and reciprocal lattice are symmetric with respect to $\mathbf{k} = 0$: interchanging $\mathbf{k}$ and $-\mathbf{k}$ makes no difference in equation (1), the Hamiltonian.

We have a more serious problem: in equation (14) we have actually assumed that $h_{\mathbf{k}}$ depends only on the numerical value of $\mathbf{k}$, regardless of whether $\mathbf{k}$ is specified by $\mathcal{N}$ or $\mathcal{U}$. Since the condition to find $h_{\mathbf{k}}$ may be different in $\mathcal{N}$ and $\mathcal{U}$, it is still possible that equation (14) could be self-contradictory, as was equation (4), in the presence of umklapp scattering. We will address this in the next section.

7. Occupancy of normal and umklapp pairs

We use equation (14) to evaluate the energy of the pair ensemble

$$W = \langle\Psi|H_{\mathrm{BCS}}|\Psi\rangle \tag{16}$$

where H_{BCS} is defined in equation (1). We find

$$W = 2\sum_{\mathbf{k}(\mathcal{N})} \epsilon_{\mathbf{k}}h_{\mathbf{k}} + 2\sum_{\mathbf{k}(\mathcal{U})} \epsilon_{\mathbf{k}}(1-h_{\mathbf{k}}) - W_{11} - W_{22} + W_{12} + W_{21} \tag{17}$$

with

$$W_{11} = \sum_{\mathbf{k}(\mathcal{N})}\sum_{\mathbf{k}'(\mathcal{N})} V_{\mathbf{k},\mathbf{k}'}\sqrt{h_{\mathbf{k}}(1-h_{\mathbf{k}})}\sqrt{h_{\mathbf{k}'}(1-h_{\mathbf{k}'})}$$

$$W_{12} = \sum_{\mathbf{k}(\mathcal{N})}\sum_{\mathbf{k}'(\mathcal{U})} V_{\mathbf{k},\mathbf{k}'}\sqrt{h_{\mathbf{k}}(1-h_{\mathbf{k}})}\sqrt{h_{\mathbf{k}'}(1-h_{\mathbf{k}'})}.$$

W_{21} and W_{22} are identical to W_{12} and W_{11}, respectively, save that $\mathcal{N}$ is replaced by $\mathcal{U}$ and vice versa.

We minimize W in equation (17) with respect to $h_{\mathbf{k}}$. When $\mathbf{k}$ is specified by $\mathcal{N}$ we have

$$\frac{\partial W}{\partial h_{\mathbf{k}}} = 2\epsilon_{\mathbf{k}} - \frac{1-2h_{\mathbf{k}}}{\sqrt{h_{\mathbf{k}}(1-h_{\mathbf{k}})}}\left[\sum_{\mathbf{k}'(\mathcal{N})} - \sum_{\mathbf{k}'(\mathcal{U})}\right] V_{\mathbf{k},\mathbf{k}'}\sqrt{h_{\mathbf{k}'}(1-h_{\mathbf{k}'})}. \tag{18}$$

Here $\epsilon_{\mathbf{k}}$ and $h_{\mathbf{k}}$ are linked together by the constraint

$$h_{\mathbf{k}} = \frac{1}{2}\left[1 - \frac{\epsilon_{\mathbf{k}}}{E(\mathbf{k})}\right] \tag{19}$$

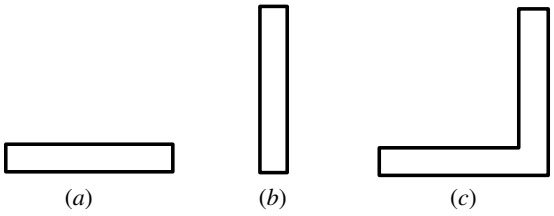

Figure 3. Configurations of (a) bar with minimum energy, (b) bar with maximum energy, and (c) two bar system.

with $E(\mathbf{k}) = \sqrt{\Delta^2(\mathbf{k}) + \epsilon_{\mathbf{k}}^2}$. Letting $\partial W/\partial h_{\mathbf{k}} = 0$, we find from equations (18) and (19)

$$\Delta(\mathbf{k}) = \left[\sum_{\mathbf{k}'(\mathcal{N})} - \sum_{\mathbf{k}'(\mathcal{U})}\right] V_{\mathbf{k},\mathbf{k}'} \frac{\Delta(\mathbf{k}')}{2E(\mathbf{k}')} \tag{20}$$

as our self-consistent equation, which is identical to the standard BCS self-consistent equation [1], save the terms in $\mathbf{k}'(\mathcal{U})$, which reduce and may even cancel the effect of the terms in $\mathbf{k}'(\mathcal{N})$.

When $\mathbf{k}$ is specified by $\mathcal{U}$, we have

$$\frac{\partial W}{\partial h_{\mathbf{k}}} = -2\epsilon_{\mathbf{k}} + \frac{1 - 2h_{\mathbf{k}}}{\sqrt{h_{\mathbf{k}}(1 - h_{\mathbf{k}})}} \left[\sum_{\mathbf{k}'(\mathcal{N})} - \sum_{\mathbf{k}'(\mathcal{U})}\right] V_{\mathbf{k},\mathbf{k}'} \sqrt{h_{\mathbf{k}'}(1 - h_{\mathbf{k}'})} \tag{21}$$

which also leads to equation (20). Apparently we have the same $\Delta(\mathbf{k})$ for the same numerical value of $\mathbf{k}$, regardless of whether $\mathbf{k}$ is specified by $\mathcal{N}$ or $\mathcal{U}$. This $\Delta(\mathbf{k})$ leads through equation (19) to $h_{\mathbf{k}}$, which also depends only on the numerical value of $\mathbf{k}$, and thus ensures that $\langle\Psi|\Psi\rangle = 1$ for equation (14).

8. Frustration of superconductivity

The principle of variation can be compared with shaking, which shapes a physical system into a configuration with minimum energy, such as the horizontal orientation of the bar in figure 3(a) in a gravitational field. However, the process of variation also produces a configuration with maximum energy, such as the vertical orientation of the bar in figure 3(b). Although we should choose the configuration with minimum energy whenever possible, some physical systems may frustrate us from doing so. For example, when the two bars are joined together to become an 'L' in figure 3(c), we cannot minimize their energy as readily as we do in figure 3(a), because minimum energy of one bar implies maximum energy of the other, and vice versa.

We have a similar situation when normal and umklapp scattering coexist. The pair occupation probability, $h_{\mathbf{k}}$, has a phase-like property, which becomes clear when we let $h_{\mathbf{k}} = \cos^2\theta_{\mathbf{k}}$, so that the normal pair generation operator in expression (5) becomes

$$\sin\theta_{\mathbf{k}} + \cos\theta_{\mathbf{k}} b_{\mathbf{k}}^{\dagger}. \tag{22}$$

The resultant wavefunction is normalized at any value of $\theta_{\mathbf{k}}$. However, in order to maximize the energy gap, we have to let

$$\cos^2\theta_{\mathbf{k}} = \frac{1}{2}\left[1 - \frac{\epsilon_{\mathbf{k}}}{E(\mathbf{k})}\right] \tag{23}$$

which is equivalent to equation (19). We can also write the umklapp pair generation operator in expression (6) as

$$\sin(\theta_{\mathbf{k}} - 90^\circ) + \cos(\theta_{\mathbf{k}} - 90^\circ) b_{\mathbf{k}}^{\dagger}. \tag{24}$$

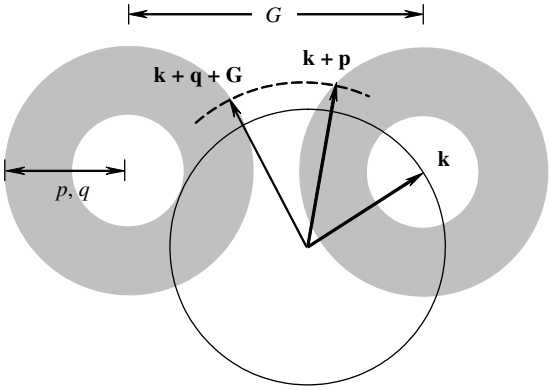

Figure 4. A spherical Fermi surface (open circle) and two identical phonon spheres, G being the lattice constant. Phonons in the unshaded circles do not invoke umklapp scattering. The particle in state $\mathbf{k}$ is scattered into $\mathbf{k}+\mathbf{p}$ and $\mathbf{k}+\mathbf{q}+\mathbf{G}$ in the normal and umklapp processes, respectively, by phonons with the same momentum. The energy of the end state in both processes is at the same level above the Fermi surface (broken arc, with an exaggerated constant height above the open circle).

It is easy to check that all the results here or in the BCS theory will not change if we replace the $-90°$ phase difference in equation (24) with $90°$.

According to equation (20) the normal pair is in a phase to sustain superconductivity, but the umklapp pair is in a phase to frustrate it. However, if we replace equation (19) with

$$h_{\mathbf{k}} = \frac{1}{2}\left[1 + \frac{\epsilon_{\mathbf{k}}}{E(\mathbf{k})}\right] \tag{25}$$

which can be written as

$$\cos^2(\theta_{\mathbf{k}} - 90°) = \frac{1}{2}\left[1 - \frac{\epsilon_{\mathbf{k}}}{E(\mathbf{k})}\right] \tag{26}$$

then in equation (20) $\mathcal{N}$ will be replaced by $\mathcal{U}$ and vice versa: umklapp pairs sustain superconductivity but normal pairs frustrate it. Apparently both normal and umklapp pairs alone may lead to an energy gap, but their coexistence mutually cancels their effect.

The $90°$ phase difference in equation (23), reminiscent of the angle between the two bars in figure 3(c), reveals an interesting dilemma. On the one hand the normal and umklapp pairs have to be locked $90°$ apart form each other in phase, otherwise our trial function, equation (14), cannot be normalized. On the other hand, we have to pay the price that either normal or umklapp scattering will be in a phase to frustrate superconductivity. Apparently only a fraction of phonons may survive cancellation to play their traditional role in the standard BCS theory and this, we suspect, was actually implied by BCS some 50 years ago.

9. Average phonon frequency

In equation (20) there can be no term in $\mathbf{k}'(\mathcal{U})$ to survive cancellation by a term in $\mathbf{k}'(\mathcal{N})$, at least for a spherical Fermi surface that does not intersect the boundary of a Brillouin zone, and with the constraint in equation (19). To see this, let $\mathbf{k}$ be a state on the Fermi surface (not in the direction of $\mathbf{G}$ for generality; see figure 4). We use $\mathbf{k}+\mathbf{p}$ to denote the end state of normal scattering, which is confined within the shaded phonon sphere, of radius p and centred at $\mathbf{k}$, as a result of momentum conservation. On the other hand, energy consideration requires that

$\mathbf{k}+\mathbf{p}$ must be at a level near the Fermi surface, which is marked as a broken arc in figure 4, somewhat exaggerated in its height above the Fermi sphere. There is an unshaded hole inside the phonon sphere (radius $\neq q_0$, because $\mathbf{k}$ and $\mathbf{G}$ are not parallel) where umklapp scattering is not invoked. We assume that $\mathbf{k}+\mathbf{p}$ is not in the hole.

If we transport the phonon sphere to the left by a reciprocal lattice constant G, then we find all the end states of umklapp scattering allowed by momentum conservation (the hole is completely outside the Fermi sphere but contacts its surface). From the intersection between the surface of the transported phonon sphere and the broken arc in figure 4, we find a state $\mathbf{k}+\mathbf{q}+\mathbf{G}$ with

$$q = p, \qquad \epsilon_{\mathbf{k}+\mathbf{q}+\mathbf{G}} = \epsilon_{\mathbf{k}+\mathbf{p}}, \tag{27}$$

i.e. both the phonon momentum and end state energy are the same in both normal and umklapp scattering. In figure 4 we have $\mathbf{k} = (k_x, k_y, 0)$. When $k_z \neq 0$ we can still find $\mathbf{k}+\mathbf{q}+\mathbf{G}$ to satisfy equation (27) by moving the phonon sphere in a proper direction over a proper distance.

We are reminded that, starting from $\mathbf{p}$, we can find more than one $\mathbf{q}$ to satisfy equation (27). However, we do have a one-to-one relation between $\mathbf{p}$ and $\mathbf{q}$. To prove this, we reverse the process in the previous two paragraphs. We start from *any* end state of umklapp scattering, $\mathbf{k}+\mathbf{q}+\mathbf{G}$, and then find $\mathbf{k}+\mathbf{p}$ to satisfy equation (27). Apparently $\mathbf{p}$ will not fall into the unshaded hole in the phonon sphere: this one-to-one relation is between the states in $\mathcal{U}$ and those states in $\mathcal{N}$ which are subject to both normal and umklapp scattering.

According to equation (27) we have

$$V_{\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G}} = V_{\mathbf{k},\mathbf{k}+\mathbf{p}} \tag{28}$$

where [1]

$$V_{\mathbf{k},\mathbf{k}+\mathbf{p}} = \frac{2\hbar\omega_{\mathbf{p}}|\mathcal{M}_{\mathbf{p}}|^2}{(\hbar\omega_{\mathbf{p}})^2 - (\epsilon_{\mathbf{k}+\mathbf{p}} - \epsilon_{\mathbf{k}})^2}, \tag{29}$$

$\mathcal{M}_{\mathbf{p}}$ being the matrix element, and $\omega_{\mathbf{p}}$ phonon frequency, both functions of p (Debye model), and $V_{\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G}}$ is defined similarly. For an isotropic energy gap we also have

$$\Delta(\mathbf{k}+\mathbf{q}+\mathbf{G}) = \Delta(\mathbf{k}+\mathbf{p}) \tag{30}$$

and hence $E(\mathbf{k}+\mathbf{q}+\mathbf{G}) = E(\mathbf{k}+\mathbf{p})$. Equations (28) and (30) lead through equation (20) to

$$\Delta(\mathbf{k}) = \sum_{\mathbf{k}'(\mathcal{B})} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta(\mathbf{k}')}{2E(\mathbf{k}')}. \tag{31}$$

$\mathcal{B}$ specifies states that do not invoke umklapp scattering, which is confined within the unshaded circle around $\mathbf{k}$ in figure 4.

We should remember that the Fermi sea and the reciprocal lattice have incompatible symmetries. Therefore in equation (31) $\mathcal{B}$ and hence Δ and E depend on the direction of $\mathbf{k}$ even when the Fermi sea is spherical. For simplicity, we have ignored the $\mathbf{k}$-dependence of $\mathcal{B}$, as a basis for deriving equation (30) from (27). In future work, we will have to generalize our proof in the previous paragraphs by replacing equations (28) and (30) with

$$V_{\mathbf{k},\mathbf{k}+\mathbf{q}+\mathbf{G}} \frac{\Delta(\mathbf{k}+\mathbf{q}+\mathbf{G})}{2E(\mathbf{k}+\mathbf{q}+\mathbf{G})} = V_{\mathbf{k},\mathbf{k}+\mathbf{p}} \frac{\Delta(\mathbf{k}+\mathbf{p})}{2E(\mathbf{k}+\mathbf{p})} \tag{32}$$

as our condition to seek $\mathbf{q}$ for a given state $\mathbf{p}$ (and vice versa). We will have to find an approximate value of $\mathbf{q}$ through the procedure in figure 4. Then we will adjust $\mathbf{q}$ slightly (assuming that phonon states are sufficiently numerous for small adjustment) to balance equation (32), which also leads to equation (31).

Equation (31) is in accord with the view that the coexistence of normal and umklapp scattering frustrates superconductivity. Indeed, if we cut the phonon frequency off at the

threshold of umklapp scattering, and go through the standard BCS formalism, then we find a self-consistent equation in exactly the same form as equation (31).

BCS introduced ω, the so-called 'average phonon frequency', to define the range of phonons when they integrated the self-consistent equation [1]. In the recent literature a liberty is often taken to replace ω with the Debye frequency ω_D. However, we see from equation (31) that the BCS average phonon frequency is based on a very deep insight. Numerically, ω is likely to be significantly lower than ω_D. According to figures 1 and 2 the phonon momentum in equation (31) cannot exceed q_0 when $\mathbf{k}$ is in the direction of $\mathbf{G}$. For a bcc lattice with valency 1 we have $q_0/k_F = 0.267$, k_F being the radius of the Fermi sphere, or $q_0/q_D = 0.212$: when $\mathbf{k}$ is in the direction of $\mathbf{G}$ the average phonon frequency of BCS is merely ~20% of the Debye frequency.

10. Excited state

For the convenience of the reader, we explain the BCS theory at finite temperatures briefly and then extend the formulation to include umklapp scattering. BCS divided reciprocal space into cells, $\Delta\mathbf{k}$, containing $N_\mathbf{k}$ pair states. There are $S_\mathbf{k}$ single particles and $P_\mathbf{k}$ excited pairs in $\Delta\mathbf{k}$, other states being occupied by ground pairs, giving

$$\frac{S_\mathbf{k}}{N_\mathbf{k}}, \qquad \frac{P_\mathbf{k}}{N_\mathbf{k}}, \qquad \frac{N_\mathbf{k} - S_\mathbf{k} - P_\mathbf{k}}{N_\mathbf{k}} \tag{33}$$

as fractions of $\Delta\mathbf{k}$ occupied by single particles, excited and ground pairs, respectively. The kinetic energy of the particle ensemble, found from equation (7), the electron term of equation (1) and the Bloch energy contribution, is

$$W_{KE} = \sum_\mathbf{k} \epsilon_\mathbf{k} \left[\frac{S_\mathbf{k}}{N_\mathbf{k}} + 2(1 - h_\mathbf{k}) \frac{P_\mathbf{k}}{N_\mathbf{k}} + 2h_\mathbf{k} \frac{N_\mathbf{k} - S_\mathbf{k} - P_\mathbf{k}}{N_\mathbf{k}} \right] \tag{34}$$

or

$$W_{KE} = 2 \sum_\mathbf{k} \epsilon_\mathbf{k} [f_\mathbf{k} + (1 - 2f_\mathbf{k}) h_\mathbf{k}] \tag{35}$$

with

$$f_\mathbf{k} = \frac{S_\mathbf{k}}{2N_\mathbf{k}} + \frac{P_\mathbf{k}}{N_\mathbf{k}}. \tag{36}$$

In equations (34) and (35) $\epsilon_\mathbf{k}$ is averaged in $\Delta\mathbf{k}$ (a cell), and $\mathbf{k}$ runs over the cells (one $\mathbf{k}$ for each cell). The interaction energy is found to be

$$W_I = -\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \sqrt{h_\mathbf{k}(1 - h_\mathbf{k})}(1 - 2f_\mathbf{k}) \sqrt{h_{\mathbf{k}'}(1 - h_{\mathbf{k}'})}(1 - 2f_{\mathbf{k}'}). \tag{37}$$

The entropy is given by

$$S = -2k_B \sum_\mathbf{k} [f_\mathbf{k} \ln f_\mathbf{k} + (1 - f_\mathbf{k}) \ln(1 - f_\mathbf{k})], \tag{38}$$

k_B being the Boltzmann constant, which leads to the free energy

$$F = W_{KE} + W_I - TS. \tag{39}$$

We have

$$\frac{\partial F}{\partial h_\mathbf{k}} = (1 - 2f_\mathbf{k}) \left\{ 2\epsilon_\mathbf{k} - \frac{1 - 2h_\mathbf{k}}{\sqrt{h_\mathbf{k}(1 - h_\mathbf{k})}} \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \sqrt{h_{\mathbf{k}'}(1 - h_{\mathbf{k}'})}(1 - 2f_{\mathbf{k}'}) \right\} \tag{40}$$

which can be compared with equation (18). When $\partial F/\partial h_{\mathbf{k}} = 0$, equation (40) leads through equation (19) to

$$\Delta(\mathbf{k}) = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta(\mathbf{k}')}{2E(\mathbf{k}')}(1 - 2f_{\mathbf{k}'}). \tag{41}$$

It is interesting that $\mathbf{k}'$ runs over the same range at any T. Therefore, when the temperature rises, ground pairs are replaced by single particles and excited pairs gradually in each and every cell, $\Delta\mathbf{k}'$, rather than being driven out altogether cell by cell. We also have

$$\frac{\partial F}{\partial f_{\mathbf{k}}} = 2E(\mathbf{k}) + 2k_{\mathrm{B}}T \ln \frac{f_{\mathbf{k}}}{1 - f_{\mathbf{k}}} \tag{42}$$

or

$$1 - 2f_{\mathbf{k}} = \tanh \frac{E(\mathbf{k})}{2k_{\mathrm{B}}T} \tag{43}$$

when $\partial F/\partial f_{\mathbf{k}} = 0$. Combining equations (41) and (43), we find

$$\Delta(\mathbf{k}) = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta(\mathbf{k}')}{2E(\mathbf{k}')} \tanh \frac{E(\mathbf{k}')}{2k_{\mathrm{B}}T} \tag{44}$$

which is the self-consistent equation at $T > 0$ in the BCS theory [1].

Equation (44), though sophisticated and elegant, manifests a simple idea, namely that all states fall into two categories: those allowed at $T = 0$ and those not, to evaluate the entropy in equation (38). Once we endorse this idea, the rest of the derivation is automatic. For each $\mathbf{k}$ we have three configurations, whose contributions to the ensemble energy are well-defined. Thermodynamics governs the number of the particles in each of the configurations, which in turn governs the magnitude of the energy gap. Apparently, this simple idea will not change when umklapp scattering is included.

In the presence of umklapp scattering, we replace equation (7) with

$$|\Psi\rangle_{\mathrm{exc}} = \prod_{\mathbf{k}''(\mathcal{S}_1)} \prod_{\mathbf{k}''(\mathcal{S}_2)} a^{\dagger}_{\mathbf{k}''\sigma} \prod_{\mathbf{k}'(\mathcal{P}_1)} \prod_{\mathbf{k}'(\mathcal{G}_2)} \left(\sqrt{1 - h_{\mathbf{k}'}}\, b^{\dagger}_{\mathbf{k}'} - \sqrt{h_{\mathbf{k}'}}\right) \prod_{\mathbf{k}(\mathcal{G}_1)} \prod_{\mathbf{k}(\mathcal{P}_2)} \left(\sqrt{1 - h_{\mathbf{k}}} + \sqrt{h_{\mathbf{k}}}\, b^{\dagger}_{\mathbf{k}}\right)|0\rangle \tag{45}$$

where $\mathcal{G}$ and $\mathcal{P}$ specify ground and excited pairs, respectively, $\mathcal{S}$ specifies single particles, as in equation (7), and the indices 1 and 2 specify the normal and umklapp processes, i.e. we separate $\mathcal{N}$ and $\mathcal{U}$ into $\mathcal{S}_1$, $\mathcal{P}_1$, $\mathcal{G}_1$ and $\mathcal{S}_2$, $\mathcal{P}_2$, $\mathcal{G}_2$, respectively. Note that, when ground pairs are generated by expression (5), we use expression (6) to generate excited pairs, similar to the arrangement in equation (7). On the other hand, when ground pairs are generated by expression (6), we use expression (5) to generate excited pairs, which raises the energy of the pair ensemble, in recognition that umklapp pairs make less negative contribution to that energy the fewer their number.

We divide $\mathcal{N}$ and $\mathcal{U}$ into cells $\Delta\mathbf{k}_1$ and $\Delta\mathbf{k}_2$ respectively. We have

$$\frac{S_{1\mathbf{k}}}{N_{1\mathbf{k}}}, \qquad \frac{P_{1\mathbf{k}}}{N_{1\mathbf{k}}}, \qquad \frac{N_{1\mathbf{k}} - S_{1\mathbf{k}} - P_{1\mathbf{k}}}{N_{1\mathbf{k}}} \tag{46}$$

as fractions of $\Delta\mathbf{k}_1$ occupied by single particles, excited and ground pairs. We also have

$$\frac{S_{2\mathbf{k}}}{N_{2\mathbf{k}}}, \qquad \frac{P_{2\mathbf{k}}}{N_{2\mathbf{k}}}, \qquad \frac{N_{2\mathbf{k}} - S_{2\mathbf{k}} - P_{2\mathbf{k}}}{N_{2\mathbf{k}}} \tag{47}$$

as fractions of $\Delta\mathbf{k}_2$ occupied by single particles, excited and ground pairs. Letting

$$f_{\mathbf{k}} = \frac{S_{1\mathbf{k}}}{2N_{1\mathbf{k}}} + \frac{P_{1\mathbf{k}}}{N_{1\mathbf{k}}} \qquad \text{or} \qquad \frac{S_{2\mathbf{k}}}{2N_{2\mathbf{k}}} + \frac{P_{2\mathbf{k}}}{N_{2\mathbf{k}}} \tag{48}$$

for $\mathbf{k}$ specified by $\mathcal{N}$ or $\mathcal{U}$ respectively, we find

$$W_{\mathrm{KE}} = \sum_{\mathbf{k}(\mathcal{N})} 2\epsilon_{\mathbf{k}}\big[f_{\mathbf{k}} + (1-2f_{\mathbf{k}})h_{\mathbf{k}}\big] + \sum_{\mathbf{k}(\mathcal{U})} 2\epsilon_{\mathbf{k}}\big[f_{\mathbf{k}} + (1-2f_{\mathbf{k}})(1-h_{\mathbf{k}})\big] \quad (49)$$

as the kinetic energy, which can be compared with equation (35). We also find

$$W_{\mathrm{I}} = -W_{11} - W_{22} + W_{12} + W_{21} \quad (50)$$

with

$$W_{11} = \sum_{\mathbf{k}(\mathcal{N})} \sum_{\mathbf{k}'(\mathcal{N})} V_{\mathbf{k},\mathbf{k}'} \sqrt{h_{\mathbf{k}}(1-h_{\mathbf{k}})} \sqrt{h_{\mathbf{k}'}(1-h_{\mathbf{k}'})} \times (1-2f_{\mathbf{k}})(1-2f_{\mathbf{k}'})$$

and

$$W_{12} = \sum_{\mathbf{k}(\mathcal{N})} \sum_{\mathbf{k}'(\mathcal{U})} V_{\mathbf{k},\mathbf{k}'} \sqrt{h_{\mathbf{k}}(1-h_{\mathbf{k}})} \sqrt{h_{\mathbf{k}'}(1-h_{\mathbf{k}'})} \times \ (1-2f_{\mathbf{k}})(1-2f_{\mathbf{k}'}).$$

W_{21} and W_{22} are identical to W_{12} and W_{11}, respectively, save that $\mathcal{N}$ is replaced by $\mathcal{U}$ and vice versa.

Now we minimize the free energy F, which is defined by equations (39), (49) and (50) when $\mathbf{k}$ is specified by $\mathcal{N}$. We find

$$\frac{\partial F}{\partial h_{\mathbf{k}}} = (1-2f_{\mathbf{k}}) \left\{ 2\epsilon_{\mathbf{k}} - \frac{1-2h_{\mathbf{k}}}{\sqrt{h_{\mathbf{k}}(1-h_{\mathbf{k}})}} \left[\sum_{\mathbf{k}'(\mathcal{N})} - \sum_{\mathbf{k}'(\mathcal{U})} \right] V_{\mathbf{k},\mathbf{k}'} \sqrt{h_{\mathbf{k}'}(1-h_{\mathbf{k}'})} (1-2f_{\mathbf{k}'}) \right\} \quad (51)$$

which can be compared with equation (40). When $\partial F/\partial h_{\mathbf{k}} = 0$, equation (40) leads through equation (19) to

$$\Delta(\mathbf{k}) = \left[\sum_{\mathbf{k}'(\mathcal{N})} - \sum_{\mathbf{k}'(\mathcal{U})} \right] V_{\mathbf{k},\mathbf{k}'} \frac{\Delta(\mathbf{k}')}{2E(\mathbf{k}')} (1-2f_{\mathbf{k}'}) \quad (52)$$

which can be compared with equation (41). Equations (42) and (43) do not change in the presence of umklapp scattering, and this leads through equation (52) to

$$\Delta(\mathbf{k}) = \left[\sum_{\mathbf{k}'(\mathcal{N})} - \sum_{\mathbf{k}'(\mathcal{U})} \right] V_{\mathbf{k},\mathbf{k}'} \frac{\Delta(\mathbf{k}')}{2E(\mathbf{k}')} \tanh \frac{E(\mathbf{k}')}{2k_{\mathrm{B}}T} \quad (53)$$

as the self-consistent equation for $T > 0$ in the presence of umklapp scattering. Equation (53) can be compared with equation (44).

When $\mathbf{k}$ is specified by $\mathcal{U}$ we define the free energy as

$$F = -W_{\mathrm{KE}} - W_{\mathrm{I}} - TS \quad (54)$$

which can be compared with equation (39); W_{KE} and W_{I} are defined in equations (49) and (50) respectively, and S is defined in equation (38). In equation (54) $W = W_{\mathrm{KE}} + W_{\mathrm{I}}$ is negative, because umklapp pairs make negative contributions to the energy of the pair ensemble. This means that we have $\delta Q = -\mathrm{d}W$ if the change in Q is caused by the change in the number and/or occupancy of umklapp pairs; Q stands for heat. Therefore we have to let $F = -W - TS$, in order to have $\mathrm{d}F = \delta Q - T\,\mathrm{d}S - S\,\mathrm{d}T = -S\,\mathrm{d}T$, which is the correct expression of $\mathrm{d}F$ (for constant volume). Now equation (51) becomes

$$\frac{\partial F}{\partial h_{\mathbf{k}}} = (1-2f_{\mathbf{k}}) \left\{ -2\epsilon_{\mathbf{k}} + \frac{1-2h_{\mathbf{k}}}{\sqrt{h_{\mathbf{k}}(1-h_{\mathbf{k}})}} \left[\sum_{\mathbf{k}'(\mathcal{N})} - \sum_{\mathbf{k}'(\mathcal{U})} \right] V_{\mathbf{k},\mathbf{k}'} \sqrt{h_{\mathbf{k}'}(1-h_{\mathbf{k}'})} (1-2f_{\mathbf{k}'}) \right\} \quad (55)$$

which also leads to equation (52). We still have equations (42) and (43), which lead through equation (52) to (53).

If we adopt the view that superconductivity is frustrated when normal and umklapp scattering coexist, then we can go through the standard BCS formalism at $T > 0$ to find

$$\Delta(\mathbf{k}) = \sum_{\mathbf{k}'(\mathcal{B})} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta(\mathbf{k}')}{2E(\mathbf{k}')} \tanh \frac{E(\mathbf{k}')}{2k_{\mathrm{B}}T} \tag{56}$$

which is identical to equation (53); $\mathcal{B}$ (defined in section 9) specifies the range of $\mathbf{k}'$, which does not depend on T, similar to the range of $\mathbf{k}'$ in equation (41) or (44).

11. Conclusions

In the conventional picture of single electron scattering in a metal the normal and umklapp scattering processes are associated with distinctively different ranges of momentum transfer. There is no possibility for these two processes to interfere with each other in the sense that, with the same initial state, the end states of normal and umklapp scattering do not coincide. In this picture umklapp scattering is effectively treated as normal scattering in an extended range of momentum transfer and, when applied in the BCS theory, it tells us that umklapp scattering also lowers the ensemble energy and thus enhances superconductivity [3, 12].

We recognize that, when the scattered entity is not a single electron but a pair, the end states of normal and umklapp scattering may coincide and the two processes may interfere. We find a formal deficiency in the standard BCS ground state wavefunction, which is designed to count the statistics of scattering of pairs in the normal or umklapp process alone and leads to a self-contradiction when these two processes coexist. A suitable trial function locks the end states of normal and umklapp scattering 90° apart in phase but leads to the consequence that superconductivity is frustrated when the normal and umklapp processes coexist. Then only a fraction of the phonons actually takes part in electron pairing. Our conclusion is reached within the BCS formalism which is based on the variational principle.

Another approach, the Eliashberg formalism, is based on the one-electron Green function, and here too superconductivity is enhanced when umklapp scattering is introduced [13]. However, in this formalism, which is non-variational and does not involve a trial function, the physics of pair scattering and interference effects may be manifest in a manner different from that in the BCS variational approach. Further consideration of the contribution of umklapp phonons in different formalisms would appear to be merited.

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