PHYSICAL REVIEW B VOLUME 39, NUMBER 10 1 APRIL 1989

Linear charge-density-wave instability in $YBa_2Cu_3O_{7-\delta}$ and the pair-breaking effect from Coulomb scattering with superconducting electrons

P. Hertel and J. Appel
I. Institut für Theoretische Physik, Universität Hamburg, 2000 Hamburg 36, Federal Republic of Germany

J. C. Swihart
Department of Physics, Indiana University, Bloomington, Indiana 47405
(Received 10 August 1988)

e-e scattering between charge carriers in the CuO_2 planes and a one-dimensional electron system causes a temperature-dependent pair-breaking effect on the formation of a commensurate charge-density wave (CDW) in the one-dimensional system. The effect decreases exponentially when the planes become superconducting, allowing for the CDW instability to occur at or near the superconducting transition temperature T_S. The CDW gap ratio $2\Delta_{C0}/k_BT_C$ depends on the *e-e* scattering rate Γ. The temperature dependence of the order parameter $\Delta_C(T,\Gamma)$ is affected by superconductivity in the plane and, therefore, is different from the Bardeen-Cooper-Schrieffer (BCS) gap function. In order to distinguish between the BCS and CDW states, the nuclear-spin relaxation rates due to magnetic and quadrupole coupling, R_C/R_N and Q_C/Q_N, are found as functions of T. The frequency dependence of the infrared conductivity due to single-particle excitations across the CDW gap σ_{1C} is evaluated as a function of $\Gamma(T)$, yielding the Lee-Rice-Anderson result for $T=0$.

I. INTRODUCTION

The magnitude of the energy gap in the high-T_S superconductor $YBa_2Cu_3O_{7-\delta}$ is ambiguous. Whereas recent experiments of infrared absorption, quasiparticle tunneling, and Andreev scattering give the Bardeen-Cooper-Schrieffer (BCS) gap ratio $2\Delta_{S0}/k_BT_S\sim 3.5$,[1] there are other experiments which yield a second gap with a ratio of ~ 9. The observation of the nuclear-spin-lattice relaxation, the zero-field quadrupole relaxation, and the infrared reflectance spectra give evidence for *two* different pairing energies.[2] A single large energy gap is also found in infrared experiments and nuclear-spin relaxation studies.[3] Tunneling experiments yield ratios of Δ_{S0}/k_BT_S between 1 and 13;[4] there are indications, however, that this spread is due to the glassy state of the superconductor. Some of the authors of Refs. 2 and 3 attribute the two energy gaps to two superconducting pairing energies corresponding, respectively, to the quasiparticle excitation spectrum on the chain-forming Cu(1) sites and on the plane-forming Cu(2) sites of the orthorhombic unit cell. The assignment of the nuclear quadrupole resonance (NQR) frequencies and of the spin-lattice relaxation rates to the two different Cu sites is a difficult problem. Recent NMR studies on oriented single crystals assign the 31.5-MHz NQR frequency to the Cu(2) plane sites which show the large gap in the relaxation studies.[5]

In an attempt to clarify the origin and the magnitude of the large gap, independent of the question whether it occurs in the chain or in the plane, the possibility is explored here that we are dealing with a Peierls gap due to the formation of a charge-density wave (CDW). The formation of a CDW gap Δ_C at or near the superconducting transition temperature T_S is indicated by measurements of the positron annihilation lifetime and the Doppler line shape as a function of temperature *above* and *below* the superconducting transition in compounds where $\delta\sim 0.1$ (superconducting) and $\delta\sim 1$ (nonsuperconducting).[6] Whereas x-ray and neutron-diffraction results do not find a real crystalline phase transition at T_S, the positron-annihilation parameters show significant changes near T_S. The positron lifetime is inversely proportional to the electron density at the annihilation sites. These sites are the oxygen vacancies which are the most abundant trapping sites in these ceramics and which occur in the planes containing the Cu-O chains: The increase in the electron density near the oxygen vacancies that is observed as T falls below T_S signals a change in the electronic structure as the material changes from the normal to the superconducting state. This change is also indicated by the anomaly of the orthorhombic lattice parameters in the CuO_2 planes *a-b* that are observed near T_S by high-resolution x-ray scattering.[7]

Based on these experimental facts we suggest that the change of the electronic structure consists of a linear and commensurate CDW occurring concomitantly or nearly so with the superconducting transition. The transition temperature for the CDW instability is governed by pair-breaking processes which scatter the electrons at the Fermi surface (FS) of the one-dimensional (1D) system between $-p_F$ and $+p_F$ (=Fermi momentum). Electrons and holes bound to pairs by an attractive interaction in the CDW phase have opposite charge. Therefore, momentum scattering due to charged imperfections affect the order parameter Δ_C in the same manner as magnetic-impurity scattering influences the order parameter Δ_S for the Cooper pairs of a BCS superconductor.[8] Here, *e-e* Coulomb scattering between the electrons of the 1D and 2D systems provides the intrinsic pair-breaking effect for the CDW state. This effect occurs whether the CDW instability is driven by electrons in the chain or in the plane. We comment on the chain versus plane instabilities below. The CDW state is *suppressed* by pair-breaking processes *above* T_S. It begins to form at the transition temperature T_C, that can be very close to T_S, because the *e-e* scattering rate Γ decreases exponentially below T_S when the CuO_2 planes become superconducting. We find Γ in Sec. II and discuss its pair-breaking effect on the T dependence of Δ_C. In order to distinguish between a BCS and Peierls gap, we evaluate some of the response functions. The superconducting state is characterized by the coherence factors for single-particle scattering processes. These factors have different effects on the temperature and frequency dependences of the response functions: Nuclear-spin relaxation T_1, quadrupole relaxation Q, and the ac conductivity σ_1. For the Peierls gap the coherence factors contain signs (of Δ_C^2) that are different from BCS. The results for the response functions are compared for the CDW and the BCS states in Sec. III.

II. *e-e* SCATTERING AND THE CDW GAP

To obtain $\Gamma=1/\tau$ for *e-e* scattering, we take the energy spectrum of noninteracting electrons in a 1D system, $\varepsilon_{\mathbf{p}+\mathbf{Q}/2}=(1/2m)(\mathbf{p}+\mathbf{Q}/2)^2-E_F$, where E_F is the Fermi level, and $\varepsilon_{\mathbf{p}+\mathbf{Q}/2}=-\varepsilon_{\mathbf{p}-\mathbf{Q}/2}$.[9] For simplicity, we assume a one-half filled band $Q=2p_F=\pi/a$ and $-p_F\le p\le +p_F$; a is the lattice constant. The CDW instability is caused by an effective interaction λ_C that incorporates Coulomb and phonon interactions. This instability is more likely to occur than singlet superconductivity.[10] The CuO_2 planes are Mott-Hubbard insulators if the nominal valencies of Cu and O are 2^+ and 2^-. The energy surface of the filled valence band is shown as the square in Fig. 1. By self-doping, the 2D band is only partially filled and the spectrum is given by $\xi_{\mathbf{k}}=-2t[\cos(ak_x)+\cos(ak_y)]-E_F$.[11] Superconductivity is caused in the plane by an effective-pairing interaction λ_S.

The Hamiltonian for our system consisting of 1D and 2D electron systems interacting through the Coulomb interaction $V_{\mathbf{m}}$ ($\mathbf{m}$ = momentum transfer), is given by

$$H=H_{1D}+H_{2D}+H_{\rm int}, \tag{1}$$

$$H_{1D}=\sum_{\mathbf{p},\sigma}\varepsilon_{\mathbf{p}+\mathbf{Q}/2}(c^\dagger_{\mathbf{p}+\mathbf{Q}/2,\sigma}c_{\mathbf{p}-\mathbf{Q}/2,\sigma}-c^\dagger_{\mathbf{p}-\mathbf{Q}/2,\sigma}c_{\mathbf{p}+\mathbf{Q}/2,\sigma})+\lambda_C\sum_{\substack{\mathbf{p},\mathbf{p}'\\ \sigma,\sigma'}}(c^\dagger_{\mathbf{p}+\mathbf{Q}/2,\sigma}c_{\mathbf{p}-\mathbf{Q}/2,\sigma}c^\dagger_{\mathbf{p}'+\mathbf{Q}/2,\sigma}c_{\mathbf{p}'-\mathbf{Q}/2,\sigma}+\text{H.c.})\ , \tag{2}$$

$$H_{2D}=\sum_{\mathbf{k},\sigma}\xi_{\mathbf{k}}e^\dagger_{\mathbf{k}\sigma}e_{\mathbf{k}\sigma}+\lambda_S\sum_{\mathbf{k},\mathbf{k}'}e^\dagger_{\mathbf{k}\uparrow}e^\dagger_{-\mathbf{k}\downarrow}e_{-\mathbf{k}'\downarrow}e_{\mathbf{k}'\uparrow}\ , \tag{3}$$

$$H_{\rm int}=\sum_{\substack{\mathbf{p},\mathbf{p}',\mathbf{k};\sigma,\sigma'\\ \mathbf{m}=\mathbf{p}'-\mathbf{p}-\mathbf{Q}}}V_{\mathbf{m}}(e^\dagger_{\mathbf{k}-\mathbf{m},\sigma'}e_{\mathbf{k}\sigma'}+e^\dagger_{\mathbf{k}\sigma'}e_{\mathbf{k}+\mathbf{m},\sigma'})\times c^\dagger_{\mathbf{p}'-\mathbf{Q}/2,\sigma}c_{\mathbf{p}'+\mathbf{Q}/2,\sigma}\ . \tag{4}$$

The operators $c^\dagger$ and $e^\dagger$ create electrons in the 1D and 2D systems, respectively.

We assume that the plane is in the superconducting state and introduce the Bogoliubov quasiparticle operators $\gamma_{\mathbf{k}\uparrow}=u_{\mathbf{k}}e_{\mathbf{k}\uparrow}-v_{\mathbf{k}}e^\dagger_{-\mathbf{k}\downarrow}$ and $\gamma_{\mathbf{k}\downarrow}=v_{\mathbf{k}}e^\dagger_{\mathbf{k}\uparrow}+u_{\mathbf{k}}e_{-\mathbf{k}\downarrow}$, where $u_{\mathbf{k}}=\frac{1}{2}(1+\xi_{\mathbf{k}}/E_{\mathbf{k}})^{1/2}$ and $v_{\mathbf{k}}=\frac{1}{2}(1-\xi_{\mathbf{k}}/E_{\mathbf{k}})^{1/2}$; the quasiparticle energy $E_{\mathbf{k}}=(\xi_{\mathbf{k}}^2+\Delta_{S\mathbf{k}}^2)^{1/2}$. We ignore the gap anisotropy $\Delta_{S\mathbf{k}}=\Delta_S$. The Coulomb interaction $H_{\rm int}$ is a small perturbation and a canonical transformation gives the result to second order in $V_{\mathbf{m}}$:

$$\begin{aligned}H_{\rm int}=-2\sum_{\substack{\mathbf{p},\mathbf{p}',\mathbf{m},\mathbf{k}\\ \sigma,\sigma'}}V_{\mathbf{m}}V_{-\mathbf{m}}\Bigg[&\frac{(u_{\mathbf{k}}u_{\mathbf{k}+\mathbf{m}}-v_{\mathbf{k}}v_{\mathbf{k}+\mathbf{m}})^2}{2(\varepsilon_{\mathbf{p}'-\mathbf{m}+\mathbf{Q}/2}-\varepsilon_{\mathbf{p}+\mathbf{Q}/2})-E_{\mathbf{k}}+E_{\mathbf{k}+\mathbf{m}}}(\gamma^\dagger_{\mathbf{k}\uparrow}\gamma_{\mathbf{k}\uparrow}-\gamma^\dagger_{\mathbf{k}+\mathbf{m}\uparrow}\gamma_{\mathbf{k}+\mathbf{m}\uparrow}+\gamma^\dagger_{\mathbf{k}\downarrow}\gamma_{\mathbf{k}\downarrow}-\gamma^\dagger_{-\mathbf{k}-\mathbf{m}\downarrow}\gamma_{-\mathbf{k}-\mathbf{m}\downarrow})\\&+(u_{\mathbf{k}}v_{\mathbf{k}+\mathbf{m}}+u_{\mathbf{k}+\mathbf{m}}v_{\mathbf{k}})^2\left(\frac{1-\gamma^\dagger_{\mathbf{k}\downarrow}\gamma_{\mathbf{k}\downarrow}-\gamma^\dagger_{\mathbf{k}+\mathbf{m}\uparrow}\gamma_{\mathbf{k}+\mathbf{m}\uparrow}}{2(\varepsilon_{\mathbf{p}-\mathbf{m}+\mathbf{Q}/2}-\varepsilon_{\mathbf{p}+\mathbf{Q}/2})+E_{\mathbf{k}}+E_{\mathbf{k}+\mathbf{m}}}\right.\\&\left.-\frac{1-\gamma^\dagger_{\mathbf{k}\uparrow}\gamma_{\mathbf{k}\uparrow}-\gamma^\dagger_{\mathbf{k}+\mathbf{m}\downarrow}\gamma_{\mathbf{k}+\mathbf{m}\downarrow}}{2(\varepsilon_{\mathbf{p}'-\mathbf{m}+\mathbf{Q}/2}-\varepsilon_{\mathbf{p}'+\mathbf{Q}/2})-E_{\mathbf{k}}-E_{\mathbf{k}+\mathbf{m}}}\right)\Bigg]\\&\times c^\dagger_{\mathbf{p}'-\mathbf{m}+\mathbf{Q}/2,\sigma}c_{\mathbf{p}'+\mathbf{Q}/2,\sigma}c^\dagger_{\mathbf{p}+\mathbf{m}+\mathbf{Q}/2,\sigma}c_{\mathbf{p}+\mathbf{Q}/2,\sigma}\ .\end{aligned} \tag{5}$$

We are interested in the effect of Coulomb scattering on the CDW instability. Therefore, we ignore the term on the right-hand side of Eq. (5) that gives the Coulomb effects on the superconducting electrons in the plane.[12] We also replace the operator products in Eq. (5) by their expectation values, $\langle\gamma^\dagger_{\mathbf{k}\sigma}\gamma_{\mathbf{k}\sigma}\rangle=f(E_k)$. $H_{\rm int}$ describes the scattering between two electrons of the 1D system caused by the electronic polarizability P of the superconducting plane,

$$H_{\rm int}=2\sum_{\substack{\mathbf{p},\mathbf{p}',\mathbf{m}\\ \sigma,\sigma'}}P(-\mathbf{m},\omega)c^\dagger_{\mathbf{p}'-\mathbf{m}+Q/2,\sigma}c_{\mathbf{p}'+Q/2,\sigma}c^\dagger_{\mathbf{p}+\mathbf{m}+Q/2,\sigma}c_{\mathbf{p}+Q/2,\sigma}\ , \tag{6}$$

where $\omega=\varepsilon_{\mathbf{p}-\mathbf{m}+\mathbf{Q}/2}-\varepsilon_{\mathbf{p}+\mathbf{Q}/2}$, and

$$\begin{aligned}P(-\mathbf{m},\omega)=2\sum_{\mathbf{k}}V_{\mathbf{m}}V_{-\mathbf{m}}\Bigg[&(f_{\mathbf{k}}-f_{\mathbf{k}-\mathbf{m}})\left(\frac{u_{\mathbf{k}}^2u_{\mathbf{k}-\mathbf{m}}^2-u_{\mathbf{k}}u_{\mathbf{k}-\mathbf{m}}v_{\mathbf{k}}v_{\mathbf{k}-\mathbf{m}}}{\omega+E_{\mathbf{k}}-E_{\mathbf{k}-\mathbf{m}}}-\frac{v_{\mathbf{k}}^2v_{\mathbf{k}-\mathbf{m}}^2-u_{\mathbf{k}}u_{\mathbf{k}-\mathbf{m}}v_{\mathbf{k}}v_{\mathbf{k}-\mathbf{m}}}{\omega-E_{\mathbf{k}}+E_{\mathbf{k}-\mathbf{m}}}\right)\\&+(1-f_{\mathbf{k}}-f_{\mathbf{k}-\mathbf{m}})\left(\frac{u_{\mathbf{k}-\mathbf{m}}^2v_{\mathbf{k}}^2+u_{\mathbf{k}}u_{\mathbf{k}-\mathbf{m}}v_{\mathbf{k}}v_{\mathbf{k}-\mathbf{m}}}{\omega-E_{\mathbf{k}}-E_{\mathbf{k}-\mathbf{m}}}-\frac{u_{\mathbf{k}}^2v_{\mathbf{k}-\mathbf{m}}^2+u_{\mathbf{k}}u_{\mathbf{k}-\mathbf{m}}v_{\mathbf{k}}v_{\mathbf{k}-\mathbf{m}}}{\omega+E_{\mathbf{k}}+E_{\mathbf{k}-\mathbf{m}}}\right)\Bigg]\ .\end{aligned} \tag{7}$$

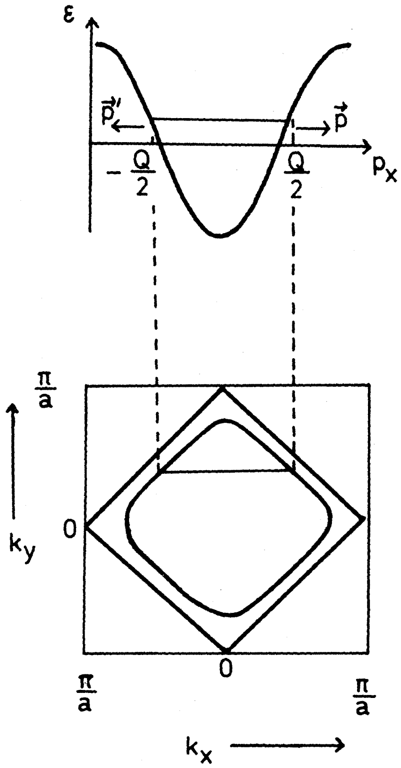

FIG. 1. Model: Energy spectrum of the one-dimensional electron system; for a half-filled band, the Fermi momentum $p_F = Q/2 = \pi/2a$. Below: Fermi surfaces for electrons on a two-dimensional square lattice (filling factors 1 and 0.75, cf. Ref. 11). Scattering between electrons of the 1D and 2D systems takes place along p_x and k_x in the phase-space regions indicated.

This function is of the same form as the density-density correlation function derived by Mahan.[13] The e-e scattering rate is determined by the spectral function of P that is given by

$$\alpha(-\mathbf{m},\omega) = \mathrm{Im} P(-\mathbf{m};\omega + i\delta) . \quad (8)$$

The function α presents the rate of making excitations with momentum transfer $\mathbf{m}$ and energy ω in the superconducting (or normal) plane. The scattering rate in the 1D system (Fig. 2) caused by excitations with momentum transfers in the plane $Q \sim 2P_F$ is given by

$$\frac{1}{\tau} = -2\sum_{\mathbf{p}'}[f(\varepsilon_{\mathbf{p}+\mathbf{Q}/2} - \varepsilon_{\mathbf{p}'-\mathbf{Q}/2}) - f(-\varepsilon_{\mathbf{p}'-\mathbf{Q}/2})] \times \alpha(\mathbf{p}-\mathbf{p}'+\mathbf{Q};\varepsilon_{\mathbf{p}+\mathbf{Q}/2} - \varepsilon_{\mathbf{p}'-\mathbf{Q}/2}) . \quad (9)$$

The scattering events take place near the Fermi surface, where $\omega = \varepsilon_{\mathbf{p}+\mathbf{Q}/2} - \varepsilon_{\mathbf{p}-\mathbf{Q}/2} \sim k_B T$. The spectral function is approximately given by $\alpha(\mathbf{p}-\mathbf{p}'+\mathbf{Q}; -\omega) = -\omega\alpha(\mathbf{Q})$, where

$$\alpha(\mathbf{Q}) = 2\pi |V_{\mathbf{Q}}|^2 \int \frac{d^2k}{(2\pi)^2}\left[-\frac{\partial f_{\mathbf{k}}}{\partial E_{\mathbf{k}}}\right]\delta(E_{\mathbf{k}} - E_{\mathbf{k}+\mathbf{Q}}) \times \frac{1}{2}\left[1 + \frac{\xi_{\mathbf{k}}\xi_{\mathbf{k}+\mathbf{Q}} - \Delta_{\mathbf{k}}^2}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{Q}}}\right] = \alpha_0 |V_{\mathbf{Q}}|^2 2f(\Delta_S) . \quad (10)$$

Here $\alpha_0 |V_Q|^2$ is a dimensionless parameter and $f(\Delta_S)$ is proportional to the density of quasiparticles at energy $\Delta_S(T)$. For the normal state in the plane, $f(\Delta_S) = \frac{1}{2}$. We carry out the $\mathbf{p}'$ integration in (9) and get

$$1/\tau = (\pi^2/3) N(E_F)(k_B T)^2 \alpha_0 |V_Q|^2 2f(\Delta_S) , \quad (11)$$

where $N(E_F)$ is the 1D density of states at E_F, including the spin degeneracy. The scattering rate $1/\tau$ plays the role of the pair-breaking parameter Γ in the Green's function theory of the CDW state.[14,15] Here Γ is temperature dependent and vanishes at $T=0$ (Fig. 3). The corresponding renormalization of the frequency and gap variables is given by

$$\tilde{\omega} = \omega + \frac{i}{2}\Gamma\tilde{\omega}/(\tilde{\omega}^2 + \tilde{\Delta}^2)^{1/2}$$

and

$$\tilde{\Delta} = \Delta - \frac{i}{2}\Gamma\tilde{\Delta}/(\tilde{\omega}^2 + \tilde{\Delta}^2)^{1/2} .$$

These two equations are to be solved simultaneously with

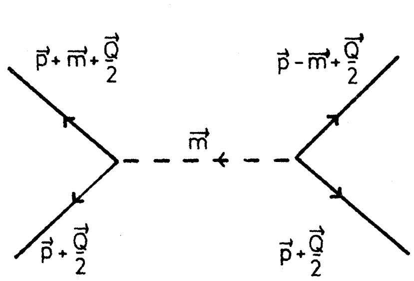

FIG. 2. e-e scattering in the 1D system.

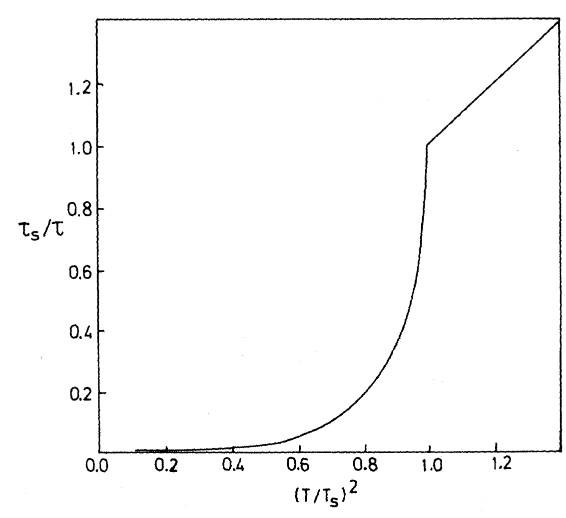

FIG. 3. T dependence of the pair-breaking parameter.

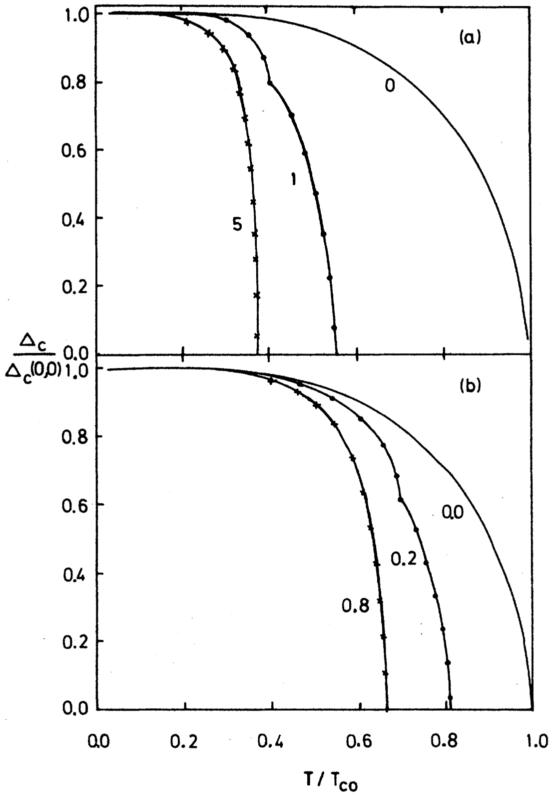

FIG. 4. Order parameter of the CDW state $\Delta_C(T,\Gamma)$. (a) and (b) correspond to $T_S/T_{C0}-0.4$ and 0.7, respectively. The parameter is γ/Δ_{C0}.

the equation for the order parameter

$$\Delta_C(\Gamma,T)=\frac{1}{2}N(\varepsilon_F)\lambda_C \times\int_0^{\varepsilon_F}d\omega\,\mathrm{Re}\left[\frac{1}{(u^2-1)^{1/2}}\right]\tanh\left[\frac{\beta\omega}{2}\right], \quad (12)$$

where $u=\tilde{\omega}/\tilde{\Delta}=(\omega/\Delta)+i(\Gamma/\Delta)u/(u^2-1)^{1/2}$. Some results for $\Delta_C(T,\Gamma)$ are shown in Fig. 4. We write $\Gamma=\gamma(T/T_{C0})^2 2f(\Delta_S)$ and parametrize the curves by the values of γ/Δ_{C0}; T_{C0} is the CDW transition temperature for $\gamma=0$, $\Delta_{C0}=\Delta_C(0,0)$. As for the scattering time τ, taking $\gamma=1$ and $T_{C0}=225$ K we get $1/\tau\sim10^9T^2\times2f(\Delta_S)\sec^{-1}\mathrm{K}^{-2}$. For Cu metal, the recent measurement of the radio-frequency size effect gives $1/\tau_{\exp}=0.33\times10^6\sec^{-1}\mathrm{K}^{-2}$.[16] The smaller scattering rate in Cu metal can be due to screening effects. Of particular interest is the case $T_S/T_{C0}=0.4$ corresponding to BCS and CDW gaps $2\Delta_{S0}=3.5k_BT_S$ and $2\Delta_{C0}=8.8k_BT_{C0}$, respectively. For $\gamma=5$, we have $T_S\sim T_C$; the pair-breaking effect is suppressed at the onset of superconductivity in the plane to allow for the formation of the CDW state. The resulting Δ_C vs T curve increases much faster below T_C than the BCS gap function ($\gamma=0$) (see Fig. 4).

III. CDW VERSUS BCS RESPONSE

We wish to compare the T and ω_0 dependences of some response functions between the BCS and CDW states, taking into account the different coherence factors of the two states and the effect of $\Gamma(T)$.

For the NMR and NQR relaxation rates, the perturbation for single-particle scattering is

$$U=\sum_{\substack{-p_F\le p,p'\le p_F\\ \sigma,\sigma'}}\Big[B_{\mathbf{p}'+Q/2,\sigma';p+Q/2,\sigma}c^\dagger_{\mathbf{p}'+Q/2,\sigma'}c_{\mathbf{p}+Q/2,\sigma}+B_{\mathbf{p}'-Q/2,\sigma';\mathbf{p}-Q/2,\sigma}c^\dagger_{\mathbf{p}'-Q/2,\sigma'}c_{\mathbf{p}-Q/2,\sigma} +\text{two corresponding terms with } \mathbf{p}'\leftrightarrow\mathbf{p}\Big]. \quad (13)$$

For the magnetic relaxation rate R, the matrix element B is determined by the contact interaction for the Cu^{2+} nuclei, due to the hyperfine coupling or the core polarization effect. For fliping down the nuclear spin,

$$B_{\pm Q/2,\uparrow;\pm Q/2,\downarrow}=(A/2)(m-1|I_-|m)(\tfrac{1}{2}|S_+|-\tfrac{1}{2}),$$

where A is the contact coupling parameter for the electrons at $\pm p_F$, m is the nuclear-spin quantum number, and I and S are the nuclear and electron spins, respectively. For the quadrupole relaxation Q, the matrix element B is determined by the quadrupole Hamiltonian H_{quad}. There is no spin conservation and

$$B_{\pm Q/2,\sigma;\pm Q/2,\sigma}=(\pm Q/2,\sigma,m'|H_{\text{quad}}|\pm Q/2,\sigma,m).$$

The matrix elements are evaluated by Mitchell.[17] Let us assume that one nuclear transition $m'\rightarrow m$ dominates the relaxation processes. In the case of ^{63}Cu, $I=\frac{3}{2}$ and $m=\frac{1}{2}$, $m'=-\frac{1}{2}$.[5] The matrix element is independent of spin σ and we take $B_{Q/2,Q/2}=B_{Q/2,-Q/2}$.

The relaxation rates for a BCS superconductor, normalized with respect to the normal state,

$$\left.\begin{array}{l}R_s/R_N\\ Q_s/Q_N\end{array}\right\}=2\int_{\Delta_S}^{\infty}N(E)N(E+\omega_0)\left[1\pm\frac{\Delta_S^2}{E(E+\omega_0}\right]\left[-\frac{\partial f_0}{\partial E}\right]dE, \quad (14)$$

are to compared with the corresponding rates for the CDW state,

$$\frac{R_C}{R_N}=\frac{Q_C}{Q_N}=2\int_0^{\infty}\mathcal{N}(\omega)\mathcal{N}(\omega+\omega_0)\left[-\frac{\partial f_0}{\partial\omega}\right]d\omega. \quad (15)$$

Here $N(E)$ is the BCS density of states normalized with respect to that of the normal state and accounting for a finite breadth of the quasiparticle states due to anisotropy in the energy gap or to lifetime effects caused by impurity and thermal phonon scattering,

$$N(E)=(2\delta)^{-1}\int_{E-\delta}^{E+\delta} d\varepsilon\,\varepsilon/(\varepsilon^2-\Delta_S^2)^{1/2} .$$

The density of states for the CDW state, $\mathcal{N}(\omega)=\mathrm{Re}[u/(u^2-1)^{1/2}]$. For the T dependences of R and Q in the BCS state shown in Fig. 5, we choose the value of $\delta/\Delta_S(T)=0.2$ so that the coherence enhancement of R_S/R_N is reduced to 1.8. The quadrupole relaxation rate Q_S/Q_N drops with infinite slope below T_S, corresponding to case I of BCS.[18]

A sharp decrease of the nuclear-spin-lattice relaxation data is observed below T_S by different experimenters and is attributed to a gap ratio of the order of 9 (Warren *et al.*,[2] Mali *et al.*,[2] Kitaoka *et al.*,[3] and Markert *et al.*[3]). We attribute this large gap to the appearance of a linear CDW and not to superconductivity. The large gap can occur either in the chain or in the plane. In the first case, the formation of the CDW occurs as the usual Peierls-type transition. The results obtained here also remain valid in the second case[5] where a different mechanism can be responsible for the linear CDW of a two-dimensional energy band. The only difference is that the *e-e* scattering rate of the normal state $1/\tau$ can be different from T^2. The formation of the CDW state in the plane becomes possible when the *e-e* pair breaking effect is suppressed by the superconductivity in the plane. In any case, the CDW state is also felt by the Y ions because Markert *et al.*[3] observed a large gap ratio (~ 11) in the magnetic spin-lattice relaxation of the spin-$\frac{1}{2}$ yttrium nuclei. The conduction electrons near the Y sites which cause the nuclear-spin relaxation via the core-polarization effect do not have spatial overlap with the superconducting electron system in the CuO_2 planes. Otherwise the substitution of ^{89}Y by magnetic ^{170}Yb ions would have some effect on the planar superconductivity. There is no significant effect on T_S and Mössbauer absorption measurements show magnetic ordering of the Yb sublattice at the very low temperature of 0.35 K.[19] For these reasons the large gap near the Y sites is probably caused by a change of the electronic structure at or near T_S, and not by superconductivity.

We mention that no experimenter so far has observed an enhancement peak of R_S/R_N below T_S at the Cu sites

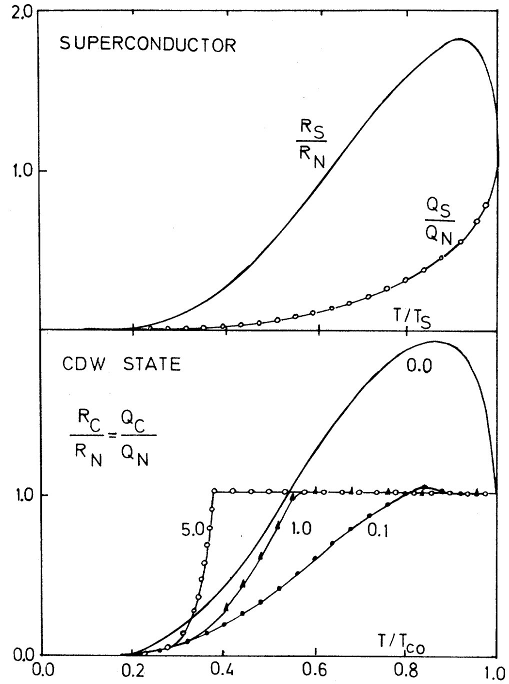

FIG. 5. Comparison between nuclear magnetic and quadrupole spin-lattice relaxation for a superconductor and for a charge-density-wave state.

(Fig. 5). The absence of this peak is expected if quadrupole relaxation processes dominate or, in the case of magnetic relaxation, if the breadth effect or if spin-fluctuation effects are sufficiently strong.

Finally, we obtain the ac conductivity that governs the absorption of the low-frequency electromagnetic radiation in the presence of a CDW. For a BCS superconductor the real part of the conductivity, $\sigma_{1S}(\omega_0)/\sigma_N$ at $T=O$, has a δ-function peak at $\omega_0=0$ due to the Meissner effect, and a contribution from quasiparticle excitations across the gap, corresponding to case II of BCS. In contrast, for a CDW state there is no Meissner effect and the response function can refer to a longitudinal vector potential.[20] The frequency-dependent conductivity $\sigma_{1C}(\omega_0)$ has a δ-function part at $\omega_0=0$, due to the unpinned collective mode, and a single-particle contribution from interband transitions. In the presence of pair breaking, the interband conductivity can be found from Ref. 20; the result is

$$\frac{\sigma_{1C}(\omega_0)}{\omega_p^2}=\frac{1}{4\pi\omega_0\Delta_C}\left\{\mathrm{Im}\int_{\Omega_C}^{\infty}dx\left[\frac{1+A_+A^*-BB^*}{C^*-C_++i\tilde{\Gamma}}+\frac{1-A_+A+B_+B}{C+C_+-i\tilde{\Gamma}}\right]\left[\tanh\left(\frac{\beta(x+\omega_0)}{2}\right)-\tanh\left(\frac{\beta x}{2}\right)\right]\right.$$
$$\left.+\mathrm{Im}\int_{\Omega_C-\omega_0}^{-\Omega_C}dx\left[\frac{1+A_+A^*-B_+B^*}{C^*-C_++i\tilde{\Gamma}}+\frac{1-A_+A+B_+B}{C+C_+-i\tilde{\Gamma}}\right]\tanh\left(\frac{\beta(x+\omega_0)}{2}\right)\right\}. \qquad (16)$$

Here

$$A=u(x+i\delta)/[u^2(x+i\delta)-1]^{1/2},\ B=1/[u^2(x+i\delta)-1]^{1/2},\ C=[u^2(x+i\delta)-1]^{1/2},\ \tilde{\Gamma}=\Gamma/\Delta_C,\ \omega_p^2=4\pi ne^2/m ,$$

where the plasma frequency ω_p depends on the electron density $n(\mathrm{cm}^{-3})$. The energy gap is given by $\Omega_C=\Delta_C[1-(\Gamma/\Delta_C)^{3/2}]^{2/3}$. For $\Delta_C=0$, we get the dc conductivity $\sigma_N=2ne^2/\Gamma m$. In the limit $T\to 0$, Eq. (16) gives the re-

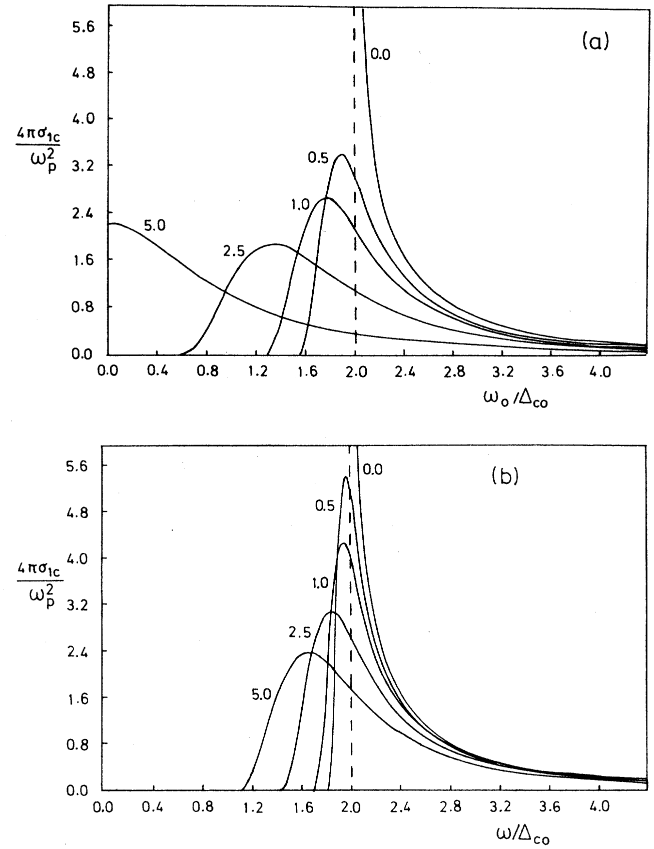

FIG. 6. (a) The real part of the interband conductivity in the absence of superconductivity ($T_S/T_{C0}=0$) for the temperature $T/T_{C0}=0.3$. The parameter is γ/Δ_{C0}. (b) The effect of superconductivity $T_S/T_{C0}=0.4$.

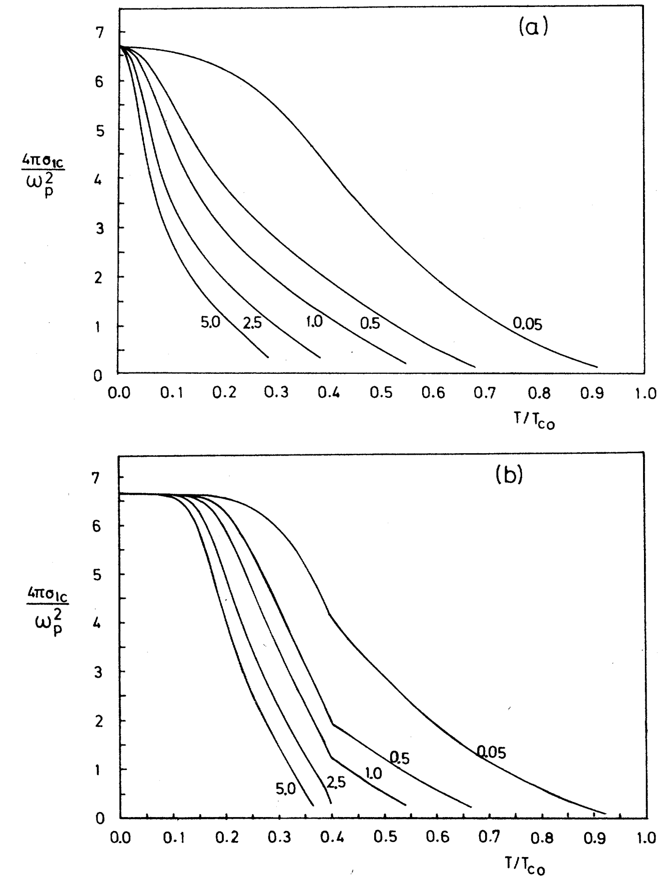

FIG. 7. The temperature dependence of $\sigma_{1C}(\Gamma)$ at $\omega_0=2.05\Delta_{C0}$ in (a) the absence and (b) presence of superconductivity.

sult of Lee, Rice, and Anderson,[21]

$$\sigma_{1C}(\omega_0)=(2ne^2\Delta_C^2/m\omega_0^2)/(\omega_0^2-\omega^2)^{1/2}.$$

The pair-breaking effect on the interband conductivity in the *absence* of superconductivity is seen in Fig. 6(a), where $\sigma_{1C}(\omega_0)/\omega_p^2$ is plotted for a fixed temperature. By comparison, the effect of superconductivity is shown in Fig. 6(b). We see how the suppression of the pair-breaking effect in the superconducting state narrows the σ_{1C} curves towards those for $\gamma=0$ at a finite value of T. The temperature dependence of σ_{1C} for a fixed frequency above the gap in the presence and absence of superconductivity in the plane is shown in Figs. 7(a) and 7(b), respectively.

IV. DISCUSSION

We study the T-dependent pair-breaking effect on the formation of a linear and commensurate CDW caused by Coulomb scattering of the 1D electrons by the electrons in the plane. We assume that we are dealing with two different electron systems, separated in coordinate *or* momentum space. The first case holds for the chain electrons which have no direct overlap with the electrons in the plane. The second case can apply to the **k** space near the FS of the 2D band shown in Fig. 1. The **k**-space "pockets" near the *saddle points* at the corners of the square can lead to a singular behavior of the wave-vector-dependent susceptibility $\chi(\mathbf{q}\sim\mathbf{Q})$, where $\mathbf{Q}$ connects two saddle points. The Fermi-surface topology of our 2D system is similar to that of layer compounds where a CDW instability due to "nesting" of saddle-point pockets is suggested by Rice and Scott.[22] This mechanism can cause the large gap at the Cu(2) sites observed in recent NMR and NQR experiments.

The order parameter for the CDW state exhibits a steep increase below T_C if due to pair breaking $T_C\sim T_S$. The gap Ω_C, measured by optical absorption, approaches Δ_C when the onset of superconductivity freezes out e-e scattering, as is seen in Fig. 3.

To distinguish between BCS and CDW states, the results for some response functions are compared in Figs. 5–7. Whereas the T dependences of the NMR and NQR relaxation rates are different for a BCS superconductor (cases I and II, respectively), they are found to be the same for the CDW state (Fig. 5). The enhancement of $R_C/R_N=Q_C/Q_N$ is suppressed by a weak-pair-breaking effect $\gamma=0.1$. For a larger value of the parameter $\gamma \sim 5$, the ratio remains flat below T_{C0} until a steep decrease occurs at the onset of superconductivity.

The optical conductivity $\sigma_1(\omega_0)$ determines the absorption of an electromagnetic wave of frequency ω_0. For a BCS superconductor at $T=0$, the Mattis-Bardeen result for $\sigma_{1S}(\omega_0)/\sigma_N$ rises from zero with finite slope at $\omega_0=2\Delta_{S0}$ and slowly approaches one for large values of ω_0 (coherence case II).[23] In contrast, the optical conductivity for single-particle excitations in the CDW state exhibits a square-root singularity at $\omega_0=2\Delta_{C0}$ that, for finite values of γ, becomes a peak that broadens as γ increases (Fig. 6). In the presence of the superconducting state in the plane, the peaks sharpen due to the freezing out of pair breaking. The temperature dependence of $\sigma_{1C}(\Gamma)$ (Fig. 7) also shows the suppression of pair breaking when the plane becomes superconducting at $T_S \sim 0.4 T_{C0}$.

ACKNOWLEDGMENTS

We would like to thank H. J. Schulz and J. Sprengel for useful comments and H. Appel and A. Kitz for their help with the numerical work. Financial support from the Deutsche Forschungsgemeinschaft is gratefully acknowledged. One of us (J.C.S.) is grateful to the I. Institut für Theoretische Physik, Universität Hamburg for its hospitality and to the Universität Hamburg—Indiana University Exchange Program for financial support making possible a visit to Hamburg. J.C.S. was also supported by National Science Foundation Grant No. DMR 8701583.

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