

Coherent Excited States in the Theory of Superconductivity: Gauge Invariance and the Meissner Effect

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We discuss the coherent states generated in the Bardeen, Cooper, and Schrieffer theory of superconductivity by the momentum displacement operator $\rho_{\mathbf{Q}} = \sum_n \exp(i\mathbf{Q} \cdot \mathbf{r}_n)$. Without taking into account plasma effects, these states are like bound Cooper pairs with momentum $\hbar\mathbf{Q}$ and energies lying in the gap, and they play a central role in the explanation of the gauge invariance of the Meissner effect. Long-range Coulomb forces recombine them into plasmons with equations of motion unaffected by the gap. Central to the argument is the proof that the non-gauge-invariant terms in the Hamiltonian of Bardeen, Cooper, and Schrieffer have an effect on these states which vanishes in the weak-coupling limit.

I. INTRODUCTION

BUCKINGHAM¹ has questioned whether an energy-gap model of superconductivity, such as that of Bardeen, Cooper, and Schrieffer,² can explain the Meissner effect without violating a certain identity derived by Schafroth³ on the basis of gauge invariance, and by Buckingham using essentially an f -sum rule. This identity is what causes the insulator, which also has an energy gap, to fail to show a Meissner effect; thus, Buckingham and Schafroth⁴ argue, a proof of gauge invariance lies at the core of the problem of superconductivity, especially since the Hamiltonian used in B.C.S. is not gauge-invariant.

Bardeen⁵ argues that the matrix elements and energy states involved in the gauge problem bring in coherent excitations which will be strongly coupled to the plasma modes, a high-frequency phenomenon presumably unaltered by superconductivity. Unfortunately, while we find that this is indeed exactly the situation, the insulator also often has normal plasma modes. Thus, while the B.C.S. calculation in the London gauge is probably entirely correct, and justifiable on physical grounds, it throws little light on the basic differences between the three cases—insulator, metal, and superconductor.

We also noticed that the operator which is central in the gauge problem as well as the plasma theory,

$$\begin{aligned} \rho_{\mathbf{Q}} &= \sum_n \exp(i\mathbf{Q} \cdot \mathbf{r}_n) \\ &= \sum_{\mathbf{k}, \sigma} c_{\mathbf{k}+\mathbf{Q}, \sigma}^* c_{\mathbf{k}, \sigma}, \end{aligned} \quad (1)$$

has another interesting property: its separate components $c_{\mathbf{k}+\mathbf{Q}, \sigma}^* c_{\mathbf{k}, \sigma}$, when applied to the B.C.S. ground-state wave function Ψ_0 , create excited pairs of electrons $\mathbf{k}_1, \mathbf{k}_2$ with momentum pairing

$$\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{Q} \quad (2)$$

¹ M. J. Buckingham, *Nuovo cimento* **5**, 1763 (1957).

² Bardeen, Cooper, and Schrieffer, *Phys. Rev.* **106**, 162 (1957); **108**, 1175 (1957). The latter we call B.C.S., and we shall follow its notation as far as possible.

³ M. R. Schafroth, *Helv. Phys. Acta* **24**, 645 (1951).

⁴ M. R. Schafroth (private communication). I am indebted to G. Wentzel for an elegant presentation of these questions in a series of discussions, to which M. Lax and C. Herring also contributed.

⁵ J. Bardeen, *Nuovo cimento* **5**, 1765 (1957).

instead of zero. The total operator applied to Ψ_0 leads to a linear combination of such states, which can be thought of as equivalent to a Cooper bound state⁶ of a pair of electrons with nonzero momentum, superimposed on the B.C.S. ground state.

Our discussion of these problems is based on the following physical picture: any transverse excitation involves breaking up the phase coherence over the whole Fermi surface of at least one pair in the superconducting ground state, and so involves a loss of attractive binding energy. This causes the Meissner effect. Longitudinal excitations, however, such as those generated by $\rho_{\mathbf{Q}}$, do not break up phase coherence in the superconducting state, and so their energies involve only kinetic energy, or electromagnetic energy when plasma effects are included. Thus longitudinal and transverse excitations are different in the superconductor, in a sense in which they are not in either the metal or the insulator, and it turns out to be this difference which allows a gauge-invariant explanation of the Meissner effect.

We proceed further in two stages. First, we discuss the fictitious problem in which the only plasma effect is the screening of the long-range repulsion. In this stage gauge invariance requires, and we indeed find, that the states

$$\Psi_{\mathbf{Q}} = \rho_{\mathbf{Q}} \Psi_0 \quad (3)$$

have energies in the energy gap and proportional to Q^2 . In a perfectly gauge-invariant theory, their energy would be just the kinetic energy

$$E_{\mathbf{Q}} = (\hbar^2 Q^2 / 2m) (2\epsilon_f / 3\pi\epsilon_0), \quad (4)$$

but we find a small correction going to zero in the weak-coupling limit. Equation (4) follows from the same f -sum rule which leads to gauge invariance.

There is a fundamental difference, which we demonstrate, between the ways in which superconducting and normal substances satisfy this sum rule. Both normal metals and insulators (leaving out the rather confusing effects of long-range Coulomb forces which can be studied later) satisfy this rule with ordinary excitations in such a way that the more familiar optical sum rule—

⁶ L. N. Cooper, *Phys. Rev.* **104**, 1189 (1956).

which in turn leads to normal diamagnetism—also follows. In these normal cases the states (3) can be shown not to exist separately from the ordinary excitations. In the superconductor, however, the rule is satisfied by matrix elements involving only the longitudinal excitations (3), while the optical sum rule and Meissner effect involve transverse excitations with entirely different behavior from the longitudinal ones. Basically, these transverse excitations involve combinations of pair states which have a finite angular as well as linear momentum and cannot be bound into quasi-“Cooper pairs” like the longitudinal excitations. This difference is the basis for the electromagnetic properties of superconductivity.

At this stage any number of $\mathbf{Q} \neq 0$ pairs could be incorporated into the state with little loss of energy. This alleviates the rigidity of the B.C.S. ground state to some extent, making it easier to fit physical boundary conditions. On the other hand, we will find that when plasma effects are included the $\mathbf{Q} = 0$ pairing condition is again enforced, except possibly in particular geometrical situations for very long wavelengths.

In the second stage of the calculation we discuss these plasma effects. Our procedure corresponds to that of Nozières and Pines,⁷ who find that the f -sum rules, and particularly the relationship of the optical and longitudinal forms, are best discussed prior to including the long-range Coulomb effects. Appealing to the random-phase approximation, which allows separation of the different momenta \mathbf{Q} , we show that the longitudinal f -sum rule becomes the commutation rule of plasma coordinates and momenta, while the transverse behavior is unaffected, whether normal or superconducting, when the long-range Coulomb interactions are included. The states $\Psi_{\mathbf{Q}}$ are recombined to make the plasma excitations, which now have large excitation energies and do not affect the energy gap.

II. COMMUTATORS AND ENERGIES OF COHERENT STATES

In this section we carry out the first stage of the program in the introduction. We naively ignore plasma effects and subsidiary conditions and study the energies of coherent excited states, and the f -sum rules, using the B.C.S. ground state derived from phonon and screened Coulomb interactions.

The initial Hamiltonian used by B.C.S. contains the kinetic energy and the second-order phonon interaction between electrons, but ignores the self-energy as well as higher-order terms. It is

$$H = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} n_{\mathbf{k}, \sigma} + \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}', \sigma, \sigma', \kappa} 2\hbar\omega_{\kappa} |M_{\kappa}|^2 \times [(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\kappa})^2 - (\hbar\omega_{\kappa})^2]^{-1} c_{\mathbf{k}'-\kappa, \sigma'}^* c_{\mathbf{k}', \sigma'} \times c_{\mathbf{k}+\kappa, \sigma}^* c_{\mathbf{k}, \sigma} + H_{\text{Coul}} \quad (5)$$

⁷ P. Nozières and D. Pines, Phys. Rev. **109**, 741 (1958).

Almost immediately B.C.S. drop, except for later perturbation calculations, all terms except $\mathbf{k}' = -\mathbf{k}, \sigma' = -\sigma$; and they replace the coefficient by a constant unless either $|\epsilon_{\mathbf{k}}|$ or $|\epsilon_{\mathbf{k}+\kappa}| > \hbar\omega$, in which case it is zero. The resulting Hamiltonian is their H_{red} .

The Hamiltonian (5) is already not gauge-invariant, if it is to be used with the usual expressions for the current and for the perturbation of an electromagnetic field, because it depends on \mathbf{k} as well as κ . Fortunately, however, we shall show that the important difficulties are not connected with the momentum dependence of (5) but with the simplification to H_{red} . The difficulty is that in calculating the properties of coherent excited states of the B.C.S. theory one must take into account more than just the $\mathbf{k}' - \mathbf{k}$ terms of the interaction.

When this is done we shall show that the corrections caused by the \mathbf{k} dependence of (5) in the important sum rules and energies become negligible in a well-defined limit which is that applying to most superconductors.

The entire argument is based on a commutation relation used by Buckingham¹ in this connection and by Nozières and Pines⁷ for other reasons:

$$[H_{\mathbf{K}}, \rho_{\mathbf{Q}}] = (-\hbar^2/2m) i\mathbf{Q} \cdot \sum_n [\nabla_n \exp(i\mathbf{Q} \cdot \mathbf{r}_n) + \exp(i\mathbf{Q} \cdot \mathbf{r}_n) \nabla_n] = (\hbar^2/2m) \sum_{\mathbf{k}, \sigma} \mathbf{Q} \cdot (2\mathbf{k} + \mathbf{Q}) c_{\mathbf{k}+\mathbf{Q}, \sigma}^* c_{\mathbf{k}, \sigma} \quad (6)$$

where $H_{\mathbf{K}}$ is the kinetic energy and $\rho_{\mathbf{Q}}$ is defined in (1). In the case of most simple kinds of forces, which are functions only of coordinates or at most of relative momenta, $\rho_{\mathbf{Q}}$ commutes with the potential energy. Then (6) may be written, using

$$[H, \rho_{\mathbf{Q}}] = [H_{\mathbf{K}}, \rho_{\mathbf{Q}}],$$

as

$$(E_m - E_{m'}) (m | \rho_{\mathbf{Q}} | m') = (\hbar^2/2m) \mathbf{Q} \cdot \sum_j (m | \nabla_j \exp(i\mathbf{Q} \cdot \mathbf{r}_j) + \exp(i\mathbf{Q} \cdot \mathbf{r}_j) \nabla_j | m'). \quad (7)$$

We may also deduce from (7) the basic f -sum rule:

$$[[H, \rho_{\mathbf{Q}}], \rho_{-\mathbf{Q}}] = N\hbar^2 Q^2/m; \quad (8)$$

$$\sum_{m'} (E_m - E_{m'}) | (m | \rho_{\mathbf{Q}} | m') |^2 = \frac{1}{2} N\hbar^2 Q^2/m,$$

or

$$\sum_{m'} | (m | \mathbf{Q} \cdot \sum_j [\nabla_j \exp(i\mathbf{Q} \cdot \mathbf{r}_j) + \exp(i\mathbf{Q} \cdot \mathbf{r}_j) \nabla_j] | m') |^2 \times (E_m - E_{m'})^{-1} = 2mN Q^2/\hbar^2. \quad (9)$$

Now in the case of (5) the potential energy does not commute with $\rho_{\mathbf{Q}}$. However, what we can show is that the commutator can be made arbitrarily small compared to (7).

In doing this we shall not use the explicit form (5) but shall carry out the first stage—the cutoff—of the simplification to H_{red} , in full confidence that the results would be practically the same if we used (5) itself, because the new potential is no less k -dependent than the old in the region of interest. One can then show that the full interaction energy, corresponding to the $\mathbf{k}' = -\mathbf{k}$ terms

of the B.C.S. H_{red} , is

$$H_V = -\frac{1}{2}V \sum_{\mathbf{q}} \left[\sum_{\mathbf{k}' \neq \mathbf{k} (\epsilon_{\mathbf{k}'} < \hbar\omega)} \sum_{\mathbf{k} (\epsilon_{\mathbf{k}} < \hbar\omega)} + \sum_{\mathbf{k}' \neq \mathbf{k} (\epsilon_{\mathbf{k}'} - \mathbf{q} < \hbar\omega)} \sum_{\mathbf{k} (\epsilon_{\mathbf{k}} - \mathbf{q} < \hbar\omega)} \right] (c_{\mathbf{k}'\uparrow}^* c_{-\mathbf{k}'+\mathbf{q}\downarrow}^* c_{-\mathbf{k}+\mathbf{q}\downarrow} c_{\mathbf{k}\uparrow}). \quad (10)$$

(All notations are as used in B.C.S.) Then first of all we have to calculate the commutator of this with $\rho_{\mathbf{Q}}$. This is done in the Appendix, and the result is:

$$[H_V, \rho_{\mathbf{Q}}] = \frac{1}{2}V \left[\sum_{\mathbf{k}' \neq \mathbf{k}} \sum_{\mathbf{k} (\epsilon_{\mathbf{k}} < \hbar\omega, \epsilon_{\mathbf{k}+\mathbf{Q}} > \hbar\omega)} - \sum_{\mathbf{k}' \neq \mathbf{k}} \sum_{\mathbf{k} (\epsilon_{\mathbf{k}} > \hbar\omega, \epsilon_{\mathbf{k}+\mathbf{Q}} < \hbar\omega)} + (\text{same with } \mathbf{k} \rightarrow \mathbf{k}', \mathbf{k}' \rightarrow \mathbf{k}) \right] \\ \times (c_{\mathbf{k}'+\mathbf{Q}\uparrow}^* c_{-\mathbf{k}'+\mathbf{q}\downarrow}^* c_{-\mathbf{k}+\mathbf{q}\downarrow} c_{\mathbf{k}\uparrow} - c_{\mathbf{k}'-\mathbf{q}\uparrow}^* c_{-\mathbf{k}'\downarrow}^* c_{-\mathbf{k}-\mathbf{Q}\downarrow} c_{\mathbf{k}-\mathbf{q}\uparrow}). \quad (11)$$

These terms already refer only to \mathbf{k} states within \mathbf{Q} of the cutoff surface, and contain subtractions which make them depend on only the derivatives of the wave function near this surface. Thus, (11) will always be small acting on states close to the ground state, at least for small Q .

We shall see that the most important measure of this smallness is the scalar product.

$$(\rho_{\mathbf{Q}} \Psi_{\mathbf{g}}, [H_V, \rho_{\mathbf{Q}}] \Psi_{\mathbf{g}}), \quad (12)$$

where $\Psi_{\mathbf{g}}$ is the B.C.S. ground state. This will be computed in the Appendix also, but first we will need to compute the wave function

$$\Psi_{\mathbf{Q}} = \rho_{\mathbf{Q}} \Psi_{\mathbf{g}}, \quad (13)$$

and its normalization. Consider a particular term of $\rho_{\mathbf{Q}}$,

$$(\rho_{\mathbf{Q}}^{\kappa})_+ = c_{\kappa+\mathbf{Q}\uparrow}^* c_{\kappa\uparrow}, \quad (14a)$$

or

$$(\rho_{\mathbf{Q}}^{\kappa})_- = c_{-\kappa\downarrow}^* c_{-\kappa-\mathbf{Q}\downarrow}. \quad (14b)$$

Then

$$(\rho_{\mathbf{Q}}^{\kappa})_+ \Psi_{\mathbf{g}} = \prod_{\mathbf{k} \neq \kappa, \kappa+\mathbf{Q}} [(1-h_{\mathbf{k}})^{\frac{1}{2}} + h_{\mathbf{k}}^{\frac{1}{2}} b_{\mathbf{k}}^*] \\ \times (1-h_{\kappa+\mathbf{Q}})^{\frac{1}{2}} h_{\kappa}^{\frac{1}{2}} c_{\kappa+\mathbf{Q}\downarrow}^* c_{-\kappa\uparrow} \Psi_{\mathbf{v}},$$

$\Psi_{\mathbf{v}}$ being the vacuum state. Thus

$$(\rho_{\mathbf{Q}}^{\kappa})_+ \Psi_{\mathbf{g}} = h_{\kappa}^{\frac{1}{2}} (1-h_{\kappa+\mathbf{Q}})^{\frac{1}{2}} \Psi_{-\kappa, \kappa+\mathbf{Q}}, \quad (15)$$

where the last notation refers to the presence of a pair of real "single" excitations in the B.C.S. sense in states $-\kappa\downarrow$ and $\kappa+\mathbf{Q}\uparrow$. Similarly,

$$(\rho_{\mathbf{Q}}^{\kappa})_- \Psi_{\mathbf{g}} = h_{\kappa+\mathbf{Q}}^{\frac{1}{2}} (1-h_{\kappa})^{\frac{1}{2}} \Psi_{-\kappa, \kappa+\mathbf{Q}}, \quad (16)$$

and

$$\Psi_{\mathbf{Q}} = \rho_{\mathbf{Q}} \Psi_{\mathbf{g}} \cong 2 \sum_{\kappa} h_{\kappa}^{\frac{1}{2}} (1-h_{\kappa})^{\frac{1}{2}} \Psi_{-\kappa, \kappa+\mathbf{Q}}. \quad (17)$$

Thus $\Psi_{\mathbf{Q}}$ is indeed a certain linear superposition of pair excitations with momentum \mathbf{Q} . Its normalization factor is

$$(\Psi_{\mathbf{Q}}, \Psi_{\mathbf{Q}}) = 4 \sum_{\kappa} h_{\kappa} (1-h_{\kappa}) \\ \cong 2\pi \epsilon_0 N(0), \quad (18)$$

which is finite—a vital point, since the corresponding quantity in metal or insulator approaches zero with \mathbf{Q} . Equation (18) already implies the presence of long-range order in the ground state, as we shall see.

Now we can compute the quantity (12) in the Appendix. The result is

$$(\rho_{\mathbf{Q}} \Psi_{\mathbf{g}}, [H_V, \rho_{\mathbf{Q}}] \Psi_{\mathbf{g}}) = \frac{2}{3} \epsilon_0^2 N(0) \hbar^2 k_F^2 Q^2 / m^2 \omega^2. \quad (19)$$

In order to get a measure of the magnitude of (19), and for later work, let us also calculate the kinetic energy commutator (6). This is also done in Appendix I, and the result is

$$(\rho_{\mathbf{Q}} \Psi_{\mathbf{g}}, [H_K, \rho_{\mathbf{Q}}] \Psi_{\mathbf{g}}) \\ = \frac{\hbar^2}{2m} (\rho_{\mathbf{Q}} \Psi_{\mathbf{g}}, \sum_{\mathbf{k}, \sigma} \mathbf{Q} \cdot (2\kappa + \mathbf{Q}) c_{\kappa+\mathbf{Q}, \sigma}^* c_{\kappa, \sigma} \Psi_{\mathbf{g}}) \\ = \frac{4}{3} (\hbar^2 Q^2 / 2m) N(0) \epsilon_F. \quad (20)$$

This value is shown there to be essentially independent of the exact structure of the wave function if it resembles a Fermi sea at all.

We can now, first of all, get a numerical measure of the relative magnitude of the ordinary terms (6) and the non-gauge-invariant terms (11) by taking the ratio of (19) to (20). The result is

$$(19)/(20) = 2\epsilon_0^2 / \hbar^2 \omega^2 = 2 \exp[-2/N(0)V], \quad (21)$$

which is completely negligible for most superconductors, and zero in the weak-coupling limit (when, of course, in principle superconductivity still exists). Thus we have proved our first contention: that, although exact gauge invariance is still not present except in the weak-coupling limit, the inclusion of the $\mathbf{Q} \neq 0$ terms of H_V restores gauge invariance well enough so that no difficulties of principle are encountered by ignoring the terms (11).

We now can use (19), (20), and (18) to show that in this stage, before the introduction of specific plasma effects, states closely related to $\rho_{\mathbf{Q}} \Psi_{\mathbf{g}}$ must lie in the energy gap. To show this we use the identity

$$E_{\mathbf{Q}} (\rho_{\mathbf{Q}} \Psi_{\mathbf{g}}, \rho_{\mathbf{Q}} \Psi_{\mathbf{g}}) = (\rho_{\mathbf{Q}} \Psi_{\mathbf{g}}, H \rho_{\mathbf{Q}} \Psi_{\mathbf{g}}) \\ = (\rho_{\mathbf{Q}} \Psi_{\mathbf{g}}, [H \rho_{\mathbf{Q}} - \rho_{\mathbf{Q}} H] \Psi_{\mathbf{g}}) \\ + E_0 (\rho_{\mathbf{Q}} \Psi_{\mathbf{g}}, \rho_{\mathbf{Q}} \Psi_{\mathbf{g}}), \quad (22).$$

using the fact that the ground state is an eigenstate. (The first equality defines $E_{\mathbf{Q}}$ as the energy of $\Psi_{\mathbf{Q}}$.)

Thus

$$(E_Q - E_0) = (\rho_Q \Psi_g, \rho_Q \Psi_g)^{-1} (\rho_Q \Psi_g, [H, \rho_Q] \Psi_g) \approx \frac{2}{3\pi} \left(\frac{\epsilon_F}{\epsilon_0} \right) \frac{\hbar^2 Q^2}{2m}. \quad (23)$$

Since ρ_Q is a state of momentum $\hbar\mathbf{Q}$, it is orthogonal to the ground state; thus some eigenstate must lie below E_Q . One guesses that Ψ_Q is really a very good approximation to this state.⁸

These states, if they existed, would have interesting properties. Their effective mass is about 10^{-4} electron mass. Therefore the specific heat would be tiny and probably below the accuracy of present measurements. The states would exist distinct from the individual particles only up to the energy gap, so that the maximum \mathbf{Q} would be about $m\epsilon_0/\hbar^2 k_F \approx 10^4/\text{cm}$. Another fact about them is that they cannot be correctly calculated directly from the excitation energies of the pair states and the appropriate matrix elements of H_V . This is because the B.C.S. ground state, while nearly exact, does not diagonalize H well enough for this purpose; we shall discuss this point later.

It is the uniqueness of the states Ψ_Q which will be the central feature in the explanation of the Meissner effect. Ψ_Q is a longitudinal excitation; the corresponding transverse excitations are of a completely different character. Study of the steps which lead to Eq. (11), or a little thought about the properties of Cooper pairs, quickly convinces us that no energy advantage is gained by making an excitation which does not have the

same amplitude at all points of the Fermi surface. Any transverse excitation is of this form, and thus necessarily has a finite excitation energy as its wave number approaches zero. An equivalent statement is that no excitation possessing a finite angular momentum exists in the energy gap, since Cooper pairs have no bound state with nonzero angular momentum.

To understand the effect of these statements let us return to the fundamental sum rule (8). [From here on, we consider the question of the gauge invariance of the Hamiltonian itself closed. All statements are exactly true only in the weak coupling limit in which (11) $\equiv 0$.] Equations (8) and (9) are general statements, and indeed are used in the Nozières-Pines plasmon theory,⁷ since they involve only longitudinal excitations. Actually, in the solid as in the atom the more familiar form of (9) is the optical (i.e., transverse) sum rule, to derive which one takes the limit as $Q \rightarrow 0$ and assumes

$$\frac{2mN}{\hbar^2} = \lim_{Q \rightarrow 0} Q^{-2} \sum_{m'} (E_{m'} - E_m)^{-1} \times |(m|\mathbf{Q} \cdot \sum [\nabla_j \exp(i\mathbf{Q} \cdot \mathbf{r}_j) + \exp(i\mathbf{Q} \cdot \mathbf{r}_j) \nabla_j]|m')|^2 = \frac{1}{3} \sum_{m'} (E_{m'} - E_m)^{-1} |(m|2 \sum_j \nabla_j|m')|^2. \quad (24)$$

The condition for the validity of this limit process has not been previously discussed; we shall find that it involves the absence of a certain type of long-range order, which is, however, present in a superconductor, in that there is a qualitative difference between transverse and longitudinal excitations even as $\mathbf{Q} \rightarrow 0$ and in the absence of Coulomb forces.

III. RELATIONSHIP OF SUM RULES AND ELECTROMAGNETIC PROPERTIES; COMPARISON OF NORMAL AND SUPERCONDUCTING CASES

In this section we shall show how the mathematical questions of the sum rules (6)–(9) and (24) are related to the physical questions of gauge invariance and the Meissner effect. Figure 1 is a schematic diagram of the rather complex relationships involved. The core of the argument is that it is the longitudinal sum rule (9) which implies gauge invariance. As we have pointed out (9) is always true. On the other hand, normal diamagnetism is a consequence of the optical sum rule (24). We shall then show that the normal cases obey the optical sum rule, while the B.C.S. superconductor need not because of the distinction between the states Ψ_Q and the transverse excitations. B.C.S. have in fact shown, in deriving the Meissner effect, that it does not, and there is no need to repeat their calculation here.

To do this we must write down the two quantities involved in the calculation of electromagnetic effects, the current operator:

$$\mathbf{J}(\mathbf{r}) = (ie\hbar/2m) (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) - (e^2/mc) \Psi^* \mathbf{A} \Psi = \mathbf{J}_p + \mathbf{J}_d, \quad (25)$$

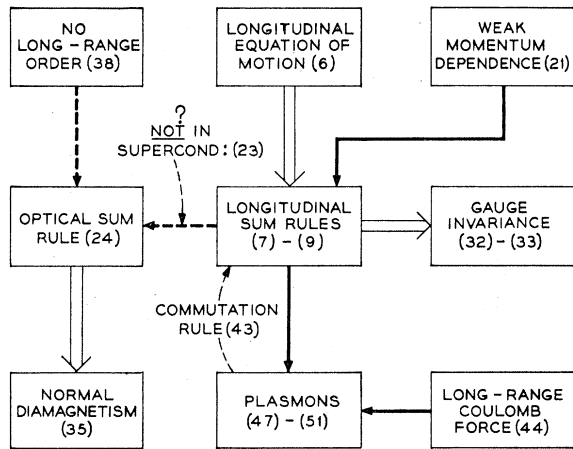


FIG. 1. Logical relations among diamagnetism, sum rules, gauge invariance, and plasmons. Wide arrows are general theorems, solid arrows mean "valid for superconductors at least," and heavy dashed arrows are theorems for normal but not superconducting cases. The numbers in parentheses refer to equations in the text.

⁸ J. Bardeen has pointed out to me that (23) could also be derived by the method of R. P. Feynman [Phys. Rev. **94**, 262 (1954)] using the B.C.S. calculation of the correlation function. Feynman also presents arguments that $\rho_Q \Psi_g$ is nearly the eigenstate.

and the perturbation to the Hamiltonian caused by the vector potential \mathbf{A} :

$$H_1 = (ie\hbar/2m) \int dr \Psi^* (\mathbf{A} \cdot \nabla + \nabla \cdot \mathbf{A}) \Psi. \quad (26)$$

The vector potential may be expanded in Fourier series:

$$\mathbf{A} = \sum_{\mathbf{Q}} \mathbf{a}_{\mathbf{Q}} \exp(i\mathbf{Q} \cdot \mathbf{r}),$$

and one can calculate the appropriate Fourier components of the current $\mathbf{J}_{\mathbf{Q}}$. If we set

$$\mathbf{J}_{\mathbf{Q}} = -K_{\mathbf{Q}} \mathbf{a}_{\mathbf{Q}}, \quad (27)$$

then it is well known that the Meissner effect follows when in the London gauge:

$$\begin{aligned} \nabla \cdot \mathbf{A} &= 0, \\ \lim_{Q \rightarrow 0} K_{\mathbf{Q}} &= \text{finite}. \end{aligned} \quad (28)$$

On the other hand, in a longitudinal gauge there can be no physical current:

$$\begin{aligned} \nabla \times \mathbf{A} &= 0, \\ K_{\mathbf{Q}} &\equiv 0. \end{aligned} \quad (29)$$

The problem is to reconcile these two [(28) and (29)].

In an energy-gap model, (28) is true because the \mathbf{J}_p term of (25) either is small or vanishes, as a result of small matrix elements and finite energy denominators in perturbation theory. But the finite energy denominators must not cause \mathbf{J}_p to vanish in the longitudinal case (29) (see reference 4).

Let us take up the longitudinal case first. Then a typical component is

$$\mathbf{A} = \nabla \exp(i\mathbf{Q} \cdot \mathbf{r}). \quad (30)$$

The \mathbf{Q} th Fourier component of the resulting paramagnetic current is, in perturbation theory,

$$\begin{aligned} \mathbf{J}_p &= \sum_{m'} \left(\frac{e^2 \hbar^2}{4m^2 c} \right) \\ &\times (0 | \sum_n [\exp(i\mathbf{Q} \cdot \mathbf{r}_n) \nabla_n + \nabla_n \exp(i\mathbf{Q} \cdot \mathbf{r}_n)] | m') \\ &\times (m' | i\mathbf{Q} \cdot \sum_n [\exp(i\mathbf{Q} \cdot \mathbf{r}_n) \nabla_n + \nabla_n \exp(i\mathbf{Q} \cdot \mathbf{r}_n)] | 0) \\ &\times (E_{m'} - E_0)^{-1} + \text{complex conj.} \end{aligned} \quad (31)$$

From the sum rule (9),

$$\mathbf{Q} \cdot \mathbf{J}_p = iQ^2 N e^2 / mc, \quad (32)$$

which is exactly the negative of

$$\mathbf{Q} \cdot \mathbf{J}_a = - (N e^2 / mc) (\mathbf{Q} \cdot \mathbf{A}). \quad (33)$$

Thus (9) ensures gauge invariance, and our proof that

to a certain order of accuracy (7) is maintained in B.C.S. is a proof of gauge invariance to that order.

Now consider the real diamagnetism problem in which

$$\mathbf{A} = \mathbf{a}_{\mathbf{Q}} \exp(i\mathbf{Q} \cdot \mathbf{r}); \quad \mathbf{a}_{\mathbf{Q}} \cdot \mathbf{Q} = 0. \quad (34)$$

Now,

$$\begin{aligned} \mathbf{J}_p &= \sum_{m'} (e^2 \hbar^2 / 4m^2 c) \\ &\times (0 | \sum_n [\exp(i\mathbf{Q} \cdot \mathbf{r}_n) \nabla_n + \nabla_n \exp(i\mathbf{Q} \cdot \mathbf{r}_n)] | m') \\ &\times (m' | \sum_n [\exp(i\mathbf{Q} \cdot \mathbf{r}_n) \mathbf{a}_{\mathbf{Q}} \cdot \nabla_n + \nabla_n \cdot \mathbf{a}_{\mathbf{Q}} \exp(i\mathbf{Q} \cdot \mathbf{r}_n)] | 0) \\ &\times (E_{m'} - E_0)^{-1} + \text{complex conj.} \end{aligned} \quad (35)$$

As far as possible constant terms are concerned, if the optical sum rule (24) is valid, then (35) is also equal to the corresponding \mathbf{J}_a and normal diamagnetism follows.

Having thus shown how the gauge invariance and sum rule questions are the same, let us compare how the three cases—superconductor, insulator, and normal metal—obey the sum rules (7) and (9). In the normal metal, the ground state may be approximated by a Fermi sea. The appropriate excited states are single-particle excitations from \mathbf{k} to $\mathbf{k} + \mathbf{Q}$, whose excitation energies are proportional to \mathbf{Q} . Equation (7) is satisfied by finite matrix elements of $\rho_{\mathbf{Q}}$ and small excitation energies. However, we can see from (8) that the sum

$$\sum_{m'} | (0 | \rho_{\mathbf{Q}} | m') |^2 = (\Psi_{\mathbf{Q}}, \Psi_{\mathbf{Q}}) \quad (36)$$

vanishes as Q when $Q \rightarrow 0$, as a result of the small number of possible excitations as $Q \rightarrow 0$. This means that the identity (22) does not cause any anomalous excited states to appear as $Q \rightarrow 0$.

The insulator behaves in an even more regular way. In the insulator there is an automatic energy gap between the ground state and all excitations, but (7) can be satisfied because $(0 | \rho_{\mathbf{Q}} | m) \rightarrow 0$. This in turn is simply a consequence of the fact that excited states are orthogonal to the ground state. The sum (36) in the insulator vanishes as Q^2 , and again (22) does not cause any special excited states to appear.

We see, then, that the failure of (36) to vanish in the superconductor is the major difference from the normal state. We now show that this is related to the presence of a kind of long-range order in the electrons' wave function. A unified way to prove that (36) vanishes in the normal cases is to write the wave function as a determinant of localized one-electron functions:

$$\Psi_0 = \sum_P (-1)^P \prod_{j=1}^N \Psi(\mathbf{r}_j - \mathbf{R}_{P(j)}). \quad (37)$$

In the insulator case, the Ψ 's are the usual Wannier functions. Equation (37) is not in the literature for the case of the Fermi sea, but may be derived as a limit from the insulator by increasing the lattice spacing and combining more and more Brillouin zones to approxi-

mate a sphere. Then, as we approach $Q=0$,

$$\begin{aligned} \rho_Q \Psi_0 &= \sum_j \sum_P (-1)^P \exp(i\mathbf{Q} \cdot \mathbf{r}_j) \prod_{i=1}^N \Psi(\mathbf{r}_j - \mathbf{R}_{P(i)}) \\ &= [\sum_j \exp(i\mathbf{Q} \cdot \mathbf{R}_j)] \Psi_0 + \sum_{P,j} (-1)^P \\ &\quad \times \exp(i\mathbf{Q} \cdot \mathbf{R}_{P(j)}) \mathbf{Q} \cdot (\mathbf{r}_j - \mathbf{R}_{P(j)}) \\ &\quad \times \prod_j \Psi(\mathbf{r}_j - \mathbf{R}_{P(j)}) \cdots = 0 + o(Q). \end{aligned} \quad (38)$$

In the real physical case, one-electron determinants

The sum rule we start from may also be written in the mixed form

$$\sum_m (0 | \mathbf{Q} \cdot \sum_j [\nabla_j \exp(-i\mathbf{Q} \cdot \mathbf{r}_j) + \exp(-i\mathbf{Q} \cdot \mathbf{r}_j) \nabla_j] | m) (m | \exp(i\mathbf{Q} \cdot \mathbf{r}_j) | 0) + c.c. = 2NQ^2. \quad (39)$$

The above is simply the scalar product

$$(\sum_{P,j} (-1)^P \exp(i\mathbf{Q} \cdot \mathbf{R}_{P(j)}) 2\mathbf{Q} \cdot \nabla_j \prod \Psi(\mathbf{r}_j - \mathbf{R}_{P(j)}), \sum_{P,j} (-1)^P \exp(i\mathbf{Q} \cdot \mathbf{R}_{P(j)}) \mathbf{Q} \cdot (\mathbf{r}_j - \mathbf{R}_{P(j)}) \prod \Psi(\mathbf{r}_j - \mathbf{R}_{P(j)}).$$

Here we have already used (38). In any case in which the Wannier functions may be taken even or odd, this is the same as

$$\sum_j (\sum_P (-1)^P \exp(i\mathbf{Q} \cdot \mathbf{R}_{P(j)}) 2\mathbf{Q} \cdot \nabla_j \Psi(\mathbf{r}_j - \mathbf{R}_{P(j)}), \sum_{P'} (-1)^{P'} \exp(i\mathbf{Q} \cdot \mathbf{R}_{P'(j)}) \mathbf{Q} \cdot (\mathbf{r}_j - \mathbf{R}_{P'(j)}) \Psi(\mathbf{r}_j - \mathbf{R}_{P'(j)}). \quad (40)$$

Since the Ψ are localized, the scalar product will vanish for all but nearby $\mathbf{R}_{P(j)}$'s, which means that at small \mathbf{Q} the exponentials all approach unity. Clearly the only property of the wave function which has been used is the absence of long-range order. The above proof fails completely for the B.C.S. ground state, simply because (37) and (38) are not true. The matrix elements which enter in the current in the B.C.S. case can be shown to lead to states with finite angular momentum, which are orthogonal to the states Ψ_Q which satisfy the sum rule (9). For details of the actual calculation see the B.C.S. paper.

IV. PLASMA CONSIDERATIONS

So far all our work has ignored the long-range order and correlations caused by the plasma effect. The reason is now obvious: that a certain special type of long-range order is required to explain the Meissner effect, which is not at all similar to the order enforced by long-range Coulomb forces. That latter order would only serve to obscure the relationships. Prior to plasma effects, the derivation of (24) from (9) is trivial, as in the Nozières-Pines paper⁷; afterwards, it is not at all simple.

In fact, we shall simply repeat the Nozières-Pines work here, but must first briefly explain the philosophy of what we do. The interaction used in B.C.S. includes both the phonon and repulsive Coulomb interactions, the latter appropriately screened, so that our procedure does require justification, in that this screening implies that in the ground-state wave function the plasma effects have already been included.

The basis of our justification is provided by the observation of Sawada, Brueckner, Fukuda, and Brout⁹

are only an approximation. Nonetheless, if we retain the definition of "no long-range order" as meaning that the wave function is really a properly symmetrized product of factors, each referring to a volume small in comparison to the whole specimen, then the above proof still holds.

Now we come to the question of showing that (24) holds in the metal and insulator but not in the superconductor. The proof for one-electron function representations of metal and insulator is trivial, but we shall give it here in a form using (37) which indicates how it might easily be generalized to any case without long-range order.

that the plasma properties of the free-electron gas follow from a Hamiltonian in which the different \mathbf{Q} 's are completely decoupled. This observation provides a deeper justification for the "random-phase approximation" of Bohm and Pines.¹⁰ What we shall do is to retain the random-phase approximation in the superconductor.

As Sawada *et al.* show, the random-phase approximation is equivalent to assuming it more probable that Coulomb interactions return an excited particle into the Fermi sea than that they excite still another. Such terms, as shown by Brueckner and Gell-Mann,¹¹ always lead to the most singular parts of the interactions. Our rather physical argument is that we can show that the part of the interaction retained by these authors is practically unchanged by the energy gap. It is then very hard to see why the less singular parts of the Coulomb interaction would take on a new importance and overwhelm the more singular terms in the superconducting, but not the normal case.

Our procedure is in principle the following: the original B.C.S. Hamiltonian is assumed to contain all the Coulomb interaction except that part involving ρ_Q itself. Thus most of the screening is present, while all momenta except \mathbf{Q} have corresponding subsidiary conditions and plasma terms. For \mathbf{Q} , however, we can still prove (7) and (9) and study the transition from (9) to (24) as we did in the last section; the random-phase approximation tells us there is no strong coupling of \mathbf{Q} and other momenta (we shall discuss the explicit point where this is introduced later). We then show that the plasma properties follow from the sum rules, practically

¹⁰ D. Bohm and D. Pines, Phys. Rev. **85**, 338 (1952).

⁹ Sawada, Brueckner, Fukuda, and Brout, Phys. Rev. **108**, 507 (1957).

¹¹ K. A. Brueckner and M. Gell-Mann, Phys. Rev. **106**, 367 (1957).

unaffected by the gap. On the other hand, the states Ψ_Q disappear and are replaced by the plasma states at $E = \hbar\omega_p$. This means that, in a sense, the pairing criterion $Q=0$ of B.C.S. is enforced only by the subsidiary condition associated with the plasma.

To derive the plasma effects, we shall use the method of the appendix of reference 9. Define a quantity

$$\Pi_Q = (NQ^2)^{-1} \\ 2i\mathbf{Q} \cdot \sum_j [\nabla_j \exp(i\mathbf{Q} \cdot \mathbf{r}_j) + \exp(i\mathbf{Q} \cdot \mathbf{r}_j) \nabla_j]. \quad (41)$$

The commutation rule (7) gives us

$$[H, \rho_Q] = (N\hbar^2 Q^2 / mi) \Pi_Q, \quad (42)$$

while (9) gives

$$[\Pi_Q, \rho_{-Q}] = i, \quad (43)$$

so that Π_Q^* plays the role of a momentum conjugate to the coordinate ρ_Q , and the sum rule becomes their commutation relation. Now we must introduce the interaction

$$H_e = \frac{2\pi e^2}{Q^2} (\rho_Q \rho_{-Q} + \rho_{-Q} \rho_Q), \quad (44)$$

of which we write only the Q terms. We also assume the existence of a ground state of energy E_0 , which we expect to be perturbed from the Ψ_0 so far discussed in such a way as to give the part of the long-range correlation energy associated with ρ_Q , and the subsidiary condition. Finally, we observe that if ρ_Q and Π_Q are to play the role of plasma oscillation coordinates, the first excited state Ψ_1 is obtainable by

$$\Psi_1 = (\alpha\rho_Q + \beta\Pi_Q)\Psi_0, \quad (45)$$

while the energy condition

$$E_1\Psi_1 = (H_0 + H_e)\Psi_1 \quad (46)$$

is just

$$[H, (\alpha\rho_Q + \beta\Pi_Q)]\Psi_0 = E_1(\alpha\rho_Q + \beta\Pi_Q)\Psi_0, \quad (47)$$

and, as Sawada *et al.* show,⁹ the condition that Ψ_0 be the ground state is the subsidiary condition:

$$(\alpha\rho_Q + \beta\Pi_Q)\Psi_0 = 0. \quad (48)$$

The commutator in (47) with Π_Q is made up of

$$[H_e, \Pi_Q] = +4\pi e^2 Q^{-2} i\rho_Q, \quad (49)$$

and of

$$[H_0, \Pi_Q] = mi(N\hbar^2 Q^2)^{-1} [H_0, [H, \rho_Q]], \quad (50) \\ [H_0, \Pi_Q]_{mm'} = mi(N\hbar^2 Q^2)^{-1} (E_m - E_{m'})^2 (m|\rho_Q|m'),$$

in the representation in which H_0 is diagonal. The sum rules (7) and (8) show us that this is of lower order in Q than (49) except in the insulator (for which a complete discussion has been given by Nozières and Pines⁷).

The random-phase approximation consists in assuming that (49) is the only important commutator of Π_Q with any of the Coulomb terms. A discussion of this was given earlier.

We can now solve (47).

$$\alpha \left(\frac{N\hbar^2 Q^2}{mi} \right) \Pi_Q + \beta \left(\frac{4\pi e^2}{Q^2} \right) \rho_Q = E_1 (\alpha\rho_Q + \beta\Pi_Q).$$

Since ρ_Q and Π_Q are independent, this can be solved to give

$$E_1^2 = 4\pi n e^2 \hbar^2 / m = (\hbar\omega_p)^2, \quad (51)$$

$$\alpha/\beta = im\omega_p / N\hbar Q^2, \quad (52)$$

and the subsidiary condition, from (48),

$$(\alpha\rho_{-Q} - \beta\Pi_{-Q})\Psi_0 = 0, \quad (53)$$

which is the same as that of Bohm and Pines¹⁰ as $Q \rightarrow 0$, since $\alpha \gg \beta$, and the no-plasmon states have almost no $Q \neq 0$ pairs present. The old states Ψ_0 and Ψ_1 more or less as eigenfunctions of momentum are to the harmonic oscillator eigenfunctions. The derivation of (51) and (53) completes our program of showing that only (7) and (44) are necessary to normal plasmon behavior.

V. CONCLUSION

The above is by no means a rigorous and complete answer to the original question of whether the B.C.S. theory satisfies gauge invariance and the sum rules and still shows a Meissner effect. Although most of it is fairly rigorous, a few parts have to be considered as a map for how things might be, rather than a proof of how they are. A few points which would bear further discussion follow.

The first one is the question of rigorous rather than approximate gauge invariance. To show rigorous gauge invariance we would have to show that the corrections to \mathbf{J} and H_1 always canceled the momentum dependence of H_0 . Many arguments indicate that this is not a basic difficulty. For instance, one can always make a superconductor of arbitrarily large transition temperature by letting $\hbar\omega \rightarrow \infty$ and $\exp[-1/N(0)V] \rightarrow 0$ simultaneously, thus satisfying gauge invariance arbitrarily well.

Second is the random-phase approximation in the superconductor. As this is an incompletely solved question for normal metals, we have little hope of making much more headway here.

The most serious question revolves around the correctness of calculating E_Q by the commutator argument rather than directly from B.C.S. excited-state energies and matrix elements. These latter are all calculated ignoring the higher order corrections of $Q \neq 0$ interactions as well as the fact that the B.C.S. ground state is not the exact solution of the reduced Hamiltonian. We believe that the argument is as sound as that of any such intermediate coupling method, in that what has to be assumed is that certain properties of the ground state—the energy commutator, which is very insensitive, and the normalization of Ψ_Q , equivalent to the correlation

function of the electrons⁸—are more stable against perturbations than the actual matrix elements themselves. In calculating frequencies of other coherent elementary excitations, such as sound waves or spin waves in metals, the same situation often arises—the energy calculated directly from what appears to be the correct wave function is not the same as that calculated from the equations of motion.

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APPENDIX. COMPUTATIONS OF COMMUTATORS

The interaction H_V is given in Eq. (10). We divide ρ_Q into two parts:

$$\rho_Q = \rho_Q^+ + \rho_Q^- = \sum_{\mathbf{K}} (c_{\mathbf{K}+\mathbf{Q}\uparrow}^* c_{\mathbf{K}\uparrow} + c_{-\mathbf{K}\downarrow}^* c_{-\mathbf{K}-\mathbf{Q}\downarrow}), \quad (\text{A1})$$

and by direct computation:

$$H_V \rho_Q^+ - \rho_Q^+ H_V = V \sum_{\mathbf{q}} \left(\sum_{\mathbf{k}(\epsilon_{\mathbf{k}} < \hbar\omega)} \sum_{\mathbf{k}' \neq \mathbf{k}(\epsilon_{\mathbf{k}'} < \hbar\omega)} + \sum_{\mathbf{k}(\epsilon_{\mathbf{k}-\mathbf{q}} < \hbar\omega)} \sum_{\mathbf{k}' \neq \mathbf{k}(\epsilon_{\mathbf{k}'-\mathbf{q}} < \hbar\omega)} \right) \\ \times (c_{\mathbf{k}'+\mathbf{Q}\uparrow}^* c_{-\mathbf{k}'+\mathbf{q}\downarrow}^* c_{-\mathbf{k}+\mathbf{q}\downarrow} c_{\mathbf{k}\uparrow} - c_{\mathbf{k}'\uparrow}^* c_{-\mathbf{k}'+\mathbf{q}\downarrow}^* c_{-\mathbf{k}+\mathbf{q}\downarrow} c_{\mathbf{k}-\mathbf{Q}\uparrow}). \quad (\text{A2})$$

In the case of ρ_Q^- , the summations are the same but the last parentheses read:

$$(c_{\mathbf{k}'\uparrow}^* c_{-\mathbf{k}'+\mathbf{q}+\mathbf{Q}\downarrow}^* c_{-\mathbf{k}+\mathbf{q}\downarrow} c_{\mathbf{k}\uparrow} - c_{\mathbf{k}'\uparrow}^* c_{-\mathbf{k}'+\mathbf{q}\downarrow}^* c_{-\mathbf{k}+\mathbf{q}-\mathbf{Q}\downarrow} c_{\mathbf{k}\uparrow}). \quad (\text{A3})$$

In both (A2) and (A3) the second term can be made to correspond with the first by the appropriate substitutions: in (A2) by

$$\mathbf{k}' - \mathbf{Q} \rightarrow \mathbf{k}', \quad \mathbf{k} - \mathbf{Q} \rightarrow \mathbf{k}, \quad \mathbf{q} - \mathbf{Q} \rightarrow \mathbf{q}, \quad (\text{A4})$$

and in (A3) simply by

$$\mathbf{q} - \mathbf{Q} \rightarrow \mathbf{q}. \quad (\text{A5})$$

If Q is small, (A4) and (A5) have no effect on the large majority of terms, so that the appropriate parts of the second term cancel the first. Near the cutoff surface, the substitutions affect the presence or absence of the terms: (A4) when the cutoff depends on \mathbf{k} and \mathbf{k}' , (A5) when it depends on $\mathbf{k} - \mathbf{q}$, $\mathbf{k}' - \mathbf{q}$. The resulting terms near the cutoff surface are given in (11) of the text.

It is also necessary to use Eq. (11) to compute $(\rho_Q \Psi_\theta, [H_V, \rho_Q] \Psi_\theta)$. Equation (17) of the text shows us that only terms of the commutator which break up only two pairs can contribute to the scalar product. Examination of (11) reveals that two types of term can appear. These are the terms involving $\mathbf{q} = 0$ or $\mathbf{q} = -\mathbf{Q}$. Upon taking this into account, the important part of (11) becomes

$$\frac{1}{2} V \left\{ \sum_{\mathbf{k}' \neq \mathbf{k}} \left[\sum_{\mathbf{k}(\epsilon_{\mathbf{k}} < \hbar\omega, \epsilon_{\mathbf{k}+\mathbf{Q}} > \hbar\omega)} - \sum_{\mathbf{k}(\epsilon_{\mathbf{k}} > \hbar\omega, \epsilon_{\mathbf{k}+\mathbf{Q}} < \hbar\omega)} \right] + \text{same with } \mathbf{k}' \rightarrow \mathbf{k}, \mathbf{k} \rightarrow \mathbf{k}' \right\} \\ \times (c_{\mathbf{k}'+\mathbf{Q}\uparrow}^* c_{-\mathbf{k}'\downarrow}^* c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + c_{\mathbf{k}'+\mathbf{Q}\uparrow}^* c_{-\mathbf{k}'-\mathbf{Q}\downarrow}^* c_{-\mathbf{k}-\mathbf{Q}\downarrow} c_{\mathbf{k}\uparrow} - c_{\mathbf{k}'\uparrow}^* c_{-\mathbf{k}'\downarrow}^* c_{-\mathbf{k}-\mathbf{Q}\downarrow} c_{\mathbf{k}\uparrow} - c_{\mathbf{k}'+\mathbf{Q}\uparrow}^* c_{-\mathbf{k}'\downarrow}^* c_{-\mathbf{k}-\mathbf{Q}\downarrow} c_{\mathbf{k}+\mathbf{Q}\uparrow}). \quad (\text{A6})$$

The effect of the terms in parentheses in this equation on the B.C.S. Ψ_θ may now be computed:

$$(\quad) \Psi_\theta = \left\{ \prod_{\mathbf{K} \neq \mathbf{k}', \mathbf{k}'+\mathbf{Q}, \mathbf{k}} [(1-h_{\mathbf{K}})^{\frac{1}{2}} + h_{\mathbf{K}}^{\frac{1}{2}} b_{\mathbf{K}}^*] h_{\mathbf{k}}^{\frac{1}{2}} (1-h_{\mathbf{k}'})^{\frac{1}{2}} (1-h_{\mathbf{k}'+\mathbf{Q}})^{\frac{1}{2}} c_{\mathbf{k}'+\mathbf{Q}\uparrow}^* c_{-\mathbf{k}'\downarrow}^* \right. \\ - \prod_{\mathbf{K} \neq \mathbf{k}, \mathbf{k}+\mathbf{Q}, \mathbf{k}'+\mathbf{Q}} [(1-h_{\mathbf{K}})^{\frac{1}{2}} + h_{\mathbf{K}}^{\frac{1}{2}} b_{\mathbf{K}}^*] (1-h_{\mathbf{k}'+\mathbf{Q}})^{\frac{1}{2}} h_{\mathbf{k}}^{\frac{1}{2}} h_{\mathbf{k}+\mathbf{Q}}^{\frac{1}{2}} b_{\mathbf{k}'+\mathbf{Q}}^* c_{\mathbf{k}+\mathbf{Q}\uparrow}^* c_{-\mathbf{k}\downarrow}^* \\ + \prod_{\mathbf{K} \neq \mathbf{k}, \mathbf{k}+\mathbf{Q}, \mathbf{k}'} [(1-h_{\mathbf{K}})^{\frac{1}{2}} + h_{\mathbf{K}}^{\frac{1}{2}} b_{\mathbf{K}}^*] h_{\mathbf{k}}^{\frac{1}{2}} h_{\mathbf{k}+\mathbf{Q}}^{\frac{1}{2}} (1-h_{\mathbf{k}'})^{\frac{1}{2}} b_{\mathbf{k}'}^* c_{\mathbf{k}+\mathbf{Q}\uparrow}^* c_{-\mathbf{k}\downarrow}^* \\ \left. - \prod_{\mathbf{K} \neq \mathbf{k}', \mathbf{k}+\mathbf{Q}, \mathbf{k}'+\mathbf{Q}} [(1-h_{\mathbf{K}})^{\frac{1}{2}} + h_{\mathbf{K}}^{\frac{1}{2}} b_{\mathbf{K}}^*] h_{\mathbf{k}+\mathbf{Q}}^{\frac{1}{2}} (1-h_{\mathbf{k}'})^{\frac{1}{2}} (1-h_{\mathbf{k}'+\mathbf{Q}})^{\frac{1}{2}} c_{\mathbf{k}'+\mathbf{Q}\uparrow}^* c_{-\mathbf{k}'\downarrow}^* \right\} \Psi_\theta.$$

Now we combine this with (23) and (24) to compute the scalar product:

$$\begin{aligned}
 (\rho_Q \Psi_g, [H_V, \rho_Q] \Psi_g) = & \frac{1}{2} V \left[\sum_{\mathbf{k} (\epsilon_{\mathbf{k}} < \hbar\omega, \epsilon_{\mathbf{k}+\mathbf{Q}} > \hbar\omega)} \sum_{\mathbf{k}' \neq \mathbf{k}} - \sum_{\mathbf{k} (\epsilon_{\mathbf{k}} > \hbar\omega, \epsilon_{\mathbf{k}+\mathbf{Q}} < \hbar\omega)} \sum_{\mathbf{k}' \neq \mathbf{k}} + \sum_{\mathbf{k}' (\epsilon_{\mathbf{k}'} < \hbar\omega, \epsilon_{\mathbf{k}'+\mathbf{Q}} > \hbar\omega)} \sum_{\mathbf{k} \neq \mathbf{k}'} - \dots \right] \\
 & \times \{ [h_{\mathbf{k}'}^{\frac{1}{2}}(1-h_{\mathbf{k}'+\mathbf{Q}})^{\frac{1}{2}} + h_{\mathbf{k}'+\mathbf{Q}}^{\frac{1}{2}}(1-h_{\mathbf{k}'})^{\frac{1}{2}}] (1-h_{\mathbf{k}'})^{\frac{1}{2}} (1-h_{\mathbf{k}'+\mathbf{Q}})^{\frac{1}{2}} \\
 & \times [h_{\mathbf{k}}^{\frac{1}{2}}(1-h_{\mathbf{k}})^{\frac{1}{2}} - h_{\mathbf{k}+\mathbf{Q}}^{\frac{1}{2}}(1-h_{\mathbf{k}+\mathbf{Q}})^{\frac{1}{2}}] + [h_{\mathbf{k}}^{\frac{1}{2}}(1-h_{\mathbf{k}+\mathbf{Q}})^{\frac{1}{2}} + h_{\mathbf{k}+\mathbf{Q}}^{\frac{1}{2}}(1-h_{\mathbf{k}})^{\frac{1}{2}}] \\
 & \times h_{\mathbf{k}}^{\frac{1}{2}} h_{\mathbf{k}+\mathbf{Q}}^{\frac{1}{2}} [h_{\mathbf{k}'}^{\frac{1}{2}}(1-h_{\mathbf{k}'})^{\frac{1}{2}} - h_{\mathbf{k}'+\mathbf{Q}}^{\frac{1}{2}}(1-h_{\mathbf{k}'+\mathbf{Q}})^{\frac{1}{2}}] \}.
 \end{aligned}$$

If in the first term we interchange the labels \mathbf{k} and \mathbf{k}' , it becomes very similar to the second, and the whole sum is symmetric in \mathbf{k} and $\mathbf{k}+\mathbf{Q}$, and antisymmetric in \mathbf{k}' and $\mathbf{k}'+\mathbf{Q}$. We therefore have left only twice the limited sum over \mathbf{k}' :

$$\begin{aligned}
 (\rho_Q \Psi_g, [H_V, \rho_Q] \Psi_g) = & V [h_{\mathbf{k}}^{\frac{1}{2}}(1-h_{\mathbf{k}+\mathbf{Q}})^{\frac{1}{2}} + h_{\mathbf{k}+\mathbf{Q}}^{\frac{1}{2}}(1-h_{\mathbf{k}})^{\frac{1}{2}}] \\
 & \times [h_{\mathbf{k}}^{\frac{1}{2}} h_{\mathbf{k}+\mathbf{Q}}^{\frac{1}{2}} + (1-h_{\mathbf{k}})^{\frac{1}{2}}(1-h_{\mathbf{k}+\mathbf{Q}})^{\frac{1}{2}}] [h_{\mathbf{k}'}^{\frac{1}{2}}(1-h_{\mathbf{k}'})^{\frac{1}{2}} - h_{\mathbf{k}'+\mathbf{Q}}^{\frac{1}{2}}(1-h_{\mathbf{k}'+\mathbf{Q}})^{\frac{1}{2}}]. \quad (\text{A7})
 \end{aligned}$$

In view of the symmetry in \mathbf{k} and $\mathbf{k}+\mathbf{Q}$ and the fact that Q is very small, the \mathbf{k} sum may be simplified to $2V \sum_{\mathbf{k}} [h_{\mathbf{k}}(1-h_{\mathbf{k}})]^{\frac{1}{2}} = 2\epsilon_0$. The \mathbf{k}' sum is an integral over the cutoff surface $|\epsilon| = \hbar\omega$. When \mathbf{k}' points at an angle θ to \mathbf{Q} , the energy difference is

$$\delta\epsilon = \epsilon_{\mathbf{k}'+\mathbf{Q}} - \epsilon_{\mathbf{k}'} = (\hbar^2 k_F Q \cos\theta)/m, \quad (\text{A8})$$

and the number of states in the surface element at this angle is $\frac{1}{2} \sin\theta d\theta N(0) \delta\epsilon$. Thus

$$\sum_{\mathbf{k}} \Delta [h_{\mathbf{k}}^{\frac{1}{2}}(1-h_{\mathbf{k}})^{\frac{1}{2}}] = 4N(0) \frac{1}{2} \int_0^{\pi/2} \sin\theta d\theta \left[\left(\frac{\hbar^2}{m} \right) k_F Q \cos\theta \right]^2 \frac{d}{d\epsilon} [\frac{1}{2} \epsilon_0 (\epsilon^2 + \epsilon_0^2)^{-\frac{1}{2}}]_{\epsilon=\hbar\omega} = \frac{1}{3} \frac{N(0) \hbar^2 k_F^2 Q^2 \epsilon_0}{(m^2 \omega^2)}, \quad (\text{A9})$$

which gives the value (19) of the text.

Finally, we compute the commutator involved in the kinetic energy:

$$\begin{aligned}
 \sum_{\mathbf{K}, \sigma} \mathbf{Q} \cdot (2\mathbf{K} + \mathbf{Q}) c_{\mathbf{K}+\mathbf{Q}, \sigma}^* c_{\mathbf{K}, \sigma} \Psi_g = & \mathbf{Q} \cdot \sum_{\mathbf{K}} (2\mathbf{K} + \mathbf{Q}) (c_{\mathbf{K}+\mathbf{Q}\uparrow}^* c_{\mathbf{K}\uparrow} - c_{-\mathbf{K}\downarrow}^* c_{-\mathbf{K}-\mathbf{Q}\downarrow}) \Psi_g \\
 = & \mathbf{Q} \cdot \sum_{\mathbf{K}} (2\mathbf{K} + \mathbf{Q}) [h_{\mathbf{K}}^{\frac{1}{2}}(1-h_{\mathbf{K}+\mathbf{Q}})^{\frac{1}{2}} - h_{\mathbf{K}+\mathbf{Q}}^{\frac{1}{2}}(1-h_{\mathbf{K}})^{\frac{1}{2}}] \Psi_{-\mathbf{K}, \mathbf{K}+\mathbf{Q}}, \quad (\text{A10})
 \end{aligned}$$

using (14)–(16). Again using (15) and (16), we get

$$(\rho_Q \Psi_g, [H_{\mathbf{K}}, \rho_Q] \Psi_g) = (\hbar^2/2m) \sum_{\mathbf{K}} \mathbf{Q} \cdot (2\mathbf{K} + \mathbf{Q}) (h_{\mathbf{K}} - h_{\mathbf{K}+\mathbf{Q}}). \quad (\text{A11})$$

For small Q , this is almost exactly

$$-(\hbar^2/m) \sum_{\mathbf{K}} (\mathbf{Q} \cdot \mathbf{k}) \mathbf{Q} \cdot \nabla_{\mathbf{k}} (h_{\mathbf{k}}) = (\hbar^2/m)^2 \sum_{\mathbf{K}} (\mathbf{Q} \cdot \mathbf{k})^2 (dh/d\epsilon). \quad (\text{A12})$$

In this form it is clearly independent of the exact form of the distribution, and thus is practically the same as the identical quantity for a Fermi sea. Evaluating (A12) (the assumption must be made that ϵ_0 is small), we get the result quoted as (20) of the text.