Competition of pairing and Peierls–charge-density-wave correlations in a two-dimensional electron-phonon model

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Monte Carlo simulations are used to investigate the competition between superconducting and Peierls–charge-density-wave (CDW) correlations in a two-dimensional electron-phonon system. The dependence of these correlations on the band filling $\langle n \rangle$, phonon frequency ω_0, and electron-phonon coupling g is examined. The Peierls-CDW correlations are favored as $\langle n \rangle$ moves towards half-filling, ω_0 decreases, and g increases. When the Peierls-CDW correlations are weak, the Monte Carlo results for the superconducting correlations are found to be in excellent agreement with the results obtained using the well-known Eliashberg approximation.

The relationship between superconductivity and insulating phases such as the Peierls-CDW phase is not yet fully understood. In general they compete, such that the onset of strong correlations of one kind suppresses the development of correlations of the other kind. However, near the boundary between the phases, both types of correlations must be taken into account. In order to obtain a better understanding of this competition, we have carried out Monte Carlo simulations for a two-dimensional (2D) electron-phonon (Holstein) model. Here we present results showing how the strength of the pairing and CDW correlations vary with the band filling, the bare phonon frequency,[1] and the electron-phonon coupling strength. We compare the Monte Carlo results for pairing with the well known Eliashberg approximation[2] and find that when the Peierls-CDW response is weak, the Eliashberg approximation is remarkably accurate.

In the Holstein model the one-electron site energy is coupled to the displacement of an Einstein phonon

$$H = -t \sum_{i,j,\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) - \mu \sum_{i\sigma} n_{i\sigma} + g \sum_i (b_i^\dagger + b_i) n_i + \omega_0 \sum_i b_i^\dagger b_i \; . \tag{1}$$

Here, $c_{i\sigma}^\dagger$ creates an electron of spin σ on site i, and $b_i^\dagger$ is the creation operator for a local phonon mode of bare frequency ω_0 located at site i. The electrons have a one-electron overlap t between near-neighbor sites on a square lattice, μ is the chemical potential which determines the band filling, and g is the electron-phonon coupling constant.

The basic electron-electron interaction arises from the exchange of phonons and in lowest-order perturbation theory is given by

$$V(i\omega_m) = -\frac{2g^2\omega_0}{\omega_m^2 + \omega_0^2} \tag{2}$$

with $\omega_m = 2m\pi T$. This interaction is attractive, giving rise to the possibility of a Peierls-CDW or a superconducting state. For the simple square lattice with a near-neighbor one-electron overlap, the single-particle band energies are given by

$$E_k = -2t(\cos k_x + \cos k_y) \; ,$$

and for a half-filled band $<n>=1$, the Fermi surface is perfectly nested. For ω_0/t finite, this leads to a low-temperature Peierls-CDW insulating phase. When the system is doped away from half-filling, it has the possibility of becoming superconducting, depending upon the band filling $<n>$, the phonon frequency ω_0/t, and the relative strength of the coupling $g^2/\omega_0 t$.

One measure of the strength of the superconducting correlations is the pair-field susceptibility

$$\chi_{SC} = \frac{1}{N} \int_0^\beta d\tau \langle \Delta(\tau) \Delta^\dagger(0) \rangle \; , \tag{3}$$

with

$$\Delta^\dagger = \sum_P c_{p\uparrow}^\dagger c_{-p\downarrow}^\dagger = \sum_l c_{l\uparrow}^\dagger c_{l\downarrow}^\dagger \; . \tag{4}$$

In an infinite system, χ_{SC} would diverge at the superconducting transition temperature. For the 2D system we are considering, this is expected to be a Kosterlitz-Thouless[3]-type transition. Here we will study χ_{SC} on finite 2D lattices, at temperatures above the superconducting transition. In this case, χ_{SC} serves as a probe of the strength of the pair-field correlations and their dependence on g, ω_0, and the band filling.

When the Peierls-CDW correlations are negligible and $\omega_0/8t$ is small, we expect that the Eliashberg[2]-Migdal[4] approximation for χ_{SC}, shown in Fig. 1, will be useful. This is the same type of approximation used by Eliashberg for $T \le T_c$. We will use it to calculate χ_{SC} above T_c. Here the bare phonon propagator of Eq. (2) is used, and vertex corrections are neglected. The electron self-energy is then

$$[1-Z(\omega_n)]i\omega_n=\frac{T}{N}\sum_{n'p}\frac{1}{Z(\omega_{n'})i\omega_{n'}-\epsilon_{p'}}\frac{2g^2\omega_0}{(\omega_{n'}-\omega_n)^2+\omega_0^2} , \tag{5}$$

and χ_{SC} is given by

$$\chi_{SC}=\chi_{SC}^0-\left[\frac{T}{N}\right]^2\sum_{np}\sum_{n'p'}\frac{1}{Z^2(\omega_{n'})\omega_{n'}^2+\epsilon_{p'}^2}t(\omega_{n'},\omega_n)\frac{1}{Z^2(\omega_n)\omega_n^2+\epsilon_p^2} , \tag{6}$$

with

$$\chi_{SC}^0=\frac{T}{N}\sum_{np}\frac{1}{Z^2(\omega_n)\omega_n^2+\epsilon_p^2} \tag{7}$$

and

$$t(\omega_{n'},\omega_n)=-\frac{2g^2\omega_0}{(\omega_{n'}-\omega_n)^2+\omega_0^2}+\frac{T}{N}\sum_{n''}\frac{1}{Z^2(\omega_{n''})\omega_{n''}^2+\epsilon_{p''}^2}\frac{2g^2\omega_0}{(\omega_{n''}-\omega_{n'})^2+\omega_0^2}t(\omega_{n''},\omega_n) . \tag{8}$$

Here, $\omega_n=(2N+1)\pi T$,

$$\epsilon_p=-2t(\cos p_x+\cos p_y)-\mu ,$$

and p sums over the Brillouin zone for an N site lattice. The chemical potential μ is adjusted to give the desired band filling taking Z into account self-consistently. We have solved these equations on finite lattices ranging from 4×4 to 64×64. For the temperature range $T/t\ge0.2$ considered here, an 8×8 lattice is sufficient. The solid lines in Figs. 2(a)–2(c) show the results obtained for χ_{SC} by solving Eqs. (5)–(8) with a band filling of 2/5 (e.g., $\langle n_{i\uparrow}+n_{i\downarrow}\rangle=0.8$). Here and in the following figures we will measure energies in units of t. Figure 2 shows χ_{SC} versus T for an electron-phonon coupling $g=1$ and three different phonon frequencies.

As the phonon frequency ω_0 decreases, the interaction is increasingly retarded, and the Peierls-CDW correlations can become stronger than the pairing correlations.[5]

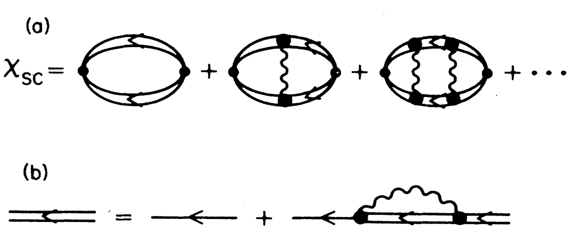

FIG. 1. (a) Eliashberg approximation for the superconducting pair field susceptibility χ_{SC}. Here the wavy line represents the bare phonon propagator, the double straight lines the electron propagator dressed within the Migdal approximation shown in (b) and the single straight line is the bare electron propagator.

This can be understood, in weak coupling, by noting that the $\omega_m=0$ limit of the electron-phonon interaction, Eq. (2), enters in calculating χ_{CDW} while finite frequencies $\omega_m\neq0$ are exchanged in the ladder graphs, Eq. (8), contributing to χ_{SC}. The interaction, Eq. (2), is clearly most attractive for $\omega_m=0$ and becomes weak when ω_m exceeds ω_0. The CDW susceptibility

$$\chi_{CDW}=\frac{1}{N}\int_0^\beta d\tau\langle\rho_q(\tau)\rho_q^\dagger(0)\rangle , \tag{9}$$

with

$$\rho_q^\dagger=\sum_{ls}e^{iq\cdot l}n_{ls} , \tag{10}$$

provides a measure of the strength of the Peierls-CDW correlations. These correlations lead to important modifications of both the phonon propagator and the electron self-energy. In the crossover regime it becomes necessary to treat both the pairing and Peierls-CDW channels on an equal footing. In order to explore these questions, we have carried out Monte Carlo calculations of χ_{SC} and χ_{CDW}. For a half-filled band, χ_{CDW} peaks at $\mathbf{q}^*=(\pi,\pi)$ corresponding to the staggered charge density

$$\rho_{q^*}=\sum_{ls}(-1)^l n_{ls} .$$

As the band filling moves away from half-filling, q^* initially remains locked at (π,π). On an 8×8 lattice, this locking occurs for $\langle n\rangle\ge0.8$, and throughout this work[6] we will show χ_{CDW} for $q^*=(\pi,\pi)$. The details of the Monte Carlo technique we use have been described elsewhere,[7] and we will turn directly to the results.

Figures 2(a)–2(c) show Monte Carlo data for χ_{SC} (solid dots) and χ_{CDW} (π,π) (triangles) versus T. At high frequencies, such as the $\omega_0=2$ data shown in Fig. 2(a), the

Monte Carlo results for χ_{SC} are in excellent agreement with the predictions (solid line) obtained by solving the Eliashberg equations for an 8×8 lattice. As previously discussed,[1] the Eliashberg results are suppressed beneath the noninteracting $g=0$ values at high temperatures, but then cross over and are enhanced over the noninteracting

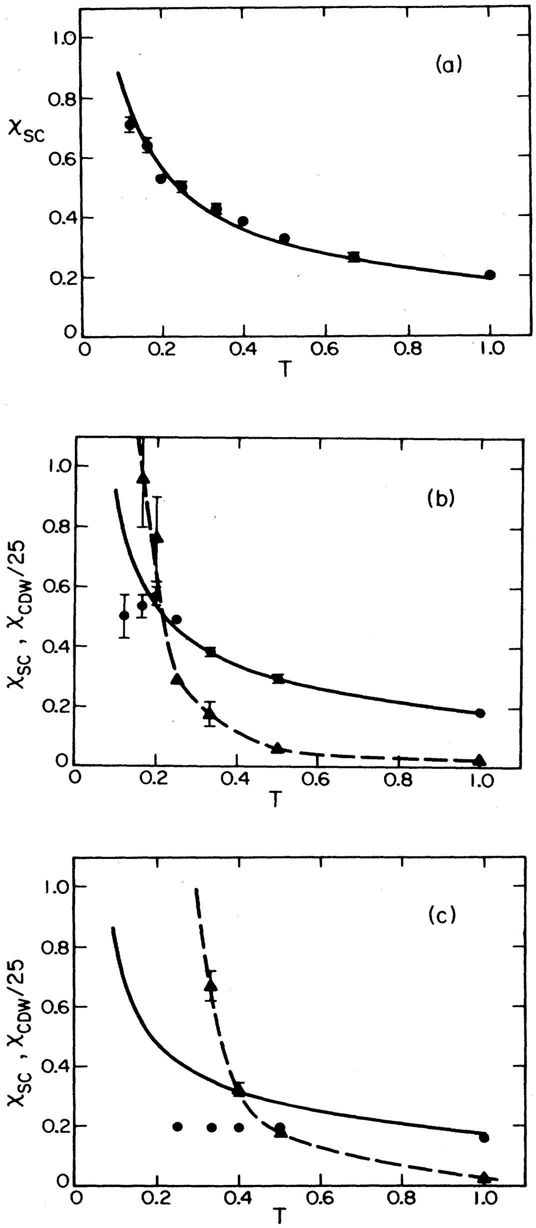

FIG. 2. (a) χ_{SC} vs T for $\langle n \rangle = 0.8$, $g=1$, and $\omega_0=2$. The solid points are Monte Carlo data and the solid line is the solution of the Eliashberg equations on an 8×8 lattice. (b) The same parameters as in (a) except $\omega_0 = 1.0$. Here the triangles are Monte Carlo results for $\chi_{CDW}/25$. The dashed line through the CDW points is a guide to the eye. (c) Similar to (b) with $\omega_0 = 0.5$.

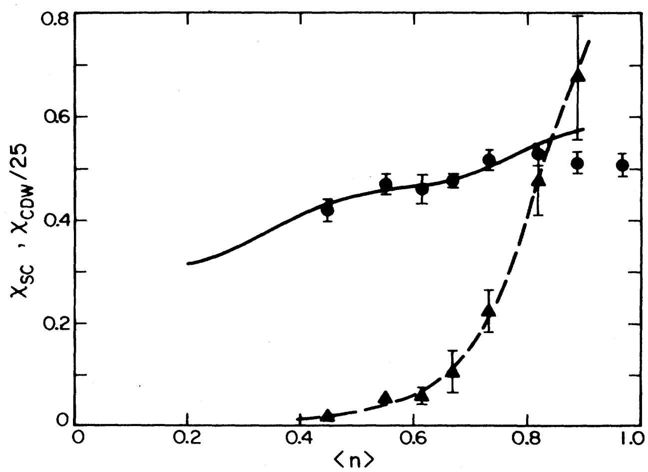

FIG. 3. χ_{SC} and $\chi_{CDW}/25$ vs $\langle n \rangle$ on an 8×8 lattice for $T=0.2$, $g=1$, and $\omega_0=1$. The solid line is the Eliashberg result, and the dashed line through the CDW points is a guide to the eye.

values at low temperatures. For $\omega_0=2$, the CDW response is weak and temperature independent. One might worry about the neglect of vertex corrections when ω_0 is large, but it appears from these results that as long as χ_{CDW} is not large, the Eliashberg approximation is quite adequate. In Fig. 2(b), ω_0 is reduced by a factor of 2 ($\omega_0 = 1.0$), and now, as the temperature is lowered, χ_{SC} initially follows the Eliashberg behavior until χ_{CDW} becomes large. At this point the Peierls-CDW correlations become dominant and the superconducting correlations are suppressed. Lowering ω_0 by another factor of 2 leads to a situation in which the Peierls-CDW correlations are dominant over the entire temperature regime, as shown in Fig. 2(c).

At large values of ω_0/t, the electron-electron interaction is effectively instantaneous, and in the limit $\omega_0/t \gg 1$ with $g^2\omega_0$ finite, one has a negative-U model. This follows simply from the fact that when $\omega_0/t \gg 1$, the band-

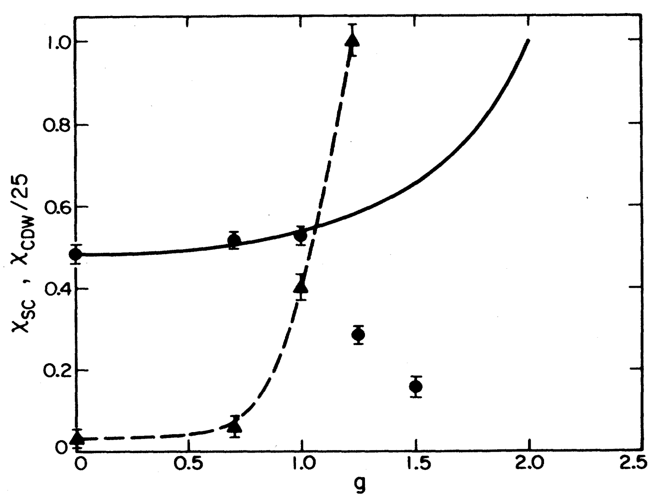

FIG. 4. χ_{SC} and $\chi_{CDW}/25$ vs g on an 8×8 lattice for $T=0.2$, $\langle n \rangle = 0.8$, and $\omega_0 = 1$.

width sets the cutoff and the phonon exchange is equivalent to a negative effective U equal to $-2g^2\omega_0$. At half-filling, the 2D negative-U model has $T_c=0$ and a ground state with both long-range CDW and pairing correlations. When a negative-U system is doped away from half-filling, the superconducting correlations dominate with a finite Kosterlitz-Thouless transition and the CDW correlations are short range.[8] However, as ω_0/t is reduced and retardation becomes important, a region of filling around the half-filled band is dominated by CDW correlations. The dependence on the band filling $\langle n \rangle$ is shown in Fig. 3 where χ_{SC} and χ_{CDW} are plotted versus $\langle n \rangle$ for $g=1$, $\omega_0=1$, and $T=0.2$. Well below half-filling, χ_{SC} follows the Eliashberg result, but as one approaches half-filling, strong Peierls-CDW correlations develop, leading to a suppression of the pairing correlations. Again, it is interesting to see how well the Eliashberg approximation does until the Peierls-CDW correlations become dominant. Figure 4 shows a similar plot versus the coupling constant g. Here $\langle n \rangle=0.8$, $\omega_0=1$, and $T=0.2$. As g increases, the superconducting susceptibility initially increases and then is suppressed when χ_{CDW} becomes large.

These results clearly show the competition between pairing and Peierls-CDW correlations which can occur in a 2D Holstein model. When the photon frequency is lowered, g increased, or $\langle n \rangle$ moved closer to half-filling, the Peierls-CDW correlations can become dominant. When they are not, we find that the Eliashberg equations provide a useful approximation[9] for χ_{SC}.

ACKNOWLEDGMENTS

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