Incompatibility of BCS pairing and the Peierls distortion in one-dimensional systems. I. Mean-field theory*

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The relationship between the BCS superconducting and Peierls insulating phase transitions in one-dimensional systems is investigated within mean-field theory. This calculation lays the essential theoretical groundwork for a treatment of fluctuations in the two order parameters which is presented in a companion paper. The model Hamiltonian used here is equivalent to the reduced BCS Hamiltonian when the Peierls gap vanishes and also equal to the mean-field approximation to the Fröhlich Hamiltonian, in the presence of electron-electron interactions, when the BCS gap is zero. The two coupled gap equations are derived and solved and it is found that the two instabilities are, in general, very incompatible. When the "bare" Peierls transition temperature T_P is greater than the "bare" BCS transition temperature T_S, the system generally orders at T_P and is a Peierls insulator at all lower temperatures. The converse is also true. Only when T_P and T_S are nearly equal will the ordered state be the "mixed" state, that in which both order parameters are simultaneously nonzero. This mixed state is shown to exhibit a "one-dimensional Meissner effect." As a side issue, the effect of electron-electron interactions on the Peierls transition (when the BCS gap is zero) is also investigated; it is shown that electron-electron interaction effects are important. Repulsive interactions lower T_P, while attractive interactions raise T_P. These effects are sufficiently severe so that in jellium, with only Coulombic interactions present, T_P is identically zero.

I. INTRODUCTION

The purpose of the present paper is to investigate the relationship between the BCS superconducting and the Peierls insulating phase transitions in one-dimensional systems. This is the first of a series of two papers and is based entirely on mean-field theory. A brief summary of these results was published previously.[1] It is important to outline clearly the predictions of mean-field theory even though, because it neglects fluctuation effects, this approximation scheme is inappropriate to strictly one-dimensional systems. Mean-field theory provides a theoretical basis for the Landau-Ginsburg fluctuation theory[2] and it is, therefore, essential that mean-field theoretic calculations be performed before fluctuation effects can be included. It is also felt that the predictions of mean-field theory will be useful as a basis for comparison with other diagrammatic approaches. The second paper in this series treats the effects of fluctuations in the BCS and Peierls order parameters within a Landau-Ginsburg framework. This paper makes use of several results, such as the expression for the free energy, obtained in the present paper. It will be shown in this next paper, that even though fluctuation effects are very important in one-dimensional systems, the conclusions reached using mean-field theory are not qualitatively different when these effects are included.

There are three important reasons for studying the relationship between the Peierls and superconducting transitions in one-dimensional systems.

(i) Little[3] has suggested that one-dimensional organic salts may be good candidates for high-temperature superconductors. However, it was pointed out a number of years ago by Peierls[4] that these one-dimensional systems also have a tendency to undergo a transition to an insulating ground state. Because of the significance of high-temperature superconductivity, it is important to determine which of the two transitions will prevail or if, in fact, they can coexist.

(ii) Recent experiments by Coleman *et al.*,[5] although controversial,[6] have been interpreted to suggest that they have observed superconducting fluctuations above the onset of a Peierls insulating phase transition in the one-dimensional organic charge-transfer salt tetrathiofulvalinium tetracyanoquinodimethan (TTF-TCNQ). The problem is, therefore, of current interest.

(iii) Finally, it is of general interest to study in detail a system which can undergo two different and competing types of phase transitions. It is hoped that the present one-dimensional calculations can provide a handle for learning about the more general problem of competing instabilities.

To investigate the coexistence of the superconducting and the Peierls insulating states we use a simple mean-field theoretic model Hamiltonian. This Hamiltonian is equivalent to the reduced BCS Hamiltonian[7] when there is no Peierls gap γ and to the usual random-phase approximation to the Fröhlich Hamiltonian[8] (in the presence of electron-electron interactions) when the BCS gap Δ_k

is zero. We derive and solve two coupled gap equations which have three types of solutions. When the "bare" Peierls transition temperature T_P is greater than the "bare" BCS transition temperature T_S, the system becomes ordered at T_P and is in the Peierls insulating state at all temperatures below T_P. Similarly, when $T_S > T_P$ the system becomes ordered at T_S and is a BCS superconductor at all lower temperatures. Only when T_P and T_S are nearly equal will the ground state be one in which both gap parameters are simultaneously nonzero. This new "mixed" state sets in at a temperature T_M which is below both T_S and T_P. Because it occurs only for very special values of the model parameters, the existence of this new state is highly improbable. Consequently we reach the very strong conclusion here that within mean-field theory *the Peierls insulating and the BCS superconducting states are almost always incompatible.*

The problem of the competition between the BCS and Peierls instabilities was first considered by Little.[3] He suggested a simple form for the BCS gap equation in the presence of a Peierls distortion and showed that his new gap equation could be nontrivially satisfied whenever the Peierls gap was small compared to the pairing interaction cutoff frequency. While his *ansatz* for the BCS-like gap equation is essentially the same as the equation which will be formally derived in the present paper, he did not solve self-consistently for the BCS and Peierls gap parameters.[9] This lack of self-consistency is an important omission and, as will be shown in Sec. V, leads to incorrect conclusions.

Bychkov, Gor'kov, and Dzyaloshinskii[10] considered the problem of the two instabilities from a different point of view. Their model Hamiltonian differs from that used here in that only electron-electron interactions are included; the electron-ion interaction is treated as an effective electron-electron interaction. In contrast to the mean-field approximation used here, they used a logarithmic approximation to solve the parquet equations and concluded that both Cooper-pair instabilities and electron-hole (Peierls) instabilities will always occur at the same temperature. Their conclusion that the two instabilities are always compatible is in disagreement with that reached in the present paper. However, it should be noted that if in the present model Hamiltonian the electron-ion interaction parameter v_Q is set equal to zero so that there are only electron-electron interactions present, and if the two electron-electron interaction parameters V_Q and $V_{kk'}$, defined below, are assumed to have the same sign, magnitude, and cutoffs then it follows from the present theory that $T_P = T_S$. This is also the case in which both γ and Δ_k are nonzero in the ordered state. Hence, our theory appears to be very similar to that of Bychkov *et al.* in this special case. However, because the parameters T_P and T_S are not, in general, restricted to be equal, it is possible here to explore a wider range of physical situations than was the case in Ref. 10.

Another investigation of the relationship between the BCS and Peierls instabilities was carried out by Patton and Sham[11] and Rice and Strässler.[11] These two groups showed that the effect of the Peierls soft phonon is to decrease the attractive pairing interaction and thus lower, or suppress altogether, the BCS transition temperature. While the present approach is complementary to that of Ref. 11, we feel the conclusions reached here regarding the incompatibility of the two phase transitions are stronger. In the present work all possible mechanisms for an attractive pairing interaction are included in a phenomenological parameter $V_{kk'}$ defined below. These include the excitonic mechanism,[3] all phonons as well as other excitations. It is found that even under circumstances which are most favorable for superconductivity (i.e., even if the nature of the pairing interaction is such that it is not substantially weakened as the Peierls phonon goes soft), if the Peierls transition occurs, it eliminates BCS superconductivity.

The remainder of this paper is divided into five sections. In Sec. II the model is described and a mean-field decoupling of the Hamiltonian $\mathcal{H}^{\text{eff}}$ is performed. This mean-field Hamiltonian $\mathcal{H}^{\text{eff}}$ is seen to be equivalent to the reduced BCS[7] and to the mean-field approximation to the Fröhlich Hamiltonian[8] in the appropriate limits. In contrast to previous treatments,[8,12] electron-electron interactions are also included in the Peierls transition. In Sec. III the two coupled equations for the gap parameters γ and Δ_k are derived. This derivation involves a sequence of three steps. First, the Bogoliubov transformation for $\mathcal{H}^{\text{eff}}$ is obtained and the Hamiltonian is thus written in diagonal form. Second, by evaluating the expectation value of $\mathcal{H}^{\text{eff}}$ the free energy is obtained, and third the two gap parameters are determined variationally by setting the derivative of the free energy with respect to each gap equal to zero. It is shown that the two equations thus obtained reduce to the usual BCS or Peierls gap equations when γ or Δ_k are, respectively, zero. The solution of the coupled gap equations is deferred until Sec. V so that a more detailed discussion of the Peierls gap equation (when $\Delta_k = 0$) in the presence electron-electron interactions can be given. This discussion is presented in Sec. IV wherein it is shown that within mean-field theory repulsive electron-electron interactions lower the Peierls transition temperature while attractive electron-electron interactions raise T_P. In jellium, with only Coulombic

interactions present T_P is identically zero. It is also demonstrated that the phonon frequency for wave vector $Q = 2k_F$ becomes zero at T_P. This last derivation serves to underline the importance of including electron-electron interactions in the Peierls transition, for it shows explicitly that in the defining equations for T_P, the electron-electron interaction appears multiplied by the singular (at zero temperature) electronic susceptibility function.

In Sec. V the coupled gap equations are solved. The phase diagram for the system at temperature $T = 0$ is presented and it is demonstrated that only when T_P and T_S are nearly equal will both order parameters be nonzero in the ground state. Except in this special case, there is no switching as a function of temperature from one type of ordered state to the other. The shape of the free-energy surface as a function of γ and Δ_k for a range of temperatures is discussed, and it is shown that (when there is no mixed state) below both critical temperatures, the lower-critical-temperature order parameter corresponds to a saddle point in the free-energy surface while the upper-critical-temperature order parameter corresponds to a true minimum. The properties of the mixed state are discussed in Sec. VI. The temperature dependence of the gap parameters in the mixed state is obtained in Sec. VI A, and in Sec. VI B the electromagnetic response of the system at $T = 0$ is calculated. It is shown that as long as $\Delta_k \neq 0$, there is a nonvanishing (negative) coefficient of proportionality between the current and the vector potential in the direction along the chain. Hence there is a "one-dimensional Meissner effect"[7] in the mixed state. An explicit expression is given for this coefficient.

II. MODEL HAMILTONIAN

In this section a simple mean-field theoretic model Hamiltonain will be derived from a more general phenomenological Hamiltonian which describes a one-dimensional system of electrons which interact with each other as well as with ions in the solid. This general Hamiltonian is

$$\mathcal{H} = \sum_{k,\sigma} \epsilon(k)\, C^\dagger_{k\sigma} C_{k\sigma} + \sum_{\substack{k,\sigma \\ q}} v_q\, C^\dagger_{k+q\sigma} C_{k\sigma} u_q + \sum_{\substack{kk' \\ \sigma\sigma' \\ q}} V_{qkk'}\, C^\dagger_{k+q\sigma} C_{k\sigma} C^\dagger_{k'-q\sigma'} C_{k'\sigma'} , \tag{2.1}$$

where $\epsilon(k)$ is the one-electron energy measured relative to the Fermi level, v_q is the electron-phonon interaction for longitudinal phonons, and the electron-electron interaction is given by

$$V_{qkk'} = (\tfrac{1}{2} V^{\mathrm{Coul}}_q + \overline{V}_{q,k'-q,k'}) . \tag{2.2}$$

The operators $C^\dagger_{k\sigma}$ and u_q are, respectively, the creation operator for electrons of wave vector k and spin σ and the ionic displacement operator of wave vector q. $\overline{V}_{q,k'-q,k'}$ is a phenomenological indirect attractive electron-electron interaction[13] and V^{Coul}_q is the ordinary repulsive Coulomb interaction. We now perform a mean-field decoupling of the Hamiltonian: Only the expectation values $\langle C^\dagger_{k+Q\sigma} C_{k\sigma}\rangle$, $\langle C^\dagger_{k\uparrow} C^\dagger_{-k\downarrow}\rangle$ and their complex conjugates are assumed to be nonzero and the ionic displacement operator u_Q is replaced by its mean value $\langle u_Q\rangle$. Here $Q \equiv 2k_F$.[14] Formally we replace the operator $C^\dagger C$ by $\langle C^\dagger C\rangle + (C^\dagger C - \langle C^\dagger C\rangle)$. This form is inserted into the Hamiltonian and only terms first order in the fluctuations of $C^\dagger C$ from its mean value $\langle C^\dagger C\rangle$ are retained. Thus, contributions quadratic in $(\cdots)$ are ignored. Finally, we define the effective electron-electron interaction in the Peierls channel

$$V_Q \equiv V^{\mathrm{Coul}}_Q + \overline{V}_{Q,k'-Q,k'} + \overline{V}_{-Q,k+Q,k} , \tag{2.3}$$

and the effective electron-electron interaction in the BCS channel[15]

$$V_{kk'} \equiv \overline{V}_{k'-k,-k',-k} + \tfrac{1}{2} V^{\mathrm{Coul}}_{k-k'} . \tag{2.4}$$

The latter interaction is assumed to be of the form

$$V\Theta(|\epsilon(k)| - \omega_c)\,\Theta(|\epsilon(k')| - \omega_c) ,$$

where ω_c is a phenomenological cutoff parameter and Θ is the step function. While the form of the very complicated electron-electron interaction is simplified considerably, this approach follows the spirit of the BCS theory. Both V_Q and $V_{kk'}$ are treated as phenomenological interaction parameters and it is assumed that all possible attractive electron-electron interactions, such as those proposed by Little,[3] are included in $V_{kk'}$ so that $V_{kk'}$ and V_Q are independent phenomenological parameters. The mean-field theoretic model Hamiltonian is then of the form

$$\mathcal{H}^{\mathrm{eff}} = \sum_{k,\sigma} \epsilon(k)\, C^\dagger_{k\sigma} C_{k\sigma} + \sum_{k,\sigma} \gamma C^\dagger_{k+Q\sigma} C_{k\sigma} - \sum_k \Delta_k C_{-k\downarrow} C_{k\uparrow} + E^0 + \mathrm{c.c.} , \tag{2.5}$$

where the gap parameters γ and Δ_k are given by

$$\gamma \equiv v_Q \langle u_Q\rangle + V_Q \langle \rho^{\mathrm{el}}_Q\rangle \tag{2.6}$$

and

$$\Delta_k \equiv -\sum_{k'} V_{k'k} \langle C^\dagger_{k'\uparrow} C^\dagger_{-k'\downarrow}\rangle . \tag{2.7}$$

In Eq. (2.6) $\langle \rho^{\mathrm{el}}_Q\rangle = \sum_{k\sigma} \langle C^\dagger_{k-Q\sigma} C_{k\sigma}\rangle$ is the expectation value of the electronic number density. The quantity E^0 is a c number given by

$$E^0 = -V_Q |\langle \rho^{\mathrm{el}}_Q\rangle|^2 + \omega_Q^2 |\langle u_Q\rangle|^2 - \sum_{kk'} V_{kk'} \eta_k \eta^*_{k'} , \tag{2.8}$$

where the second term represents the elastic energy of the lattice associated with the distortion of wave vector Q and $\eta_k \equiv \langle C^\dagger_{k\uparrow} C^\dagger_{-k\downarrow} \rangle$. The first and third terms in Eq. (2.8) arise from the mean-field decoupling scheme.

The Hamiltonian in Eq. (2.5) thus describes a system of electrons which can undergo both a BCS superconducting and a Peierls insulating transition. When $\gamma \to 0$, $\mathcal{H}^{\rm eff}$ reduces to the usual BCS Hamiltonian and when $\Delta_k \to 0$, $\mathcal{H}^{\rm eff}$ is equivalent to the mean-field theoretic approximation to the Fröhlich Hamiltonian. It should be noted from the definition of γ that electron-electron interactions, which were not considered by Fröhlich or Peierls are also included in the present treatment of the Peierls interaction. As will be discussed in Sec. IV, they play an important role in determining the Peierls transition temperature T_P. The two gap parameters γ and Δ_k are determined self-consistently from two coupled gap equations in Sec. III.

III. DERIVATION OF GAP EQUATIONS

In this section the gap equations are obtained in a sequence of three steps. (i) $\mathcal{H}^{\rm eff}$ is written in diagonal form, i.e., the Bogoliubov[7] transformation for the coupled BCS-Peierls system is obtained; (ii) the expectation value $\langle \mathcal{H}^{\rm eff} - TS \rangle = F^{\rm MF}$, where S is the entropy and $F^{\rm MF}$ is the mean-field free energy, is calculated; and (iii) the equations for γ and Δ_k are determined variationally from $F^{\rm MF}$, thus yielding the two coupled gap equations.

The Hamiltonian in Eq. (2.5) may be written in diagonal form provided the Peierls interaction [the second term on the right-hand side of Eq. (2.5)] only mixes those pairs of states involving one positive and one negative wave vector k. Since only these states can be degenerate or nearly degenerate in energy these interactions dominate and all others can be treated perturbatively. It suffices, then, to consider only those states in $\mathcal{H}^{\rm eff}$ with $|k| \le Q$. Writing out these terms explicitly, it follows from Eq. (2.5) that

$$\mathcal{H}^{\rm eff} \cong \sum_{0 \le k \le k_F} \mathcal{H}_+(k) + \sum_{-k_F \le k \le 0} \mathcal{H}_-(k) + E^0 , \tag{3.1}$$

where

$$\begin{aligned}\mathcal{H}_+(k) = [&\epsilon(k)(C^\dagger_{k\uparrow} C_{k\uparrow} + C^\dagger_{-k\downarrow} C_{-k\downarrow}) \\ &+ \epsilon(k-Q)(C^\dagger_{k-Q\uparrow} C_{k-Q\uparrow} + C^\dagger_{-k+Q\downarrow} C_{-k+Q\downarrow}) \\ &+ \gamma^*(C^\dagger_{k-Q\uparrow} C_{k\uparrow} + C^\dagger_{-k\downarrow} C_{-k+Q\downarrow} \\ &+ \gamma(C^\dagger_{k\uparrow} C_{k-Q\uparrow} + C^\dagger_{-k+Q\downarrow} C_{-k\downarrow}) - \Delta_k C_{-k\downarrow} C_{k\uparrow} \\ &- \Delta^*_k C^\dagger_{k\uparrow} C^\dagger_{-k\downarrow} - \Delta_{k-Q} C_{-k+Q\downarrow} C_{k-Q\uparrow} \\ &- \Delta^*_{k-Q} C^\dagger_{k-Q\uparrow} C^\dagger_{-k+Q\downarrow}] . \end{aligned} \tag{3.2}$$

The terms with γ^* and Δ^*_k come from the complex-conjugate term in Eq. (2.5) and $\mathcal{H}_-(k)$ can be obtained from $\mathcal{H}_+(k)$ by replacing Q by $-Q$. It may be seen that $\mathcal{H}_\pm(k)$ only mixes the four operators $C_{k\uparrow}$, $C^\dagger_{-k\downarrow}$, $C_{k\mp Q\uparrow}$, and $C^\dagger_{-k\pm Q\downarrow}$. For simplicity, in what follows, the gap parameters are assumed to be real (this does not affect the derivation of the free-energy or the gap equations), and for k positive (negative) Δ_k and Δ_{k-Q} (Δ_{k+Q}) are assumed to be equal. Because the k dependence of the gap parameter is later shown to be of the BCS form $\Delta_k = \Delta\Theta(|\epsilon(k)| - \omega_c)$, this last approximation can be shown to be valid *a posteriori* providing the cutoff frequency in the pairing interaction, ω_c, is small compared to the Fermi energy (which assumption is expected to be reasonable for most physical systems). This leads to considerable simplification of the algebra. The Hamiltonians $\mathcal{H}_\pm(k)$ can be written in the basis

$$\begin{pmatrix} C_{k\uparrow} \\ C^\dagger_{-k\downarrow} \\ C_{k\mp Q\uparrow} \\ C^\dagger_{-k\pm Q\downarrow} \end{pmatrix} ,$$

as

$$\begin{pmatrix} \epsilon(k) & -\Delta_k & -\gamma & 0 \\ -\Delta_k & -\epsilon(k) & 0 & -\gamma \\ \gamma & 0 & \epsilon(k \mp Q) & -\Delta_k \\ 0 & -\gamma & -\Delta_k & -\epsilon(k \mp Q) \end{pmatrix} , \tag{3.3}$$

where we have used the fermion commutation relations in obtaining the signs in some of the matrix elements.

The four energy eigenvalues for $\mathcal{H}_+(k)$ are

$$\begin{aligned}&\pm[\Delta_k^2 + \tfrac{1}{4}([\epsilon(k) + \epsilon(k-Q)] \\ &\quad \pm\{[\epsilon(k) - \epsilon(k-Q)]^2 + 4\gamma^2\}^{1/2})^2]^{1/2} , \end{aligned} \tag{3.4}$$

and the corresponding eigenvectors are labeled $\psi^{++}(k)$, $\psi^{-+}(k)$, $\psi^{+-}(k)$, and $\psi^{--}(k)$, where the two superscripts correspond in order to the choices of plus and minus signs appearing in Eq. (3.4). It should be noted that when $\gamma = 0$ or $\Delta_k = 0$ the correct results for the energy eigenvalues for the BCS or mean-field Fröhlich Hamiltonians are obtained from Eq. (3.4). Because of the complicated form of the eigenvectors of Eq. (3.3) it is not convenient to evaluate them directly from the eigenvalue equation. To obtain the unitary matrix U which diagonalizes $\mathcal{H}_\pm(k)$ we first note that it follows from the eigenvalue equations that the following identities among the eigenvectors hold:

$$\frac{\psi_1^{lm}}{\psi_3^{lm}} = \frac{\psi_2^{lm}}{\psi_4^{lm}} , \quad l = \pm , \quad m = \pm , \tag{3.5}$$

$$\frac{\psi_1^{++}}{\psi_3^{++}} = \frac{\psi_1^{-+}}{\psi_3^{-+}} , \quad \frac{\psi_1^{--}}{\psi_3^{--}} = \frac{\psi_1^{+-}}{\psi_3^{+-}} , \tag{3.6}$$

$$\frac{\psi_2^{-+}}{\psi_1^{-+}} = \frac{-\psi_1^{++}}{\psi_2^{++}}, \quad \frac{\psi_2^{--}}{\psi_1^{--}} = \frac{-\psi_1^{+-}}{\psi_2^{+-}}, \tag{3.7}$$

and

$$\frac{\psi_1^{--}}{\psi_3^{--}} = \frac{-\psi_3^{++}}{\psi_1^{++}}, \tag{3.8}$$

where we have, for convenience, omitted the argument k from the ψ's and the subscripts, $i=1-4$, denote the ith component of the eigenvector. It follows at once from these identities and from the normalization and orthogonalization relations of the eigenvectors that the unitary matrix which diagonalizes $\mathcal{H}_+(k)$ can be written

$$U = \begin{pmatrix} \alpha_1 & -\alpha_2 & \beta_2 & \beta_1 \\ \alpha_2 & \alpha_1 & -\beta_1 & \beta_2 \\ \alpha_1/\nu & -\alpha_2/\nu & \beta_2\nu & -\beta_1\nu \\ \alpha_2/\nu & \alpha_1/\nu & \beta_1\nu & -\beta_2\nu \end{pmatrix}. \tag{3.9}$$

In Eq. (3.9) $\alpha_1+i\alpha_2=[\nu^2/(1+\nu^2)]^{1/2}e^{i\varphi_\alpha}$ and $\beta_1+i\beta_2=(1+\nu^2)^{-1/2}e^{i\varphi_\beta}$ where $\nu=\psi_1^{++}/\psi_3^{++}$. Each column of the unitary matrix U gives the coefficients of the four operators $C_{k\uparrow}$, $C_{-k\downarrow}^\dagger$, $C_{k\mp Q\uparrow}$, and $C_{-k\pm Q\downarrow}^\dagger$, and corresponds to one of the four eigenvectors of $\mathcal{H}_\pm(k)$. In what follows we shall present all results for $\mathcal{H}_+(k)$. The corresponding results for $\mathcal{H}_-(k)$ can be obtained from those for $\mathcal{H}_+(k)$ by replacing Q by $-Q$. Thus, Eq. (3.9) gives the generalized Bogoliubov transformation for the coupled BCS-Peierls system in terms of the unknown parameters φ_α, φ_β, and ν. To obtain these three unknowns we evaluate the matrix $U^{-1}\mathcal{H}_+(k)\,U$ and require that its off-diagonal elements are zero. This gives six different equations. Four of these reduce to the defining equation for ν

$$\nu = 2\gamma[\epsilon(k-Q)-\epsilon(k)+\overline{E}]^{-1}, \tag{3.10}$$

where

$$\overline{E} \equiv \{[\epsilon(k)-\epsilon(k-Q)]^2+4\gamma^2\}^{1/2}. \tag{3.11}$$

The remaining equations imply

$$\sin 2\varphi_\alpha = -\Delta_k/E^-(k) \tag{3.12}$$

and

$$\sin 2\varphi_\beta = \Delta_k/E^+(k), \tag{3.13}$$

where $E^+(k)$ and $E^-(k)$ are the two positive energy eigenvalues of $\mathcal{H}_+(k)$ which can be obtained from Eq. (3.4). These are given by

$$E^\pm(k) = \{\Delta_k^2+\tfrac{1}{4}[\epsilon(k)+\epsilon(k-Q)\pm\overline{E}]^2\}^{1/2}. \tag{3.14}$$

Once the Bogoliubov transformation is found it is then straightforward to write $\mathcal{H}^{\rm eff}$ [Eq. (2.5)] in diagonal form. Equation (3.9) may be inverted to obtain the four operators $C_{k\uparrow}$, $C_{-k\downarrow}^\dagger$, $C_{k-Q\uparrow}$, and $C_{-k+Q\downarrow}^\dagger$ in terms of the eigenvectors $\psi^{++}(k)$, $\psi^{-+}(k)$, $\psi^{+-}(k)$, and $\psi^{--}(k)$. Substituting these into Eq. (3.2) we obtain

$$\begin{aligned}\sum_{0\le k\le k_F}\mathcal{H}_+(k) = &\sum_{0\le k\le k_F} E^+(k)\{[\psi^{++}(k)]^\dagger \\ &\times\psi^{++}(k)+\psi^{-+}(k)[\psi^{-+}(k)]^\dagger\} \\ &+\sum_{0\le k\le k_F} E^-(k)\{[\psi^{+-}(k)]^\dagger\psi^{+-}(k) \\ &+\psi^{--}(k)[\psi^{--}(k)]^\dagger\} \\ &+\sum_{0\le k\le k_F}[\epsilon(k)+\epsilon(k-Q)-E^+(k)-E^-(k)]\,.\end{aligned} \tag{3.15}$$

Using Eq. (3.1) $\mathcal{H}^{\rm eff}$ may then be written in diagonal form.

The mean-field (MF) free energy $F^{\rm MF}$ is calculated from

$$F^{\rm MF} = \langle \mathcal{H}^{\rm eff} - TS\rangle\,. \tag{3.16}$$

To evaluate $\langle\mathcal{H}^{\rm eff}\rangle$ it is convenient to change variables ($k\to -k+Q$) in the first sum on the right-hand side of Eq. (3.15) so that the limits of summation are from k_F to $2k_F$. Defining

$$\begin{aligned} f(k) &\equiv \langle[\psi^{+-}(k)]^\dagger\psi^{+-}(k)\rangle \\ &= \langle\psi^{--}(k)[\psi^{--}(k)]^\dagger\rangle, \quad \text{for } 0<k<k_F\,, \end{aligned}$$

and

$$\begin{aligned} f(k) &\equiv \langle[\psi^{++}(k)]^\dagger\psi^{++}(k)\rangle \\ &= \langle\psi^{-+}(k)[\psi^{-+}(k)]^\dagger\rangle\,, \quad \text{for } k_F<k<2k_F\,, \end{aligned}$$

it follows that

$$\begin{aligned} F^{\rm MF} = &\frac{1}{4}{\sum_{k,k'}}' V_{kk'}\sin 2\theta_k \sin 2\theta_{k'}(1-2f_k)(1-2f_{k'}) \\ &+{\sum_k}'[\epsilon(k)+\zeta_k\cos 2\theta_k] \\ &-2{\sum_k}'\zeta_k\cos 2\theta_k f_k+\omega_Q^2|\langle u_Q\rangle|^2-V_Q|\langle\rho_Q^{\rm el}\rangle|^2-TS \end{aligned} \tag{3.17}$$

where the prime on $\sum$ denotes that all wave vectors lie between $\pm 2k_F$ and where S is the usual entropy term:

$$S = -2k_B T{\sum_k}'[f_k\ln f_k+(1-f_k)\ln(1-f_k)]\,.$$

Finally,

$$\sin 2\theta_k = \Delta_k/(\Delta_k^2+\zeta_k^2)^{1/2} \tag{3.18}$$

and

$$\cos 2\theta_k = -\zeta_k/(\Delta_k^2+\zeta_k^2)^{1/2}, \tag{3.19}$$

and ζ_k for $k>0$ is

$$\zeta_k = \tfrac{1}{2}[\epsilon(k)+\epsilon(k-Q)+\mathrm{sgn}(|k|-k_F)\,\overline{E}]\,, \tag{3.20}$$

which is just the dispersion relation for a Peierls insulator. The quantity f_k, which describes the

occupation number for excitations denoted by wave number k, will be determined variationally. In obtaining (3.17) terms like $(\zeta_k^2+\Delta_k^2)^{1/2}$ which appear in Eq. (3.17) have been written as $\zeta_k^2/(\zeta_k^2+\Delta_k^2)^{1/2}+\Delta_k^2/(\zeta_k^2+\Delta_k^2)^{1/2}$ and those terms proportional to Δ_k^2 have been combined with the last term in E^0 [Eq. (2.8)]. It can be seen that in the limit $\gamma\to 0$ the free energy reduces to that obtained in the BCS theory[7]; in the limit $\Delta_k\to 0$, the free energy is equivalent to that obtained in the usual Peierls theory.[8] This special case will be discussed in Sec. IV. The gap equations can be obtained by finding the extrema of F^{MF} with respect to the four quantities f_k, $\langle u_Q\rangle$, $\langle \rho_Q^{el}\rangle$, and Δ_k, and by using Eq. (2.6). As in previous theories of the Peierls limit,[8] at the free-energy minimum $\langle u_Q\rangle$ and $\langle \rho_Q^{el}\rangle$ are proportional:

$$(\omega_Q^2/v_Q)\langle u_Q\rangle = -\langle \rho_Q^{el}\rangle \ . \tag{3.21}$$

Defining

$$\lambda = V_Q\,\omega_Q^2/|v_Q|^2 \ , \tag{3.22}$$

the equations for the three remaining unknowns are

$$\gamma = \left(\frac{1-\lambda}{\lambda}\right) V_Q \sum_k{}' (1-2f_k)\,[|\zeta_k|/(\Delta_k^2+\zeta_k^2)^{1/2}]\,\frac{\gamma}{\bar{E}} \ , \tag{3.23}$$

$$\Delta_k = -\frac{1}{2}\sum_{k'}{}' V_{kk'}(1-2f_{k'})\,\Delta_{k'}/(\Delta_{k'}^2+\zeta_{k'}^2)^{1/2} \ , \tag{3.24}$$

$$f_k = \{\exp[(\zeta_k^2+\Delta_k^2)^{1/2}/k_B T]+1\}^{-1} \ . \tag{3.25}$$

The quantity $\bar{E}$ appearing in Eq. (3.23) is defined in Eq. (3.11). The gap equations contain the BCS limit when $\gamma\to 0$ and the Peierls limit when $\Delta_k\to 0$. Note that the excitation energies are given by $(\zeta_k^2+\Delta_k^2)^{1/2}$ which also reduces to the appropriate limits when Δ_k or γ are zero. Because of the form of the BCS pairing interaction $V_{kk'}$ it follows that the BCS gap parameter may be written $\Delta_k = \Delta\Theta(|\epsilon(k)|-\omega_c)$. It can be seen that the BCS-like gap equation [Eq. (3.24)] has the same form as the usual BCS gap equation except that the one-electron energy in the presence of a Peierls distortion ζ_k appears in place of $\epsilon(k)$. This gap equation is essentially that which Little proposed.[16] The way in which the Peierls-like gap equation is modified as a result of coupling to the BCS gap is less predictable from intuitive considerations. In Sec. IV the Peierls gap equation, when the BCS gap Δ is zero, is discussed. Particular emphasis is placed on the effect of electron-electron interactions on the Peierls transition temperature T_p. The solution of the coupled gap equations will be discussed in Sec. V.

IV. EFFECT OF ELECTRON-ELECTRON INTERACTIONS ON THE PEIERLS TRANSITION IN MEAN-FIELD THEORY: CASE OF ZERO BCS GAP

While there have recently appeared in the literature[11,12] numerous discussions of the Peierls transition (when the BCS gap is zero), a detailed discussion of the effect of electron-electron interactions on the transition has not yet been given. It is the purpose of this section to discuss these effects using mean-field theory and to thus show that they are generally important. We find that repulsive electron-electron interactions depress the Peierls transition temperature, while attractive electron-electron interactions raise it. This can be understood physically as arising from the fact that it costs the electrons electrostatic energy to form a charge-density wave when the electrons repel one another, whereas energy is gained upon formation of the charge-density wave when the electrons attract one another. In jellium, with only Coulombic interactions, the effect of electron-electron interactions is sufficiently severe so that the transition temperature is suppressed to zero. It is important to recognize that, however small the electron-electron interaction parameter V_Q is, in the RPA expression for the renormalized phonon frequency, it appears multipled by the singular (at $T=0$) electronic density-density correlation function. *Hence, within mean-field theory electron-electron interactions should never, at the outset, be neglected.*

The frequency of phonons of wave vector q in the presence of the electron-phonon interaction v_q is modified. This modification can be easily calculated within mean-field theory and the phonon-dispersion relation is shown to be[17]

$$\omega^2 = \omega_q^2 + \frac{|v_q|^2\chi^0(q,\omega)}{1-V_q\chi^0(q,\omega)} \ , \tag{4.1}$$

where ω_q is the bare phonon frequency and $\chi^0(q,\omega)$ is the density-density correlation function for non-interacting electrons[17]:

$$\chi^0(q,\omega) = 2\sum_k \frac{f(\epsilon(k))-f(\epsilon(k-q))}{\epsilon(k)-\epsilon(k-q)-\omega-i\eta} \ , \tag{4.2}$$

where $f(\epsilon(k))$ is the free-electron Fermi function and $\eta\to 0$ from above. Finally, V_q is the qth component of the Fourier transform of the electron-electron interaction, as in Sec. III. Equation (4.1) will be modified somewhat if the detailed effects of the periodicity of the lattice are included.[17] These were considered in the treatment of the Peierls distortion presented by Renker *et al.*[18] In one dimension $\chi^0(Q,0) = -\infty$, at $T=0$. It is this divergence which drives the phonon frequency to zero. The transition temperature corresponding to that at which $\omega\to 0$ for $q=Q$ is obtained from

the equation

$$\omega_Q^2 = -\left.\frac{|v_Q|^2\chi^0(Q,0)}{1-V_Q\chi^0(Q,0)}\right|_{T_P} . \tag{4.3}$$

There are two important points to make concerning Eq. (4.3). First, this equation yields the same transition temperature as that calculated from Eq. (3.23) with $\Delta_k = 0$; this will be shown explicitly below. Second, the electron-electron interaction V_Q is multiplied by $\chi^0(Q,0)$, the term whose singularity (at $T=0$) drives the phonon frequency to zero. Thus, because V_Q is multiplied by a singular term, arguments which have been previously presented for neglecting V_Q, because it is small compared to the bandwidth,[12] are misleading. Equation (4.3) has solutions for a nonzero temperature only when

$$V_Q < |v_Q|^2/\omega_Q^2 . \tag{4.4}$$

When the equality holds, the transition temperature is identically zero. Equation (4.4) is equivalent to the inequality $\lambda < 1$ which is required in order that Eq. (3.23) have nontrivial solutions. The condition for neglecting the electron-electron interactions in determining T_P is that V_Q be small compared to $|v_Q|^2/\omega_Q^2$. In jellium (with simple Coulombic interactions) it follows that for a chain of length L and radius r with $k_F r \ll 1$

$$\omega_Q^2 = -(2\pi ne^2/M)(Qr)^2[\ln(Qr)] ,$$

$$V_Q = (-2e^2/L)[\ln(Qr)] ,$$

and

$$v_Q = 2\pi ie^2(n/M)^{1/2}(\pi r^2 L)^{-1/2} Qr^2[\ln(Qr)] ,$$

where n is the density of ions and M is the ionic mass. It can be seen from (4.4) that in jellium $T_P = 0$. The same conclusion can be obtained using the three-dimensional jellium parameters ($k_F r \gg 1$). The physical interpretation of this result is that in jellium the attractive electron-ion interaction is exactly canceled by the repulsive electron-electron interaction so that there is no way to produce a Peierls distortion at finite temperatures. These observations were made independently by Heine and Weaire.[19] In summary, within mean-field theory, the effect of repulsive electron-electron interactions is to lower T_P while attractive electron-electron interactions raise T_P. Note also that it follows from Eq. (3.23) that an attractive electron-electron interaction will itself drive a Peierls transition even if electron-ion interactions are absent ($\lambda \to -\infty$). This picture of the Peierls transition corresponds to the model used by Bychkov *et al.*[10]

Equation (3.23) may be written (when $\Delta_k = 0$), after several algebraic steps as

$$\gamma = \left(\frac{1-\lambda}{\lambda}\right) V_Q 4\left(\sum_{0<k<k_F} (1-f_k)(\gamma/\bar{E}) - \sum_{k_F<k<2k_F} f_k\gamma/\bar{E}\right), \tag{4.5}$$

$$\gamma \cong -\left(\frac{1-\lambda}{\lambda}\right) V_Q 4\left\{\sum_{k>0} \gamma\tilde{f}_k \,\mathrm{sgn}[\epsilon(k)-\epsilon(k-Q)]\Big/\bar{E} + \sum_{k>0} \frac{\gamma\tilde{f}_k}{\epsilon(k)-\epsilon(k+Q)}\right\}, \tag{4.6}$$

where $\tilde{f}_k \equiv 1 - f_k$ if $k < k_F$ and $\tilde{f}_k \equiv f_k$ if $k > k_F$. In obtaining Eq. (4.6) from (4.5) we have included terms for $k > 2k_F$ which were not present in Eq. (4.5) since we neglected these at the outset (see Sec. III). Because the contribution of these additional terms is very small [note that $|\epsilon(2k_F) - \epsilon(k_F)| \gg k_B T$ for all reasonable T so that f_k, for $k > 2k_F$ is small], they may be added to Eq. (4.3) with negligible error. The second term in the curly brackets in Eq. (4.6) arises from the coupling of states $|k\rangle$ and $|k+Q\rangle$ with $k > 0$. This coupling, which was neglected in Sec. III since these states are always nondegenerate, is included in Eq. (4.6) using perturbation theory. The equation for T_P obtained from (4.2) and (4.6) is then

$$1 = -[(1-\lambda)/\lambda] V_Q \chi^0(Q,0)|_{T_P} . \tag{4.7}$$

This equation for T_P is seen to be identical to that obtained from Eq. (4.1). Thus, the temperature at which the phonon frequency is driven soft is identical to that at which a gap opens in the electronic energy spectrum.

A final remark should be made in this section concerning the slight difference in form between the BCS and Peierls gap equations (in the absence of coupling between the two gaps). It follows from Eqs. (3.23) and (3.24) that the two equations would have exactly the same form, except for differences in the cutoff energies of the interactions, if

$$\bar{E} \equiv \{[\epsilon(k)-\epsilon(k-Q)]^2 + 4\gamma^2\}^{1/2} = 2[\epsilon^2(k)+\gamma^2]^{1/2} .$$

Since for $k \sim k_F$, $\epsilon(k-Q) \approx -\epsilon(k)$ and since the sum in Eq. (3.23) is dominated by the contributions of wave vectors near k_F, the above equality is nearly satisfied for all important k. However, as will be discussed in Sec. V, the gap equations are not completely identical in form and this fact gives rise to certain asymmetries in the solution of the coupled gap equations. These asymmetries do not show up in the parquet diagrammatic analysis[10] in which the BCS and Peierls gap equations are found to be identical in form.

V. SOLUTION OF COUPLED GAP EQUATIONS

It can be seen from Eqs. (3.23) and (3.24) that there are three types of solutions to the coupled gap equations, each corresponding to extrema of the free-energy surface; (i) the normal-state solutions in which $\Delta = \gamma = 0$, (ii) the decoupled

solutions in which $\gamma = 0$ and $\Delta = \Delta^0$, and $\Delta = 0$ and $\gamma = \gamma^0$, where the superscript zero is used to denote the value of the gap parameters in the absence of coupling, and (iii) the solutions for which both Δ and γ are nonzero. The highest temperature at which Eq. (3.23) has a nontrivial solution when $\Delta = 0$ is T_P and that at which Eq. (3.24) has a nontrivial solution when $\gamma = 0$ is T_S. An extensive numerical study we have carried out indicates that only when Δ^0 and γ^0 are nearly equal with $\gamma^0 < \Delta^0$ can there be solutions to Eqs. (3.23) and (3.24) with γ and Δ simultaneously nonzero. This result is qualitatively independent of k_F, ω_c the cutoff frequency which appears in $V_{kk'}$, and temperature. From the numerical studies, we have constructed the phase diagram for the system at $T = 0$. This is shown in Fig. 1, for a half-filled cosine band, $\epsilon(k) = (\frac{1}{2}W)(1 - \cos k)$, where W is the bandwidth and the lattice constant is assumed to be unity. The vertical axis plots the BCS gap (in the absence of coupling) divided by W and the horizontal axis plots the normalized Peierls gap (in the absence of coupling). The upper and right-hand axes plot the effective interaction strengths corresponding to γ^0 and Δ^0, respectively. Since at $T = 0$, $\Delta^0 = 1.76\, k_B T_S$, and $\gamma^0 \cong 1.76\, k_B T_P$, the axes can be viewed as plotting T_S and T_P. It follows from the figure that the ground state of the system is a BCS superconductor when $T_S > T_P$ and a Peierls insulator if the converse is true. Only when T_S and T_P are nearly equal will the system be in the mixed state with both order parameters nonzero. The corresponding parameters are indicated by the shaded region in Fig. 1. The lack of symmetry between the superconducting and Peierls insulating states in the phase diagram arises from the slight differences in form of the BCS and Peierls (decoupled) gap equations. In the half-filled cosine band case this arises only from differences in the cutoff energies. This was discussed in Sec. IV. This asymmetry would not be expected to show up in calculations based on the logarithmic approximations to the parquet equations.[10]

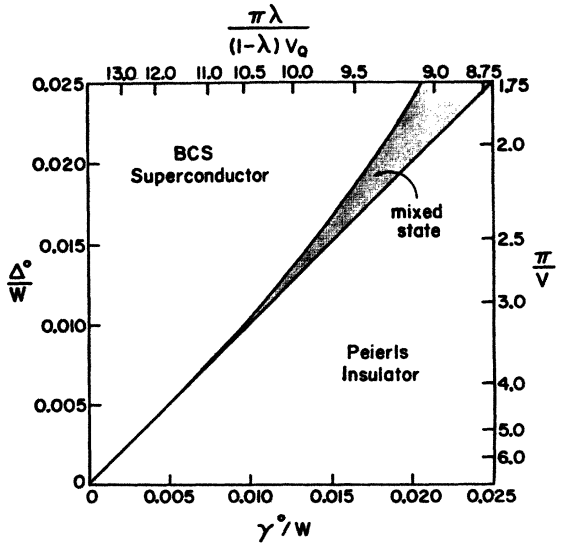

FIG. 1. Phase diagram for the coupled BCS-Peierls system at $T = 0$. The variables Δ^0 and γ^0 are the values of the gap parameters divided by bandwidth W when there is no coupling between the two gap equations. The vertical axis on the right and upper horizontal axis give the effective interaction strengths corresponding to Δ^0 and γ^0, respectively. In the shaded region the ground state is one in which both gap parameters are simultaneously nonzero.

We have studied the temperature dependence of the solutions of the gap equations. Except for the very special case when the mixed state occurs, the system does not switch from one type of ordering to the other. Thus, for $T_P > T_S$ the ordered state is always the Peierls insulator and for $T_S > T_P$ it is always a BCS superconductor throughout the entire temperature range. The free-energy surface as a function of the coordinates (Δ, γ) has the following behavior. Above both critical temperatures a minimum is at the origin $\Delta = 0$, $\gamma = 0$. When there is no mixed state, below the upper critical temperature, say T_P, a minimum appears at $(0, \pm\gamma^0)$ and the origin is a saddle point. Below the lower critical temperature, T_S, a saddle point develops at $(\pm\Delta^0, 0)$ and the origin is then a maximum. The minimum still occurs at $(0, \pm\gamma^0)$. This behavior continues down to zero temperature. The special behavior associated with the mixed state will be discussed in Sec. VI.

In summary, it is found by numerical solution of the coupled gap equations that the BCS superconducting and Peierls insulating states are, in general very incompatible in mean-field theory, and the system has only one phase transition, except under very special circumstances.

VI. SOME PROPERTIES OF THE MIXED STATE

While, on the basis of the present calculations, it seems very unlikely that the mixed state can be observed in any real systems, for the sake of completeness, some properties of this state will be discussed in this section.

A. Temperature dependence of the gap parameters

It is possible to show analytically that the solution of the coupled gap equations [Eqs. (3.23) and (3.24)] corresponding to $\gamma \neq 0$, $\Delta \neq 0$ can only occur when $\gamma^0 \leq \Delta^0$, whereas in Sec. V, γ^0 and Δ^0 are the temperature-dependent gap parameters in the absence of coupling. This proof is given in Appendix A which also contains a brief description of how the shaded region in Fig. 1 (which corresponds to the mixed state) was obtained. Numerical calculations substantiate these analytical re-

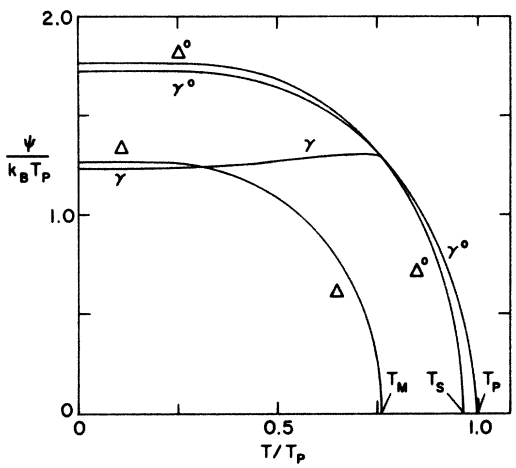

FIG. 2. Temperature dependence of the gap parameters when the mixed state having order parameters Δ, γ exists. The mixed state sets in at temperature T_M corresponding to the point at which the curves Δ^0 and γ^0 vs T (which are the solutions to the uncoupled gap equations) cross.

sults. It is also found numerically that the mixed state always appears at a temperature T_M which coincides with an intersection of the curves Δ^0 and γ^0 plotted as a function of temperature. Thus the mixed state is found to occur only when $T_P \gtrsim T_S$ and $\gamma^0 \leq \Delta^0$. These results are illustrated in Fig. 2 which plots the gap parameters as a function of temperature for a half-filled cosine band. The parameters are chosen as follows: $V_Q = V = 1.0$ in units of bandwidth and $\lambda = 0.766$. As before, the parameters Δ and γ are the solutions to Eqs. (3.23) and (3.24) associated with the mixed state. It follows from Fig. 2 and from considering the state of lowest free energy that for $T_P > T > T_M$ the BCS gap parameter is zero and the Peierls gap parameter γ is monotonically increasing until $T = T_M$. Below this temperature Δ begins to grow and γ to decrease until the zero temperature limit is reached. As shown Appendix A, $\Delta^2 + \gamma^2 = (\Delta^0)^2$.

The free energy as a function of (Δ, γ) has the following behavior. For $T > T_P$ a minimum in the free energy surface is at the origin (0, 0). For $T_S < T < T_P$ the points $(0, \pm\gamma^0)$ are minima. The origin is then a saddle point. For $T_M < T < T_S$ the points $(0, \pm\gamma^0)$ are minima, $(\pm\Delta^0, 0)$ are saddle points and the origin is a maximum. For $T < T_M$ the mixed state is a minimum in the free-energy surface and the points $(0, \pm\gamma^0)$ and $(\pm\Delta^0, 0)$ are saddle points; the origin is then a maximum.

B. Electromagnetic response in the mixed state at $T=0$

Once the Bogoliubov transformation (see Sec. III) for the coupled BCS-Peierls system is obtained, it is relatively simple to calculate the electromagnetic response of the system. As was suggested by Bychkov *et al.*[10] the mixed state exhibits a "one-dimensional Meissner effect", i.e., there is a nonzero coefficient of proportionality between the current induced by an electromagnetic field $J_\parallel$ and the vector potential $A_\parallel$. The aim of this section is to calculate this coefficient. Only a one-dimensional calculation is performed here; hence the subscript $\parallel$ is used to represent the fact that the current and vector potential are along the direction of the chain. Clearly there are complicated effects which arise from three-dimensional coupling between the chains and the fields. These will not be considered here.

Define the paramagnetic current $J_\parallel^p$ as

$$J_\parallel = J_\parallel^p - ne^2 A_\parallel / mc \ , \tag{6.1}$$

where n is the density of electrons, m is their mass, and c is the velocity of light. To calculate $J_\parallel^p$ we follow Rickayzen.[7] The Hamiltonian which describes the interaction between the spatially- (z) and time- (t) dependent external field $A_\parallel(z, t)$ and the electrons is written in second-quantized form as

$$H' = \frac{-e}{2mc} \sum_{\substack{k,q \\ \sigma}} a(q,t)(2k+q)\, C^\dagger_{k+q\sigma} C_{k\sigma} \ , \tag{6.2}$$

where $a(q, t)$ is the Fourier transform of $A_\parallel(z, t)$, and the paramagnetic-current-density operator is

$$\hat{J}^p(z) = \frac{e}{2m} \sum_{\substack{k,q \\ \sigma}} C^\dagger_{k\sigma} C_{k+q\sigma} e^{iqz}(2k+q) \ . \tag{6.3}$$

The expectation value of the current density is

$$J_\parallel^p(z,t) = -i \lim_{\substack{\tau\to\infty \\ t>\tau}} \int_0^t dt' e^{-(t-t')/\tau} \times \langle [\hat{J}^p(z,t),\, H'(t')] \rangle_{\rm av} \ , \tag{6.4}$$

where we have used the Heisenberg representation of the operators $\hat{J}$ and H'. We wish to evaluate the Fourier transform of Eq. (6.4), $J_\parallel^p(q, \omega)$, in the limit that first $\omega \to 0$ and then $q \to 0$. To evaluate the commutator in Eq. (6.4) is tedious but straightforward. The Bogoliubov transformation is used to express the operators $C_{k\sigma}$, etc., in terms of the ψ's defined in Sec. III. The final expression for the expectation value $J_\parallel^p$ at $T = 0$ can be shown to be

$$\frac{J_\parallel^p}{A_\parallel} = \frac{2e^2 Q^2}{m^2 c} \sum_{k=0}^{\infty} \frac{2\gamma^2}{(\bar{E})^2} \left(\frac{1}{E^+(k) + E^-(k)} \right) \times \left[1 - \frac{\nu^-(k)}{E^-(k)} \left(\frac{\nu^+(k)}{E^+(k)} \right) - \frac{\Delta_k}{E^-(k)} \left(\frac{\Delta_k}{E^+(k)} \right) \right] \ , \tag{6.5}$$

where $\bar{E}$ is given in Eq. (3.11) and $E^+(k)$ and $E^-(k)$ are defined by Eq. (3.14). Here

$$\nu^\mp(k) = \tfrac{1}{2}[\epsilon(k) + \epsilon(k-Q) \mp \bar{E}] \ . \tag{6.6}$$

In the Peierls limit $(\Delta \to 0)$ the quantity in square brackets is 2.0 for all k values. In the BCS limit

($\gamma \to 0$) $J_{\parallel}^{p} = 0$, so that only the diamagnetic contribution remains. It is shown in Appendix B that in the Peierls limit $J_{\parallel}^{p}$ exactly cancels the diamagnetic term so that there is, as expected, no "Meissner effect" in the insulator. It follows from Eqs. (3.12) and (3.13) that the quantity in square brackets is given by $[1+\cos(2\varphi_\alpha - 2\varphi_\beta)]$ which clearly lies between 0 and 2. Thus there is a *reduction* in $J_{\parallel}^{p}/A_{\parallel}$ relative to the value in the Peierls insulator, when $\Delta \to 0$. This means that the coefficient of proportionality between $J_{\parallel}$ and $A_{\parallel}$ is negative and nonzero.

Bychkov *et al.*[10] suggested that in the mixed state

$$J_{\parallel}^{p}/A_{\parallel} = (ne^2/mc)[\gamma^2/(\Delta^2+\gamma^2)] . \tag{6.7}$$

As can be seen, Eq. (6.5) differs quantitatively from this equation but the qualitative dependence $J_{\parallel}^{p}/A_{\parallel}$ on Δ and γ is the same.

ACKNOWLEDGMENTS

We wish to acknowledge helpful discussions with J. Hertz and E. Mulazzi.

APPENDIX A: PROOF THAT THE MIXED STATE OCCURS ONLY WHEN $\gamma^0 \leq \Delta^0$

Define

$$I^{\mathrm{BCS}}(\nu) = \alpha \int_{k_F}^{k_F+\Delta k} dk \, \frac{1-2f^{\mathrm{BCS}}(\nu)}{[\epsilon^2(k)+\nu^2]^{1/2}} , \tag{A1}$$

where α is an unimportant constant, Δk is the cutoff wave vector in the BCS interaction and $f^{\mathrm{BCS}}(\nu)$ is the Fermi function for excitation energies of the BCS form: $[\epsilon^2(k)+\nu^2]^{1/2}$. The decoupled BCS gap equation [Eq. (3.24) with $\gamma = 0$] can be written in terms of I^{BCS} as

$$I^{\mathrm{BCS}}(\Delta^0) = \pi/V . \tag{A2}$$

The decoupled Peierls equation [Eq. (3.23) with $\Delta_k = 0$] is

$$I^{\mathrm{BCS}}(\gamma^0) + I^{(1)}(\gamma^0) = \pi\lambda/[(1-\lambda)V_Q] , \tag{A3}$$

where we have used the fact that $\epsilon(k) \approx -\epsilon(k-Q)$ for $k \approx k_F$ and

$$I^{(1)}(\nu) \equiv \alpha \int_0^{k_F-\Delta k} \frac{1-2f^{p}(\nu)}{\frac{1}{4}[\epsilon(k)-\epsilon(k-Q)]^2+\gamma^2} . \tag{A4}$$

In Eq. (A4), $f^{p}(\nu)$ is the Fermi function for excitation energies of the Peierls form $|\zeta_k|$. The coupled gap equations are solved by γ, Δ where the BCS-like gap equation [Eq. (3.24)] implies

$$I^{\mathrm{BCS}}[(\Delta^2+\gamma^2)^{1/2}] = \pi/V . \tag{A5}$$

Thus $\Delta^2+\gamma^2 = (\Delta^0)^2$. The Peierls-like gap equation [Eq. (3.23)] implies

$$I^{\mathrm{BCS}}[(\Delta^2+\gamma^2)^{1/2}] + I^{(1)}(\gamma) = \pi\lambda/[(1-\lambda)V_Q] . \tag{A6}$$

Hence,

$$I^{(1)}(\gamma) = \pi\lambda/[(1-\lambda)V_Q] - \pi/V . \tag{A7}$$

In order for there to be a mixed state the quantity on the right-hand side of Eq. (A7) must be positive. Now $I^{\mathrm{BCS}}(\nu)$ and $I^{(1)}(\nu)$ are positive functions which rapidly decrease monotonically as ν increases. We want to show that only if $\gamma^0 \leq \Delta^0$ can we obtain solutions to Eqs. (A5) and (A6). If $\gamma^0 < \Delta^0$

$$I^{\mathrm{BCS}}(\gamma^0) \gg I^{\mathrm{BCS}}(\Delta^0) = \pi/V , \tag{A8}$$

and thus

$$I^{(1)}(\gamma^0) = \pi\lambda/[(1-\lambda)V_Q] - I^{\mathrm{BCS}}(\gamma^0) \ll \pi\lambda/[(1-\lambda)V_Q] - \pi/V . \tag{A9}$$

The Peierls-like gap equation implies

$$I^{(1)}(\gamma^0) \ll I^{(1)}(\gamma) . \tag{A10}$$

Equation (A10) implies $\gamma < \gamma^0$ and it has solutions if and only if

$$I^{(1)}(\gamma) = \pi\lambda/[(1-\lambda)V_Q] - \pi/V \leq I^{(1)}(0) . \tag{A11}$$

Since $\gamma^0 < \Delta^0$, by assumption, we conclude that $\gamma < \Delta^0$ so that Eq. (A5) is also satisfied. Had we assumed $\Delta^0 < \gamma^0$ we would have reached the conclusion $\gamma > \gamma^0 > \Delta^0$ which is inconsistent with Eq. (A5). In summary, the mixed state only occurs when

$$\gamma^0 \leq \Delta^0 ,$$

and

$$0 \leq I^{(1)}(\gamma) = \pi\lambda/[(1-\lambda)V_Q] - \pi/V \leq I^{(1)}(0) .$$

The first equation places an upper bound on γ^0. The last equation places a lower bound on γ^0. These two equations were used to plot the phase diagram in Fig. 1.

APPENDIX B: PROOF THAT $J_{\parallel}^{p} = ne^2 A_{\parallel}/mc$ IN THE PEIERLS INSULATOR

From Eq. (6.5) we have (when $\Delta_k = 0$)

$$\frac{J_{\parallel}^{p}}{A_{\parallel}} = \frac{8e^2Q^2}{m^2c} \sum_{k=0}^{\infty} \frac{\gamma^2}{(\bar{E})^2}\left(\frac{1}{E^+(k)+E^-(k)}\right) , \tag{B1}$$

$$\frac{J_{\parallel}^{p}}{A_{\parallel}} = \frac{8e^2Q^2\gamma^2}{2\pi m^2c} \int_0^{\infty} \frac{dk}{[E^+(k)+E^-(k)]^3} . \tag{B2}$$

For simplicity we assume $\epsilon(k) = k^2/2m$. The results should be valid for any band shape. From Eq. (3.14) we have

$$\frac{J_{\parallel}^{p}}{A_{\parallel}} = \frac{4e^2Q^2\gamma^2}{2\pi m^2c} \frac{m^3}{Q^3} \int_{-\infty}^{\infty} \frac{dk}{[(k+\frac{1}{2}Q)^2+(2m\gamma/Q)^2]^{3/2}} . \tag{B3}$$

Defining $k+\frac{1}{2}Q = (2m\gamma/Q)x$ gives

$$\frac{J_{\parallel}^{p}}{A_{\parallel}} = \frac{8e^2Q}{mc8\pi} \int_0^{\infty} \frac{dx}{(1+x^2)^{3/2}} . \tag{B4}$$

The number of electrons per unit length (including spin) is

$$n = 2k_F/\pi = Q/\pi \ . \qquad \text{(B5)}$$

Evaluation of Eq. (B4) yields the desired result

$$J_{\parallel}^{p}/A_{\parallel} = ne^2/mc \ . \qquad \text{(B6)}$$

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[9]This lack of self-consistency was, however, mentioned in a note added in proof in Ref. 3. A brief discussion of the solution of a pair of coupled gap equations at $T=0$ for a particular model of the competition between BCS pairing and the Overhauser instability in one dimension [see A. Overhauser, Phys. Rev. Lett. 4, 415 (1960)] has been presented by E. M. Henley and L. Wilets [Ann. Phys. 14, 120 (1961)]. These authors find that the presence of correlations of the Overhauser type suppress the binding energy of the BCS state, a conclusion consistent with ours for the appropriate choice of parameters in our model Hamiltonian.

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[11]B. Patton and L. J. Sham, Phys. Rev. Lett. 31, 631 (1973); M. J. Rice and S. Strässler, Solid State Commun. 13, 697 (1973).

[12]P. A. Lee, T. M. Rice, and P. W. Anderson, Phys. Rev. Lett. 31, 462 (1973); David Allender, J. W. Bray, and John Bardeen, Phys. Rev. B 9, 119 (1974).

[13]For example, the attractive phonon-induced interaction is of the form

$$\bar{V}_{q,k',-q,k'} = \omega_q \mid M_q \mid^2 / \{[\epsilon(k') - \epsilon(k'-q)]^2 - (\omega_q)^2\},$$

where ω_q is the phonon frequency and M_q is a matrix element whose exact form is not important here.

[14]Only for this single value of q will the mean value of the ionic displacement be assumed to be nonzero. It is clear that if Q and the reciprocal-lattice vector are commensurate additional gaps may be opened (besides that at $2k_F$) in the electronic spectrum arising from the change in lattice symmetry. Because they are away from the Fermi energy, these gaps are unimportant for the purposes of the present calculation and will be neglected here as in previous treatments (see, for example Refs. 8, 11, and 12).

[15]It is necessary to neglect the k and k' dependence of the interaction V_Q in order that the mean-field equations be solvable. This assumption is made in the same spirit as the BCS treatment of the pairing interaction. Whether $V_{kk'}$ and V_Q are chosen as independent parameters does not affect the conclusions reached here.

[16]Little's *Ansatz* differs from Eq. (3.24) in that ξ_k^2 is replaced by $\epsilon_k^2+\gamma^2$. This represents a reasonable approximation to Eq. (3.24) whenever the cutoff frequency ω_c is small compared to the Fermi energy, which assumption is expected to be valid in most physical systems.

[17]David Pines, *Elementary Excitations in Solids* (Benjamin, New York, 1963).

[18]B. Renker, H. Rietschel, L. Pintschovius, W. Glaser, P. Brüesch, D. Kuse, and M. J. Rice, Phys. Rev. Lett. 30, 1144 (1973).

[19]V. Heine and D. Weaire, in *Solid State Physics*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1965), Vol. 24.

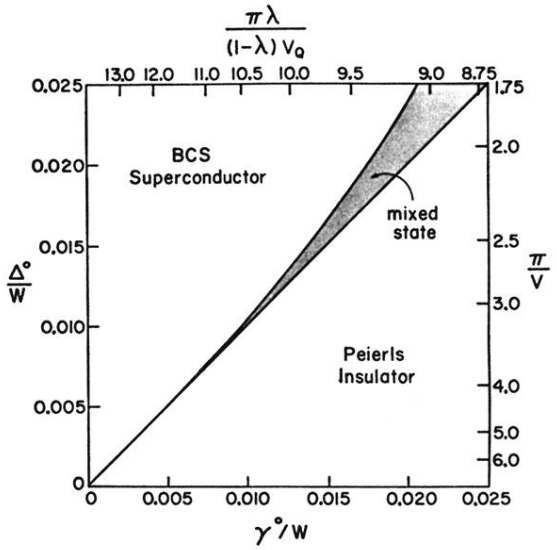

FIG. 1. Phase diagram for the coupled BCS-Peierls system at $T=0$. The variables Δ^0 and γ^0 are the values of the gap parameters divided by bandwidth W when there is no coupling between the two gap equations. The vertical axis on the right and upper horizontal axis give the effective interaction strengths corresponding to Δ^0 and γ^0, respectively. In the shaded region the ground state is one in which both gap parameters are simultaneously nonzero.