Umklapp Frustration and Field-theoretic Approach to Superconductivity

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The formula of Gell-Mann and Low can be applied to both the Stark effect and superconductivity. The standard version of the field-theoretic approach fits the Stark effect, because in this version electrons have identical initial and end states, so that the energy of each and every electron acquires a shift in the same direction. A preliminary alternative version of the field-theoretic approach is introduced, in which the electrons have different initial and end states, to accommodate superconductivity. Consequently the energy of the electrons acquires a random shift, which will cancel macroscopically, unless the electrons are paired. It also becomes apparent that superconductivity is frustrated when normal and umklapp scattering coexist.

I. INTRODUCTION

In umklapp scattering a Cooper pair may contest a state which is the destination of another pair in normal scattering (FIG. 1). Consequently the contribution to superconductivity is frustrated. We find that on average only 15% of phonons are involved in pairing electrons in 12 common superconductive metals. Were the frustration effect of umklapp scattering lifted, metals would be superconductive at remarkably high temperatures, for example 980 K in the case of tin [2]. This result is found from the original approach of Bardeen, Cooper and Schrieffer (BCS), based on the method of variation [3]. It is natural to ask if the same result could be found from the standard field-theoretic approach, based on the method of the Green function [4, 5].

The Green function method can be highly sophisticated. As a first attempt, we follow a relatively simple approach which, to our knowledge, was pioneered by Hubbard [4] to describe collective motions in terms of many-body perturbation theory, with many features common to the standard field-theoretic approach. For example both approaches start with the formula of Gell-Mann and Low [2], which involves an expansion of the scattering matrix or s-matrix. In both approaches the treatment of Wick is applied in order to reduce the operator chain into a c-number [5]. The diagram technique is also used in both approaches to identify the relevant physical process and facilitate calculation, etc. Detailed knowledge about one approach will certainly help us to understand the other.

In a field-theoretic approach it is customary to start with an ensemble of free particles. Then the interaction is switched on adiabatically in time. According to Gell-Mann and Low an eigen-state of the free particles evolves adiabatically and eventually becomes an eigen-state of the ensemble with interaction. Apparently this approach is applicable to say the Stark effect, which can be literally switched on adiabatically, and is characterized by either of the following chains of events:

\[(k, \sigma) \rightarrow (k + q, \sigma) \rightarrow (k, \sigma)\]

(1)

\[(k + q, \sigma) \rightarrow (k, \sigma) \rightarrow (k + q, \sigma)\]

k and q being the wave-vectors of the electron and photon respectively, \(\sigma = \uparrow,\downarrow\) spin. In the first line of Eq. (1) the electron absorbs a photon from the external field and then emits it. In the second line the electron emits a photon and then absorbs one again. In both cases the electron returns to its original state, reflecting that the external field alters the electron orbit, rather than forces the electron to jump orbit.

We find through this simple version of the field-theoretic approach that, when we switch on the electron-
phonon interaction in a particle ensemble, the ensemble energy changes. Apart from an additional factor of 2, the strength of the interaction is the same as that in the BCS theory. The electrons always return to their original state, a situation similar to the Stark effect, but different from the picture of the BCS theory. Indeed, we find that the energy change of each and every electron is of the same sign and they do not cancel. There is no need to pair the electrons. Consequently there can be no umklapp frustration of superconductivity. We emphasize we are not criticizing the work of Hubbard: he did not employ his approach to study superconductivity \[6\]. We alter the path of scattering so that the electrons no longer return to their original state. Pairing becomes necessary, otherwise there will be no change of the ensemble energy. Now the process is characterized by the following event:

\[
(k, \uparrow) \rightarrow (k + q, \uparrow)
\]

\[
(-k, \downarrow) \rightarrow (-k - q, \downarrow)
\]

Here the two electrons jump orbits after exchanging virtual phonons. The energy of the electron ensemble is lowered, not because some slowly introduced interaction alters the energy of the electron orbits. Rather, when the two electrons jump orbits in a coherent manner, they are in a configuration of a lower energy. We also find umklapp frustration.

This communication is arranged as follows. In Section \( II \) we introduce the Hamiltonian of the electron-phonon system. In Sections \( III \) - \( V \) we derive the energy shift according to the scenario Eq. \( 1 \). In Section \( VI \) we derive the energy shift according to the scenario Eq. \( 2 \). In Section \( VII \) we show that pairing in necessary for this second scenario. In Section \( VIII \) we reveal umklapp frustration to superconductivity. In Section \( IX \) we discuss Coulomb repulsion. In Section \( X \) we outline a possible path to a self-consistent solution of our alternative field-theoretic approach. In Section \( XI \) we comment on the standard field-theoretic approach. We give a brief conclusion in Section \( XII \).

**II. ELECTRON-PHONON SYSTEM**

Unless stated otherwise, we always use the Schrödinger representation. We separate the Hamiltonian into two parts:

\[
H = H_0 + H'
\]

where \( H_0 \) and \( H' \) are Hamiltonians of free particles and interaction, respectively, of which the later will be considered as perturbation. In an electron-phonon system we have

\[
H_0 = H_e + H_p
\]

where \( H_e \) and \( H_p \) are electron and phonon Hamiltonian respectively. In second quantization we have

\[
H_e = \sum_{k,\sigma} \epsilon_0(k)a_{k,\sigma}^\dagger a_{k,\sigma}, \quad (5)
\]

\[
H_p = \sum_{q, l} \hbar \omega_l(q) \left( c_{q,l}^\dagger c_{q,l} + 1/2 \right), \quad (6)
\]

\( a^\dagger \) and \( a \) being the electron generation and destruction operators, \( \epsilon_0 \) and \( k \) electron energy and wave vector in the absence of interaction, \( c^\dagger \) and \( c \) phonon generation and destruction operators, \( \omega \) and \( q \) phonon frequency and wave vector and \( l \) identifies phonon polarization. The interaction Hamiltonian turns out to be

\[
H' = \sum_{k,\sigma, q, l} M_{q,l} c_{q,l}^\dagger a_{k+q,\sigma}^\dagger a_{k,\sigma} + h.c. \quad (7)
\]

\( h.c. \) stands for Hermitian conjugate. Here we neglect the slight dependence of the matrix element \( M \) on \( k \). Note that in Eq. \( 7 \) an electron has the same spin before and after being scattered by a phonon.

**III. IDENTICAL INITIAL AND END STATES**

Gell-Mann and Low proved the following important formula \[4, 7\]:

\[
|\psi\rangle = S(t)|\psi_0\rangle/\langle\psi_0|S(0)|\psi_0\rangle. \quad (8)
\]

where \( |\psi\rangle \) and \( |\psi_0\rangle \) satisfy

\[
H|\psi\rangle = \epsilon|\psi\rangle \quad \text{and} \quad H_0|\psi_0\rangle = \epsilon_0|\psi_0\rangle, \quad (9)
\]

whereas

\[
S(t) = S_0(t) + S_1(t) + S_2(t) + ... \quad (10)
\]

with \( S_0(t) = 1 \),

\[
S_n(t) = \frac{1}{(ih)^n} \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \cdots \int_{-\infty}^{t_{n-1}} dt_n H'_0(t_1)H'_0(t_2)\cdots H'_0(t_n) \quad (11)
\]

which is known as the s-matrix (scattering matrix),

\[
H'_0(t) = \lim_{\alpha \to +0} e^{-H_0(t)/\hbar} H^\alpha e^{H_0(t)/\hbar} e^{\alpha t}. \quad (12)
\]

For clarity we will integrate Eq. \( 11 \) directly, instead of the usual practice in the literature of replacing \( t_1, t_2, ..., t_{n-1} \) with \( t \) in the multiple integration of time via the use of the chronological operator.

It is apparent from Eq. \( 3 \) that, when \( t = 0 \), we have \( \langle\psi_0|\psi\rangle = 1 \) and this leads through Eqs. \( 3 \) and \( 4 \) to

\[
e - \epsilon_0 = \langle \psi_0|H|\psi\rangle - \langle\psi_0|H_0|\psi_0\rangle = \langle\psi_0|H|\psi\rangle \quad (13)
\]
Combining Eqs. (8) and (13) we find
\[ \epsilon - \epsilon_0 = \frac{\langle \psi_0 | H' S(0) | \psi_0 \rangle}{\langle \psi_0 | S(0) | \psi_0 \rangle} \] (14)
or \[ \epsilon - \epsilon_0 = \epsilon_1 + \epsilon_2 + \ldots \]
with
\[ \epsilon_n = \frac{\langle \psi_0 | H' S_n(0) | \psi_0 \rangle}{\langle \psi_0 | S(0) | \psi_0 \rangle} \] (15)

Note that in Eqs. (14) and (15) the initial and end states are identical. This is why Eq. (15) vanishes with \( S_0(0) = 1 \): the phonon field in the bra is altered by the phonon operator in \( H' \) and becomes orthogonal to the phonon field in the ket (or vice versa). Apparently, \( \epsilon_1 \) is associated with the scenarios of scattering in Eq. (1), where the particle always returns to its initial state.

IV. S-MATRIX EVALUATION

We seek the matrix element of \( H'_\alpha \) in the Schrödinger representation. To this end we have to evaluate
\[ \langle 0 | a_{k+q,\sigma} H'_\alpha a_{k,\sigma}^\dagger | 0 \rangle \]
\[ \langle 0 | c_{q,l} a_{k,\sigma} H'_\alpha a_{k+q,\sigma}^\dagger | 0 \rangle \] (16)

\( | 0 \rangle \) being the electron and phonon vacuum, which tell us the probability of any event in Eqs. (11) and (12). We have
\[ e^{H_{0t}/\hbar} a_{k+q,\sigma}^\dagger | 0 \rangle = \sum_{n=0}^{\infty} \left( \frac{t/\hbar}{n!} \right)^n H_{0t}^n c_{q,l} a_{k,\sigma}^\dagger | 0 \rangle \]
\[ = \sum_{n=0}^{\infty} \left( \frac{t/\hbar}{n!} \right)^n \left[ \epsilon_0(k) + \hbar \omega_l(q) \right]^n c_{q,l} a_{k,\sigma}^\dagger | 0 \rangle \]
\[ = \exp \left\{ \left[ \epsilon_0(k) + \hbar \omega_l(q) \right] t/\hbar \right\} c_{q,l} a_{k,\sigma}^\dagger | 0 \rangle \] (17)

Similarly we have
\[ e^{H_{0t}/\hbar} a_{k+q,\sigma}^\dagger | 0 \rangle = \exp \left\{ \epsilon_0(k) + \hbar \omega_l(q) t/\hbar \right\} a_{k+q,\sigma}^\dagger | 0 \rangle \] (18)

Combining Eqs. (7), (12) and (10, 18), we find
\[ H'_\alpha = \sum_{k,\sigma,q,l} M_{q,l} c_{q,l} a_{k+q,\sigma}^\dagger a_{k,\sigma} \]
\[ \times \exp \left\{ \left[ \epsilon_0(k) + \hbar \omega_l(q) - \epsilon_0(k + q) \right] t/\hbar \right\} \]
\[ + \sum_{k,\sigma,q,l} M_{q,l} c_{q,l} a_{k,\sigma}^\dagger a_{k+q,\sigma} \]
\[ \times \exp \left\{ \left[ \epsilon_0(k + q) - \epsilon_0(k) - \hbar \omega_l(q) \right] t/\hbar \right\} \] (19)
where for simplicity we have dropped the factor \( \exp(\alpha t) \) in Eq. (12).

In order to evaluate the integrations in Eq. (11) at \( t = -\infty \), we add an infinitesimal positive number \( \delta \) to the argument of the exponential functions in Eq. (19). This leads to
\[ S_1(0) = \sum_{k,\sigma,q,l} M_{q,l} \left[ \frac{c_{q,l} a_{k+q,\sigma}^\dagger a_{k,\sigma}}{\epsilon_0(k) + \hbar \omega_l(q) - \epsilon_0(k + q) + i\delta} \right] \]
\[ + \frac{c_{q,l} a_{k,\sigma}^\dagger a_{k+q,\sigma}}{\epsilon_0(k + q) - \epsilon_0(k) + i\delta} \] (20)
as the \( n = 1 \) term of \( S(0) \).

V. STARK EFFECT

We substitute Eq. (20) into Eq. (15) to evaluate \( \epsilon_1 \). We find we have to evaluate the following:
\[ \langle \psi_0 | c_{q,l} a_{k,\sigma} a_{k+q,\sigma}^\dagger | \psi_0 \rangle \] (21)
\[ \langle \psi_0 | c_{q,l} a_{k+q,\sigma}^\dagger a_{k,\sigma} | \psi_0 \rangle \] (22)
\[ \langle \psi_0 | c_{q,l} a_{k+q,\sigma}^\dagger a_{k,\sigma}^\dagger | \psi_0 \rangle \] (23)
\[ \langle \psi_0 | c_{q,l} a_{k,\sigma}^\dagger a_{k+q,\sigma} | \psi_0 \rangle \] (24)

In Wick’s treatment Expressions (21 - 24) are evaluated via permutation of the operators. Description of this process in the literature is often in some special terminology, such as ‘\( N \)-product’, ‘\( T \)-product’, ‘pairing’, etc. Essentially we have to move some of the operators to the left to apply on the bra, move others to the right to apply on the ket. The transformed bra and ket must be symmetrical (that is the bra is the Hermitian conjugate of the ket and vice versa), otherwise their product will vanish. The sign of this product depends on the nature of the operators and the number of permutations we have made. Since we have two phonon generation operators in Expression (22), the bra and ket can never be transformed symmetrically, so that this expression has to vanish. For the same reason Expression (23) also has to vanish.

In Expressions (21) and (24) the bra and ket may be transformed symmetrically when the phonon operators have the same momentum and polarization. This leads to a c-number \( \delta_{q,q'} \delta_{l,l'} \), which in turn leads to
\[ \epsilon_1 = \sum_{k,k',\sigma',q,l} \overline{\langle \psi_0 | S(0) | \psi_0 \rangle} \]
\[ \times \left[ \frac{\langle \psi_0 | c_{q,l} a_{k+q,\sigma}^\dagger a_{k,\sigma}^\dagger | \psi_0 \rangle}{\epsilon_0(k) + \hbar \omega_l(q) - \epsilon_0(k + q) + i\delta} \right] \]
\[ + \frac{\langle \psi_0 | a_{k+q,\sigma}^\dagger a_{k,\sigma} | \psi_0 \rangle}{\epsilon_0(k + q) - \epsilon_0(k) + i\delta} \] (25)

Furthermore, in order to transform the bras and kets in Eq. (25) symmetrically, we have to let \( k' = k, \sigma' = \sigma \), in
accordance with the scenario in Eq. (1). We find
\[ \epsilon_1 = -2 \sum_{k} \sum_q \frac{V_{k,q}}{\langle \psi_0 | S(0) | \psi_0 \rangle} \tag{26} \]
where the factor 2 arises when we sum spin,
\[ V_{k,q} = \sum_l \frac{2\hbar \omega_l(q) \mathcal{M}_{q,l}^2}{[\hbar \omega_l(q)]^2 - [\epsilon_0(k + q) - \epsilon_0(k)]^2} \tag{27} \]
which is the same as the matrix element of the BCS reduced Hamiltonian \[2\]. Note that in the above equation we have dropped the infinitesimal number \( \delta \) in Eq. (20) since it has no numerical effect on \( V \). In Eq. (26) all the terms in \( k \) have the same sign, reflecting the nature of say the Stark effect, rather than superconductivity.

VI. DIFFERENT INITIAL AND END STATES

According to Eq. (3) we have
\[ \epsilon \langle \psi | \psi \rangle = \langle \psi | H | \psi \rangle = \langle \psi | H_0 | \psi \rangle + \langle \psi | H' | \psi \rangle \tag{28} \]
By using Eq. (8) we find
\[ \langle \psi | H' | \psi \rangle = \frac{\langle \psi | H' S(0) | \psi_0 \rangle}{\langle \psi_0 | S(0) | \psi_0 \rangle} \tag{29} \]
Similarly we find
\[ \langle \psi | H_0 | \psi \rangle = \frac{\langle \psi | S(0) H_0 | \psi_0 \rangle}{\langle \psi_0 | S(0) | \psi_0 \rangle} + \frac{\langle \psi | H_0 S(0) - S(0) H_0 | \psi_0 \rangle}{\langle \psi_0 | S(0) | \psi_0 \rangle} \tag{30} \]
where
\[ \frac{\langle \psi | S(0) H_0 | \psi_0 \rangle}{\langle \psi_0 | S(0) | \psi_0 \rangle} = \epsilon_0 \frac{\langle \psi | S(0) | \psi_0 \rangle}{\langle \psi_0 | S(0) | \psi_0 \rangle} = \epsilon_0 \langle \psi | \psi \rangle \tag{31} \]
Combining Eqs. (28, 30), we find
\[ (\epsilon - \epsilon_0) \langle \psi | \psi \rangle = \frac{\langle \psi | H_0 S(0) - S(0) H_0 | \psi \rangle}{\langle \psi_0 | S(0) | \psi_0 \rangle} + \epsilon_1 + \epsilon_2 + \ldots \tag{32} \]
with
\[ \epsilon_n = \frac{\langle \psi | H' S_n(0) | \psi_0 \rangle}{\langle \psi_0 | S(0) | \psi_0 \rangle} \tag{33} \]
which resembles Eq. (16) closely, except that in Eq. (33) the end state, \( | \psi \rangle \), is different from the initial state, \( | \psi_0 \rangle \). However we assume virtual phonons, that is the phonon states are still identical in \( | \psi_0 \rangle \) and \( | \psi \rangle \), so that Eq. (33) vanishes with \( S_0(0) = 1 \), see the text below Eq. (15).

When \( n = 1 \) we have
\[ \epsilon_1 = \sum_{k,k',\sigma,\sigma'} \sum_{q,l} \frac{\mathcal{M}_{q,l}^2}{\langle \psi_0 | S(0) | \psi_0 \rangle} \times \left[ \frac{\langle \psi | a_{k,\sigma}^\dagger a_{k+q,\sigma'}^\dagger a_{k+q,\sigma} a_{k,\sigma'} | \psi_0 \rangle}{\epsilon_0(k) + \hbar \omega_l(q) - \epsilon_0(k + q) + i\delta} \right. \]
\[ \left. + \frac{\langle \psi | a_{k+q,\sigma}^\dagger a_{k,\sigma'} a_{k+q,\sigma'}^\dagger a_{k,\sigma} | \psi_0 \rangle}{\epsilon_0(k + q) - \epsilon_0(k) - \hbar \omega_l(q) + i\delta} \right] \tag{34} \]
which apparently is associated with the scenario in Eq. 2.

Without special measures, we have \( \epsilon_1 = 0 \) in Eq. (34). To see this, let
\[ | \psi_0 \rangle = \prod_k a_k^\dagger | 0 \rangle, \quad | \psi \rangle = \prod_k a_k^\dagger | 0 \rangle \tag{35} \]
where for simplicity we do not generate phonons explicitly. In Eq. (34) \( | \psi_0 \rangle \) and \( | \psi \rangle \) are identical, except that the sequence of \( a_k^\dagger \) in \( k' \) is a random reshuffle of the sequence in \( k \), in order to model the chaotic nature of the electron-phonon interaction. Eq. (35) allows us to transform the bras and kets in Eq. (34) symmetrically after a number of permutations. However, Eq. (35) also means that terms in Eq. (34) will alter their signs randomly, due to the Fermi-Dirac statistics, and cancel 3.

The first term on the right hand side of Eq. (32) tells us that the physics associated with \( \epsilon_1, \epsilon_2, \ldots \) is not the sole effect of scattering. Indeed, in order to reveal superconductivity, Fröhlich 11 introduced the canonical transform, which cancels much of the electron-phonon interaction. However, we know from Eqs. (35), (17) and (4) that terms in
\[ H_0 S_1(0) - S_1(0) H_0 \tag{36} \]
always have an odd number of phonon operators, which cannot transform \( | \psi \rangle \) and \( | \psi_0 \rangle \) in Eq. (34) symmetrically with respect to the phonon fields, that is we can ignore the contribution by Expression (34) to \( \epsilon_1 = 0 \), as long as we have virtual phonons, see explanation below Eq. (35).

VII. COOPER PAIRS

We follow BCS 3 to let
\[ k' = -k - q, \quad \sigma = \uparrow, \quad \sigma' = \downarrow \tag{37} \]
so that Eq. (34) becomes
\[ \epsilon_1 = -\sum_k \sum_q \frac{V_{k,q}}{\langle \psi_0 | S(0) | \psi_0 \rangle} \langle \psi | b_{k+q}^\dagger b_k | \psi_0 \rangle \tag{38} \]
where
\[ b_k = a_{-k}^\dagger a_k^\dagger \tag{39} \]
are the destruction and generation operators of the Cooper pairs, which permute like Bosons [3]. Clearly here we have adopted the scenario in Eq. (2). We also replace Eq. (36) with

\[ |\psi_0\rangle = \prod_k b^\dagger_k |0\rangle, \quad |\psi\rangle = \prod_{k,q} b^\dagger_{k+q} |0\rangle \]  

(40)

which leads through Eq. (35) to

\[ \epsilon_1 = -\sum_k \sum_q \frac{V_{k,q}}{\langle \psi_0 | S(0) | \psi_0 \rangle} \]  

(41)

\( V_{k,q} \) is also defined by Eq. (27). Note that in Eq. (41) we do not sum spin, so that we do not have the factor 2, in contrast to Eq. (26).

In Eq. (40) \( k + q \) in \(|\psi\rangle\) runs over more states compared with \( k \) in \(|\psi_0\rangle\). To understand this we recall that we have

\[ \sum_q V_{k,q} = \frac{1}{\Omega_{D}} \int d \mathbf{q} V_{k,q} = \langle \psi_0 | S(0) | \psi_0 \rangle \]  

(42)

\( \Omega_{D} \) being the volume of the Debye phonon sphere. Consequently Eq. (41) can be written as

\[ \epsilon_1 = -\sum_k \frac{\langle V_{k,q} \rangle}{\langle \psi_0 | S(0) | \psi_0 \rangle} \]  

(43)

that is \( \epsilon_1 \) is averaged over many end states, with the implicit assumption that these end states can all be traced back to the same initial state, \(|\psi_0\rangle\). This situation is opposite to that in Eq. (26), where the initial and end states are the same but \( \epsilon_1 \) is averaged over many intermediate states.

\section{VIII. Umklapp Frustration}

We are reminded that in Eq. (35) we let both \( k \) and \( k' \) run over the first electron Brillouin zone. We also let both \( \sigma \) and \( \sigma' \) run over the two spins. When we pair the electrons, we must be careful that we do not neglect or double count any of the electron states. We may let the pairs be in states \((k \uparrow, -k \downarrow)\) and \((k \downarrow, -k \uparrow)\) and let \( k \) run over half the Brillouin zone. Here we let the pairs be in the state \((k \uparrow, -k \downarrow)\) and let \( k \) run over the whole Brillouin zone [1]. Either way we acknowledge that, with the same wavevector \( k \), electrons of both spins can find a partner with \(-k\) and opposite spin to form pairs. Consider two such pairs generated by the following operators:

\[ b^\dagger_k = a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} \]  

(44)

\[ b^\dagger_{-k} = a^\dagger_{-k\uparrow} a^\dagger_{k\downarrow} \]

which are in the initial state \(|\psi_0\rangle\) in Eq. (40). Since

\[ \langle 0 | b^\dagger_{-k} b^\dagger_k | 0 \rangle = \langle 0 | a_{k\downarrow} a_{-k\uparrow} a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} | 0 \rangle = 0 \]  

(45)

we have two genuinely different pairs orthogonal to each other. They are not the same pair with different names.

Now consider the end states initiated by the operators in Eq. (41). In normal scattering the end states are generated by

\[ b^\dagger_{k+q} = a^\dagger_{k+q\uparrow} a^\dagger_{-k-q\downarrow} \]  

(46)

\[ b^\dagger_{-k+q'} = a^\dagger_{-k+q'\uparrow} a^\dagger_{k-q'\downarrow} \]

which are in \(|\psi\rangle\) in Eq. (40). In umklapp scattering the end states are generated by

\[ b^\dagger_{k+q+G} = a^\dagger_{k+q+G\uparrow} a^\dagger_{-k-q-G\downarrow} \]  

(47)

\[ b^\dagger_{-k+q'-G} = a^\dagger_{-k+q'-G\uparrow} a^\dagger_{k-q'+G\downarrow} \]

which too are in \(|\psi\rangle\) in Eq. (40). In FIG. 1 we have

\[ -k + q' = k + q + G \]  

(48)

Eqs. (40) and (47) lead through (45) to

\[ b^\dagger_{k+q} b^\dagger_{-k-q}\downarrow G = b^\dagger_{k+q} b^\dagger_{k+q} = 0 \]  

(49)

\[ b^\dagger_{-k+q'} b^\dagger_{k+q'} = b^\dagger_{-k+q'} b^\dagger_{k+q'} = 0 \]

which means that superconductivity is cancelled (or frustrated) unless \( q \) in Eq. (41) is such that umklapp scattering is not invoked.

One may ask why we do not pay attention to some other conceivable cancellation. For example in FIG. 1 we may place a second electron beside \( k \) to let it compete with the first electron for end states. The answer lies in our initial state, \(|\psi_0\rangle\), in Eq. (40), where we are only allowed to have two pairs generated by Eq. (41), in order to serve the purpose of finding the energy shift for a given \( k \). Indeed both \(|\psi_0\rangle\) and \(|\psi\rangle\) are approximate. They are requested to serve their purpose without self-conflict. It is not necessary to subject them to any further scrutiny, such as what would happen when we have the second electron beside \( k \) in FIG. 1.

Could we go a step further to have only one pair in the initial state? Then umklapp frustration will vanish. Since this question carries physical consequences, it concerns situations in physics rather than formalisms in mathematics. One such situation is that either \( b^\dagger_k \) or \( b^\dagger_{-k} \) in Eq. (41) is always forbidden to generate a pair, which apparently is unreasonable. Another situation is that, when one pair is scattered in accordance with the scenario in Eq. (2), the other is left unchanged. This too is unreasonable because, apart from their spins, the two pairs generated by Eq. (41) are identical. We have no reason to treat them differently in electron-phonon scattering, not to mention that numerical test has already confirmed the existence of umklapp scattering [2].
IX. COULOMB REPULSION

So far we have not discussed Coulomb repulsion, which has been proved to have negligible effect on superconductivity, apparently due to the situation that in a metal the Coulomb force between electrons is in a balance, which can be toppled by even weak attraction due to the electron-phonon interaction. To see this, we replace $H_c$ in Eqs. [1] and [5] with $H_c + H_{\text{Col}}$, where $H_{\text{Col}}$ is the Coulomb Hamiltonian, and alter the definition of $a_{k,\sigma}^\dagger$ and $a_{k,\sigma}$ accordingly. Consequently we redefine $\epsilon_0$ as the energy of the particle ensemble with Coulomb repulsion but without the electron-phonon interaction. We also redefine $\epsilon$ as the ensemble energy with both the Coulomb and electron-phonon interaction. This has no effect on subsequent derivations, based on the very general assumption that we have Bloch particles, except that the numerical values of $V_{k,\sigma}$ in Eqs. [27] may change slightly.

X. SELF-CONSISTENT SOLUTION

We may follow the example of the standard field-theoretic approach to employ the Dyson equation to find a self-consistent solution for the superconductive energy gap. We may acquire a rough idea about the use of the Dyson equation from the familiar self-consistent equation of BCS [2]:

$$\Delta(k) = \sum_q V_{k,q} \frac{\Delta(k + q)}{2[\Delta^2(k + q) + c^2(k + q)]^{1/2}}$$  (50)

where $\Delta$ is the energy gap function, which replaces $-\epsilon_1$ in Eq. [11]. In order to find something like Eq. [51], we should be able to separate $\epsilon_1$ as a factor from $\epsilon_2, \epsilon_3, \ldots$ in Eq. [52]. We should also argue credibly that, when we add the remainder of $\epsilon_2, \epsilon_3, \ldots$, together we will recover within a constant the original series $\epsilon_1 + \epsilon_2 + \ldots$ in Eq. [52]. Further discussion, however, is beyond the scope of this communication.

XI. GREEN FUNCTION

In the standard field-theoretic approach the superconductive energy gap is identified from the high order terms of the Green function, which is of the following form:

$$G(x, x') = -i \frac{\langle \psi_0 | T \hat{\psi}(x) \hat{\psi}^\dagger(x') S(0) | \psi_0 \rangle}{\langle \psi_0 | S(0) | \psi_0 \rangle}$$  (51)

where $x = (r, t)$ denotes a set of four variables,

$$\hat{\psi}(x) = \sum_{k,\sigma} a_{k,\sigma}^\dagger \psi_{k,\sigma}(r) \exp[i\epsilon_0(k)t/\hbar]$$  (52)

$\psi_{k,\sigma}$ being the Bloch function, and $T$ is the chronological operator. When $t > t'$ we have

$$T \hat{\psi}(x) \hat{\psi}^\dagger(x') S(0) = \hat{\psi}(x) S(0) \hat{\psi}^\dagger(x')$$  (53)

otherwise, when $t \leq t'$, we have

$$T \hat{\psi}(x) \hat{\psi}^\dagger(x') S(0) = -\hat{\psi}^\dagger(x') S(0) \hat{\psi}(x)$$  (54)

On substituting Eq. [11] into Eq. [51] we find

$$G(x, x') = G_0(x, x') + G_1(x, x') + \ldots$$  (55)

with

$$G_n(x, x') = -\frac{\langle \psi_0 | T \hat{\psi}(x) \hat{\psi}^\dagger(x') S_n(0) | \psi_0 \rangle}{\langle \psi_0 | S(0) | \psi_0 \rangle}$$  (56)

where $S_n(0)$ is given in Eq. [11], $n = 0, 1, 2, \ldots$ [4].

In the literature $G_0$ is known as the Green function of free particles, of which a brief derivation is given in the Appendix, in order to demonstrate clearly that the Green function is evaluated with UNPAIRED particles. We know from discussion in this communication that in $G_1$ the events are described by the scenario in Eq. [11]. In the standard field-theoretic approach the effect of superconductivity starts to become apparent in $G_2$, which is proportional to the square of $H_{\text{Col}}$, similar to $\epsilon_1$ in Eq. [11]. In $G_2$ there is also a factor 1/2, arising from the use of $S_2(0)$ rather than $S_1(0)$, which cancels the factor 2 in Eq. [20]. However, in $G_2$ the nature of events is still similar to that described by Eq. [11], although the particles go through more intermediate states before returning to their initial state, so that the diagram technique becomes indispensable in order to facilitate calculation. Indeed there is no need to pair electrons in the standard field-theoretic approach, which indicates that we are dealing with something similar to the Stark effect rather than superconductivity. It would be difficult to identify umklapp frustration from the standard field-theoretic approach.

XII. CONCLUSION

Gell-Mann and Low devised a general formula, which is applicable to both the Stark effect (or other similar effects) and superconductivity. Therefore, when applying this formula, we must know to which process we are applying it. In the standard field-theoretic approach the electrons always return to their initial orbits. The energy of each and every orbit is perturbed in the same direction. There is no need to pair the electrons, in order for the process to manifest itself macroscopically. This communication introduces a preliminary new version of the field-theoretic approach, where the electrons do not return to their initial orbits. Then it becomes necessary to pair the electrons in order to observe an energy shift of the ensemble. Umklapp frustration emerges, which is closely associated with pairing. Apparently the standard field-theoretic approach fits the nature of the Stark effect, whereas the alternative version is more appropriate to describe superconductivity. Further work appears to be worthwhile in order to incorporate the sophistication of the standard field-theoretic approach [4] into the new version.
XIII. APPENDIX

When \( t > t' \) we have

\[
G_0(x, x') = -i\langle \psi_0 | \hat{\psi}(x) \hat{\psi}^\dagger(x') | \psi_0 \rangle
\]

(57)

where \( \hat{\psi} \) is a weighted series of particle destruction operators given by Eq. \( \text{(52)} \), in which the Bloch wave function is of the following specific form

\[
\psi_{k, \sigma}(r) = \frac{1}{\sqrt{\Omega}} u_{k, \sigma} \exp(ik \cdot r)
\]

(58)

\( \Omega \) being the volume of the metal, \( |u_{k, \sigma}|^2 = 1 \) for free particles. Combining Eqs. \( \text{(52)}, \text{(57)} \) and \( \text{(57)} \), we find

\[
G_0(x, x') = -\frac{i}{\Omega} \sum_{k, \sigma} \langle \psi_0 | a_{k, \sigma} a_{k, \sigma}^\dagger | \psi_0 \rangle \times \exp[i(k \cdot (r - r'))] \times \exp [\epsilon_0(k)(t - t')/i\hbar]
\]

(59)

Letting \( |\psi_0\rangle \) be the state of all the electrons in the Fermi sea, which are UNPAIRED, we have

\[
\langle \psi_0 | a_{k, \sigma} a_{k, \sigma}^\dagger | \psi_0 \rangle = \begin{cases} 1, & |k| > k_F \\ 0, & \text{otherwise} \end{cases}
\]

(60)

\( k_F \) being the Fermi wavenumber, so that

\[
G_0(x, x') = -\frac{i}{\Omega} \sum_{|k| > k_F} \exp[i(k \cdot (r - r'))] \times \exp [\epsilon_0(k)(t - t')/i\hbar]
\]

(61)

which can be written as

\[
G_0(x, x') = -\frac{i}{(2\pi)^3} \int \! dk \theta(|k| - k_F) \times \exp[i(k \cdot (r - r'))] \times \exp [\epsilon_0(k)(t - t')/i\hbar]
\]

(62)

where

\[
\theta(\xi) = \begin{cases} 1, & \xi > 0 \\ 0, & \text{otherwise} \end{cases}
\]

(63)

When \( t < t' \) we find through a similar procedure

\[
G_0(x, x') = -\frac{i}{(2\pi)^3} \int \! dk \theta(k_F - |k|) \times \exp[i(k \cdot (r - r'))] \times \exp [\epsilon_0(k)(t - t')/i\hbar]
\]

(64)

According to Eq. \( \text{(62)} \), we have

\[
\int_{t'}^\infty G_0(x, x') \exp[i\omega(t - t')] \, dt = \frac{\theta(|k| - k_F)}{\omega - \epsilon_0(k)/\hbar + i\delta} \exp[ik \cdot (r - r')]
\]

(65)

where we have introduced the infinitesimal number \( \delta \), in order to evaluate the integration at \( t = \infty \), as we did in Eqs. \( \text{(24)}, \text{(25)}, \text{(33)} \). On the other hand, according to Eq. \( \text{(64)} \), we have

\[
\int_{-\infty}^{t'} G_0(x, x') \exp[i\omega(t - t')] \, dt = \frac{\theta(k_F - |k|)}{\omega - \epsilon_0(k)/\hbar - i\delta} \exp[ik \cdot (r - r')]
\]

(66)

Adding Eqs. \( \text{(65)} \) and \( \text{(66)} \) together, we find through Eq. \( \text{(63)} \) that

\[
\int_{-\infty}^\infty G_0(x, x') \exp[i\omega(t - t')] \, dt = \frac{\exp[ik \cdot (r - r')]}{\omega - \epsilon_0(k)/\hbar + i\delta \text{sign}(|k| - k_F)}
\]

(67)

where \( \text{sign}(\xi) = 1 \) if \( \xi > 0 \), otherwise \( \text{sign}(\xi) = -1 \). It is easy to recognize that Eq. \( \text{(67)} \) represents the Fourier transform of \( G_0(x, x') \) with respect to \( t \). An inverse Fourier transform of the expression on the right hand side of Eq. \( \text{(67)} \) gives

\[
G_0(x, x') = \frac{1}{(2\pi)^3} \int \! d\omega \int \! dk \ G_0(k, \omega) \times \exp[ik \cdot (r - r')] \exp[-i\omega(t - t')] \]

(68)

with

\[
G_0(k, \omega) = \frac{1}{\omega - \epsilon_0(k)/\hbar + i\delta \text{sign}(|k| - k_F)}
\]

(69)

which is known as the free electron Green function in frequency and momentum space,

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