Gauge-Invariant Theory of the Dynamical Interaction of Charge Density Waves and Superconductivity

P. B. Littlewood and C. M. Varma
Bell Laboratories, Murray Hill, New Jersey 07974
(Received 15 June 1981)

The long-wavelength amplitude mode of the charge-density-wave state modulates the average density of states at the Fermi surface leading to a coupling between it and the order parameter for superconductivity. This is shown, in a gauge-invariant theory, to lead to a bound state below twice the BCS gap. Our results are discussed in the context of recent experiments on $2H$-$NbSe_2$.

PACS numbers: 74.20.Fg, 71.45.Gm, 72.15.Nj

In the charge-density-wave (CDW) state, there exist zone-center optic phonon modes, which transform with the full symmetry of the lattice. These CDW amplitude modes (CDW-AM) are accompanied by an oscillation of the CDW gap, which leads in general to a variation of the average density of states at the Fermi surface (see Fig. 1). Furthermore, if a material in a CDW state undergoes a superconducting transition, the excitation of the CDW-AM leads also to a time-dependent perturbation of the superconducting gap, since the latter depends on the density of states at the Fermi surface, $N(0)$. In this paper, we study the effects of this coupling.

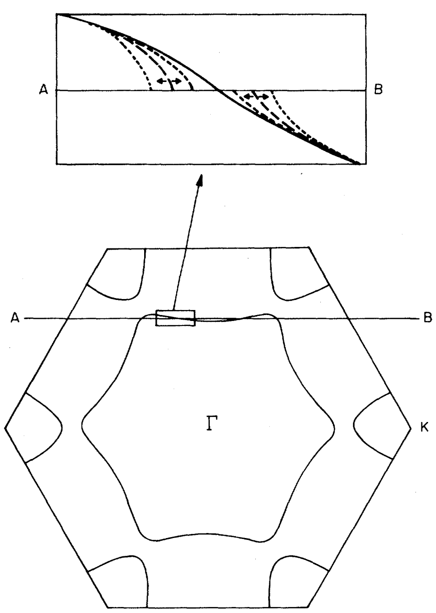

FIG. 1. A schematic picture of the Fermi surface of $2H$-$NbSe_2$ (adapted from Ref. 1) in the $k_z = 0$ plane, including the Bragg plane AB induced by a lattice distortion in the CDW state. The inset shows how the Fermi surface changes from the normal state (full line) into the CDW state (dashed line) and with further perturbation of the CDW-AM (dotted line).

We were stimulated to undertake the present study by Raman-scattering experiments of Sooryakumar and Klein (SK) on $2H$-$NbSe_2$.[2] Below the transition to the CDW state[3] at $T_d = 33$ K, they observe the CDW-AM in both A and E symmetries near 40 cm^{-1}. On further cooling below the superconductivity transition at $T_c = 7.2$ K, a new "gap" mode appears, in both symmetries, at frequencies close to the BCS gap, $2\Delta \approx 17$ cm^{-1}. SK argued that the sharpness of the new lines, as well as the transfer of oscillator strength from the gap modes to the CDW-AM with application of a magnetic field, indicate a new kind of coupled excitation of the CDW-AM and superconductivity.[2]

Static effects of the coupling mechanism between the CDW and Δ have already been invoked[4] to understand why under pressure a decrease of T_d [leading to a larger remaining $N(0)$] is accompanied by an increase of T_c. In a study of the dynamics, the leading-order coupling of the amplitude u of the CDW-AM to the superconducting gap is

$$\Delta = \Delta_0 + \Delta_1 u. \tag{1}$$

The coupling constant Δ_1 can be obtained from the variation of the BCS gap due to a change in $N(0)$ by using the BCS prescription. This gives

$$\Delta_1 = (\Delta_0/\lambda_0)[N(0)]^{-1} dN(0)/du, \tag{2}$$

where λ_0 is the BCS coupling constant.

We write the total Hamiltonian as

$$H = H_{ph} + H_{el} + H_{int}, \tag{3}$$

where in H_{ph} we consider only the $q \simeq 0$ CDW-AM,

$$H_{ph} = \hbar\omega_0 b^+ b. \tag{4}$$

H_{el} describes the electronic part which gives rise to superconductivity,

$$H_{el}=\sum_{\vec{k}}\epsilon_{\vec{k}}\Psi_{\vec{k}}^{+}\tau_3\Psi_{\vec{k}}+\tfrac{1}{2}\sum_{\vec{k}\vec{k}'\vec{q}}V(\vec{k},\vec{k}',\vec{q})(\Psi_{\vec{k}+\vec{q}}^{+}\tau_3\Psi_{\vec{k}})(\Psi_{\vec{k}'-\vec{q}}^{+}\tau_3\Psi_{\vec{k}'}), \tag{5}$$

in the Nambu notation,[5] where the electronic creation and annihilation operators are written as two-component vectors,

$$\Psi_{\vec{k}}=\begin{pmatrix} C_{\vec{k}\uparrow} \\ C_{-\vec{k}\downarrow}^{+}\end{pmatrix},\quad \Psi_{\vec{k}}^{+}=(C_{\vec{k}\uparrow}^{+},\ C_{-\vec{k}\downarrow}), \tag{6}$$

and the τ's are Pauli matrices. $V(\vec{k}\vec{k}'\vec{q})$ contains both the Coulomb repulsion and the effective attraction mediated via phonons. Following Nambu,[5] we rewrite H_{el} as the sum of the BCS reduced Hamiltonian H_0 and the rest:

$$H_{el}=H_0+H_1. \tag{7}$$

$$H_0=\sum_{\vec{k}}\Psi_{\vec{k}}^{+}(\epsilon_{\vec{k}}\tau_3+\Delta_0\tau_1)\Psi_{\vec{k}}, \tag{8}$$

$$H_1=\tfrac{1}{2}\sum_{\vec{k}\vec{k}'\vec{q}}V(\vec{k}\vec{k}'\vec{q})(\Psi_{\vec{k}+\vec{q}}^{+}\tau_3\Psi_{\vec{k}})(\Psi_{\vec{k}'-\vec{q}}^{+}\tau_3\Psi_{\vec{k}'})-\sum_{\vec{k}}\Psi_{\vec{k}}^{+}\Delta_0\tau_1\Psi_{\vec{k}}. \tag{9}$$

We write H_{int} as

$$H_{int}=H_{int}^{\Delta}+H_{int}^{\rho}, \tag{10}$$

where H_{int}^{Δ} is the part due to the effect arising from (1), which is

$$H_{int}^{\Delta}=g(b+b^{+})\sum_{\vec{k}}\Psi_{\vec{k}}^{+}\tau_1\Psi_{\vec{k}},\qquad g=\Delta_1(\hbar/2NM\omega_0)^{1/2}. \tag{11}$$

Besides (11), the phonon also couples to the electronic charge density, giving rise to

$$H_{int}^{\rho}=\lim_{\vec{q}\to 0}g'(b_{\vec{q}}+b_{-\vec{q}}^{+})\sum_{\vec{k}}\Psi_{\vec{k}+\vec{q}}^{+}\tau_3\Psi_{\vec{k}}. \tag{12}$$

For now we shall discuss H_{int}^{Δ} alone; the effect of H_{int}^{ρ}, already discussed by Balseiro and Falicov,[6] will be considered at the end and shown to be unimportant.

The phonon propagator for the $q=0$ CDW-AM is modified from its unperturbed form $D_0(\nu)$ in the absence of superconductivity ($\Delta_0=0$) to

$$D^{-1}(\nu)=D_0^{-1}(\nu)-\Sigma(\nu), \tag{13}$$

where $\Sigma(\nu)$ is the phonon self-energy. Within the BCS approximation (which involves neglecting the residual electron-electron interactions, i.e., H_1) $\Sigma(\nu)$ to lowest order is represented in Fig. 2(a) and is given by

$$\Sigma_0(\nu)=-ig^2\int d^3k\,d\omega\,(2\pi)^{-4}\,\mathrm{Tr}[\tau_1G(\vec{k},\omega+\nu)\tau_1G(\vec{k},\omega)], \tag{14}$$

where $G(\vec{k},\omega)$ is the BCS propagator

$$G^{-1}(\vec{k},\omega)=\omega I-\epsilon_{\vec{k}}\tau_3-\Delta_0\tau_1. \tag{15}$$

Equation (14) itself has few unusual consequences. An interesting result is obtained, however, if we go beyond the BCS approximation and calculate the "ladder corrections" [Fig. 2(b)] to the phonon's self-energy due to H_1. The self-energy $\Sigma(\nu)$ is then given by

$$\Sigma(\nu)=-i\int d^3k\,d\omega\,(2\pi)^{-4}\,\mathrm{Tr}[\Gamma(\vec{k},\omega;\vec{k},\omega+\nu)G(\vec{k},\omega+\nu)g\tau_1G(\vec{k},\omega)], \tag{16}$$

where the vertex Γ calculated in the ladder approximation is given by

$$\Gamma(\vec{k},\omega+\nu;\vec{k},\omega)=g\tau_1+i\int d^3k\,d\omega'\,(2\pi)^{-4}\tau_3G(\vec{k},\omega'+\nu)\Gamma(\vec{k}',\omega'+\nu;\vec{k}',\omega')G(\vec{k}',\omega')\tau_3V_{\vec{k}\vec{k}'}. \tag{17}$$

We can solve (16) exactly with $V_{\vec{k}\vec{k}'}$ of the separable BCS form. The solution leads to

$$\Sigma(\nu)=\Sigma_0(\nu)/\{1+[\lambda_0/2g^2N(0)]\Sigma_0(\nu)\}, \tag{18}$$

where $\Sigma_0(\nu)$, Eq. (14), is calculated to be

$$\mathrm{Re}\Sigma_0(\nu)=-2N(0)g^2\left[\lambda_0^{-1}-\left(\frac{4\Delta_0^2-\nu^2}{\nu^2}\right)^{1/2}\tan^{-1}x\right],\quad \text{for } \nu<2\Delta_0,$$

$$=-2N(0)g^2\left[\lambda_0^{-1}-\frac{1}{2}\left(\frac{\nu^2-4\Delta_0^2}{\nu^2}\right)^{1/2}\ln\left|\frac{1+x}{1-x}\right|\right],\quad \text{for } \nu>2\Delta_0,$$

where

$$x=\left|\frac{\nu^2}{\nu^2-4\Delta_0^2}\right|^{1/2}\left[1+\left(\frac{\Delta_0}{\hbar\omega_D}\right)^2\right]^{-1/2}, \tag{19}$$

and

$$\operatorname{Im}\Sigma_0(\nu) = 0 \quad \nu < 2\Delta_0,$$
$$= -g^2\pi N(0)\left(\frac{\nu^2 - 4\Delta_0^{\,2}}{\nu^2}\right)^{1/2}, \quad \nu > 2\Delta_0. \tag{20}$$

The first thing to note is that $\Sigma(\nu)$ is divergent for any value of the coupling constant g for $\nu \simeq 2\Delta_0$. This means that a pole necessarily appears in the phonon spectral weight

$$S(\nu) = -\pi^{-1}\operatorname{Im}D(\nu) \tag{21}$$

at a frequency ν_g below 2Δ. It is convenient to define a dimensionless coupling strength

$$\alpha = 4g^2N(0)/\lambda^2\hbar\omega_0. \tag{22}$$

For $\alpha \ll 1$, we get from $D^{-1}(\nu_g) = 0$

$$\hbar\nu_g = 2\Delta\left[1 - \frac{2\alpha^2}{\pi^2}\left(1 - \frac{4\Delta_0^{\,2}}{(\hbar\omega_0)^2}\right)^{-1}\right] \tag{23}$$

with spectral weight

$$S(\nu_g) = \frac{8\alpha^2}{\pi^2}\frac{(2\Delta/\hbar\omega_0)}{[1 - (2\Delta/\hbar\omega_0)^2]^3}. \tag{24}$$

We identify this mode with the new "gap" mode observed in Raman scattering by Sooryakumar and Klein.[2] In Fig. 3, we present the spectral weight, calculated numerically, for α varying from 0.1 to 0.5 and with $\omega_0 = 4.8\Delta_0$.

We can get a rough estimate of α from the measured variations with pressure of T_c and T_d,[4] and the estimated amplitude of the lattice distortion accompanying the CDW[3,7]; we find $\alpha = 0.3$–0.5. To obtain the result of SK that (10–15)% of the CDW-AM weight is transferred to the gap mode, we need $\alpha \approx 0.4$.

It is interesting to note that the vertex correction is necessary to keep the self-energy invariant to the transformation

$$\Psi(x) \to \exp[\alpha(x)\tau_1]\Psi(x) \tag{25}$$

(and the associated transformation of the gradient operator) under which H_{el} is invariant, but the BCS Hamiltonian H_0 is not. In fact the vertex Γ [Eq. (17)] was derived by Nambu[5] from a generalized Ward identity following from (25).

The transformation (25) is to be contrasted with the more familiar gauge transformation

$$\Psi(x) \to \exp[i\beta(x)\tau_3]\Psi(x) \tag{26}$$

(and the associated transformation of the electromagnetic field and the gradient operator) under which H_{el} is also invariant, but the BCS Hamiltonian is not. The longitudinal response of a superconductor in the BCS approximation is not gauge invariant. Vertex corrections to maintain the gauge invariance in the response give rise to bound states,[8] the so-called Bogoliubov modes, which go to zero frequency at long wavelength. However, in a charged superconductor these modes get pushed to near the plasma frequency of the metal by Coulomb interactions.

The modes calculated here are massive by contrast with a mass $\lesssim 2\Delta$. The Coulomb interactions do not affect $\Sigma(\nu)$ and our bound state. This is as it should be since $H_{\text{int}}^{\,\Delta}$ induces variations of the superconducting gap with no associated variation in the charge density.

In the above calculation we have neglected $H_{\text{int}}^{\,\rho}$

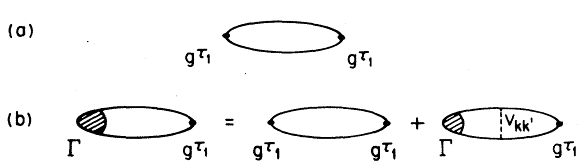

FIG. 2. (a) The phonon self-energy in lowest order from the BCS approximation Σ_0 and (b) the full self-energy Σ including the vertex correction Γ.

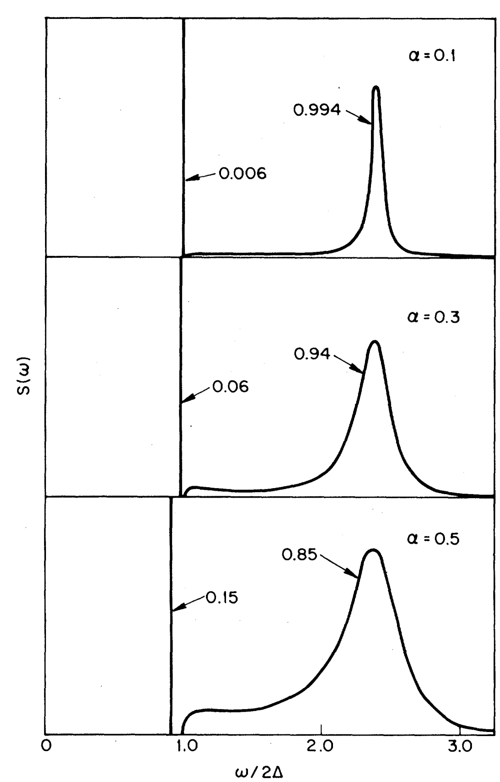

FIG. 3. The phonon spectral weight of the CDW-AM for three different values of the coupling constant α.

given by Eq. (12). $H_{\rm int}{}^{\rho}$ represents the usual coupling of phonons to the long-wavelength components of the electronic charge density. In the BCS approximation, the self-energy of a phonon due to $H_{\rm int}{}^{\rho}$ is[6]

$$\Sigma_{\rho}(\nu) = -ig'^2 \int d^3k\, d\omega\, (2\pi)^{-4} \times \mathrm{Tr}[\tau_3 G(\vec{k}, \omega+\nu)\tau_3 G(\vec{k},\omega)], \qquad (27)$$

which is the same quantity that occurs in the calculation of the longitudinal response of a superconductor. It is not invariant under the gauge transformation (26). As already discussed, a gauge-invariant treatment as well as the inclusion of Coulomb interactions within the random-phase approximation leads to features in $\Sigma_{\rho}(\nu)$ only near the plasma frequency. Thus $H_{\rm int}{}^{\rho}$ cannot be relevant to the SK experiment.

The singularity of the τ_1 vertex signifies that a massive collective mode exists in all superconductors (just as the singularity of the τ_3 vertex signifies the Bogoliubov mode). It is the special situation in $NbSe_2$ that it couples to the optic phonon mode which has led to its observation in the Raman scattering experiment by SK. The physical meaning of the mode is that it corresponds to an oscillation of the amplitude of the superconducting gap. This meaning becomes clear by analogy if one solves the charge-density-wave transition problem in a formalism analogous to Nambu's. For an incommensurate situation, there is again a singularity of the τ_3 vertex at $\omega = 0$ for $k \to 0$ signifying the phason, which is the analog of the Bogoliubov mode. There is also a singularity of the τ_1 vertex at finite frequency for $k \to 0$ which is simply the optic phonon of the CDW structure.

We shall discuss the above points as well as the finite-κ behaviors of the new collective mode in detail elsewhere.

Finally, we note that the collective mode found in this paper should be distinguished from the "exciton" modes discussed in the literature.[9] The latter arise from charge (τ_3 symmetry) couplings in $l \neq 0$ angular momentum channels for an s-wave superconducting ground state. Our mode is also distinct from the collective mode discovered by Carlson and Goldman[10] which occurs very close to T_c when the normal and superfluid components are decoupled and which are principally phase modes. To the best of our knowledge the amplitude modes of superconductors discovered here have not been discussed before. Modes derived from similar considerations, however, appear in a paper by Nambu and Jona-Lasinio[11] on a dynamical symmetry-breaking model for elementary particles.

[1]J. E. Inglesfield, J. Phys. C 13, 17 (1980).

[2]R. Sooryakumar and M. V. Klein, Phys. Rev. Lett. 45, 660 (1980).

[3]D. E. Moncton, J. D. Axe, and F. J. DiSalvo, Phys. Rev. B 16, 801 (1977).

[4]C. Berthier, P. Molinié, and D. Jérome, Solid State Commun. 18, 1393 (1976).

[5]Y. Nambu, Phys. Rev. 117, 648 (1960).

[6]C. A. Balseiro and L. M. Falicov, Phys. Rev. Lett. 45, 662 (1980).

[7]The distortion amplitude u_0 has not been accurately measured in $2H$-$NbSe_2$, but is estimated to be between $\frac{1}{2}$ and $\frac{1}{3}$ of the amplitude in $TaSe_2$ measured in Ref. 2. (D. E. Moncton, private communication.)

[8]P. W. Anderson, Phys. Rev. 110, 827 (1958), and 112, 1900 (1958); N. N. Bogoliubov, Nuovo Cimento 7, 794 (1958).

[9]These are reviewed by P. C. Martin, in *Superconductivity*, edited by R. D. Parks (Marcel Dekker, New York, 1969).

[10]R. V. Carlson and A. M. Goldman, Phys. Rev. Lett. 34, 11 (1975).

[11]Y. Nambu and G. Jona-Lasinio, Phys. Rev. 122, 345 (1961).