# Charge-Density-Wave and Pairing Susceptibilities in a Two-Dimensional Electron-Phonon Model

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We present quantum Monte Carlo results for a two-dimensional electron-phonon model. At half filling, a Peierls–charge-density-wave (CDW) instability dominates the behavior of the system and suppresses superconductivity. The CDW structure factor scales with system size and is consistent with a finite-size Ising-like scaling analysis which we use to estimate $T_c$ for the Peierls-CDW transition. Away from half filling, the Monte Carlo calculations show superconducting pairing in an $s$-wave channel, with a peak in the pair field susceptibility near a region in which there are strong Peierls-CDW correlations.

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$BaBiO_3$ has a Peierls–charge-density-wave (CDW) structural instability which disappears as one dopes with K or Pb to get the superconductors $Ba(Pb,Bi)O_3$ or $(Ba,K)BiO_3$.[1] Here we use quantum Monte Carlo simulations to explore the interplay of a Peierls-CDW instability and superconductivity in a two-dimensional electron-phonon Holstein model.[2] While the $BaBiO_3$ system is three dimensional, our two-dimensional system is more readily simulated and also exhibits a metal-insulator transition associated with a Peierls-CDW instability at half filling. In two dimensions at half filling, the Peierls-CDW transition is expected to be Ising-like while a superconducting transition should have Kosterlitz-Thouless[3] character. We present evidence that superconductivity is suppressed in the region with strong Peierls-CDW order, but that near the metal-insulator transition, there is superconducting pairing with a peak in the superconducting response. We find that the pair field susceptibility away from the region of the metal-insulator transition is sensibly approximated within the Eliashberg framework[4] and lays below the Eliashberg result for all values of the doping.

The Holstein Hamiltonian,

$$H=-t\sum_{\langle lm\rangle,\sigma}(c_{l\sigma}^\dagger c_{m\sigma}+\text{H.c.})+\omega_0\sum_l a_l^\dagger a_l -\mu\sum_{l,\sigma}n_{l\sigma}+g\sum_{l,\sigma}n_{l\sigma}(a_l^\dagger+a_l)\,, \tag{1}$$

consists of a one-electron hopping term with overlap integral $t$, Einstein phonons of frequency $\omega_0$, and an interaction which couples the on-site phonon displacement and the site charge density. The sum in the hopping term is over the set of nearest-neighbor sites on a two-dimensional square lattice. The $c_{l\sigma}$ are fermion annihilation operators on a site $l$ with spin $\sigma$, $n_{l\sigma}=c_{l\sigma}^\dagger c_{l\sigma}$, and the $a_l$ are phonon annihilation operators at site $l$. The chemical potential $\mu$ sets the band filling, and $g$ is the electron-phonon coupling constant. Since we are interested in the superconducting and CDW responses of the system, we will consider the $s$-wave superconducting pair susceptibility,

$$P_s=\frac{1}{N}\int_0^\beta d\tau\langle\Delta(\tau)\Delta^\dagger(0)\rangle\,, \tag{2}$$

where

$$\Delta^\dagger=\sum_l c_{l\uparrow}^\dagger c_{l\downarrow}^\dagger\,, \tag{3}$$

and the charge-density structure factor,

$$S(q)=(1/N)\langle\rho_q\rho_q^\dagger\rangle\,, \tag{4}$$

where

$$\rho_q^\dagger=\sum_{l,\sigma}e^{i\mathbf{q}\cdot\mathbf{l}}c_{l\sigma}^\dagger c_{l\sigma}\,. \tag{5}$$

$N$ is the number of lattice sites.

For the half-filled system, the nesting of the Fermi surface for a wave vector $\mathbf{Q}=(\pi,\pi)$ and the Van Hove singularity in the density of states, $N(\varepsilon)\simeq(1/2\pi^2t)\times\ln(16t/\varepsilon)$, lead to a Peierls-CDW instability. In the presence of a next-nearest-neighbor hopping $t'$, this Van Hove logarithmic singularity is shifted to $\varepsilon=4t'$ which can lead to an enhanced pairing response.[5] Here we will focus on the $t'=0$ model.

The simplest approximation that allows one to calculate some properties of the half-filled Peierls-CDW state is a mean-field approximation with a staggered phonon displacement

$$g\langle(a_l^\dagger+a_l)\rangle=\Delta_{\text{CDW}}(-1)^{l_x+l_y}\,. \tag{6}$$

Here $\Delta_{\text{CDW}}$ is determined by the condition

$$\frac{4g^2}{\omega_0 N}\sum_k\frac{\tanh(\beta E_k/2)}{2E_k}=1\,, \tag{7}$$

where $E_k=(\varepsilon_k^2+\Delta_{\text{CDW}}^2)^{1/2}$ with $\varepsilon_k=-2t(\cos k_x+\cos k_y)$. The mean-field critical temperature is obtained from this expression by calculating the $T_c$ at which $\Delta_{\text{CDW}}$ first becomes nonzero. In two dimensions,

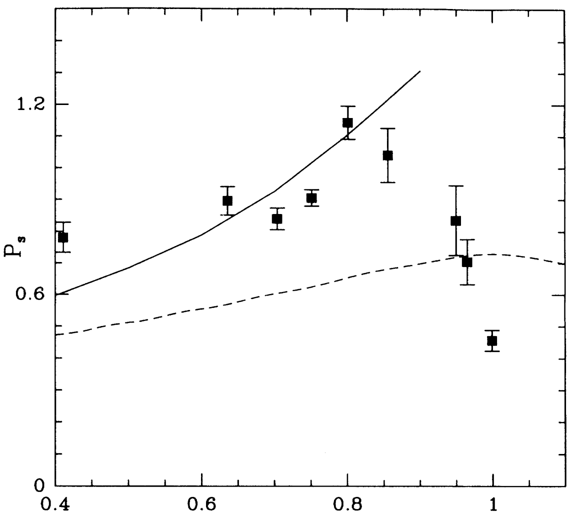


FIG. 1. The $s$-wave pair susceptibility as a function of band filling for an $8\times8$ lattice with $g=1$, $\omega_0=1$ at $\beta=12$. The squares are Monte Carlo data, the solid line shows results obtained from an Eliashberg calculation, and the dashed line gives the noninteracting susceptibility.

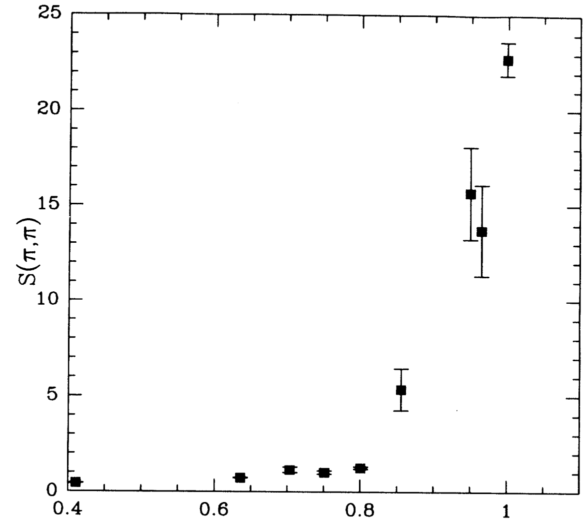


FIG. 2. The CDW structure factor $S(\pi,\pi)$ as a function of filling $\langle n\rangle$, for an $8\times8$ lattice with $g=1$, $\omega_0=1$, at $\beta=12$.

we expect that fluctuations will significantly reduce the mean-field $T_c$.

In a similar manner, one can calculate superconducting properties in mean-field theory by using the well-known Eliashberg[4] approximation. As we will discuss, these calculations are in qualitative agreement with our Monte Carlo simulations at fillings below $\langle n\rangle\equiv(1/N)\times\sum_{l,\sigma}\langle n_{l\sigma}\rangle\approx0.85$, where the Peierls-CDW correlations are relatively weak. However, our Eliashberg calculations neglect the effects of the Peierls-CDW correlations.[6] Thus these results predict a finite superconducting $T_c$ at all band fillings, with the highest $T_c$ occurring at half filling, where the density of states peaks.

This work extends earlier work by Scalettar, Bickers, and Scalapino[7] and Su,[8] who used an algorithm which becomes unstable at low temperatures, severely limiting the temperature range that could be explored, as well as work by Marsiglio,[9] which treated the half-filled-band case with a stable, low-temperature algorithm. The method we use for the quantum Monte Carlo simulations is a stable low-temperature algorithm developed by White *et al.*[10] for the repulsive-$U$ Hubbard model. In the Holstein model, the phonon field couples in the same way to both the spin-up and spin-down fermions so that the product of their determinants is positive at all fillings, eliminating the fermion sign problem.[11] For this reason, the Holstein model provides a more tractable system than the repulsive-$U$ Hubbard model[10,11] in which to study the nature of the pairing correlations near a metal-insulator transition.

Here we show results for two sets of coupling constants: $g=\omega_0=1$ and $g=2$, $\omega_0=4$. Both of these couplings have the same dimensionless strength $\lambda=2|g|^2/\omega_0 D=0.25$, where $D=8t$ is the bandwidth. However, as we will see, a lower phonon frequency favors the CDW transition which dominates as the band filling approaches half filling.

Figures 1 and 2 show the pair susceptibility $P_s$ and the structure factor $S(\pi,\pi)$ as a function of band filling for an $8\times8$ lattice with $g=1$, $\omega_0=1$, at $\beta=12$. The dashed line in Fig. 1 is the noninteracting pair susceptibility and the solid line is the result of the Eliashberg calculation. Both are calculated on a $32\times32$ lattice, which is large enough to reach the bulk limit at this temperature. For $\langle n\rangle$ greater than 0.8, the structure factor shows a very strong response and $P_s$ is suppressed below the noninteracting susceptibility as $\langle n\rangle$ approaches 1. Within the momentum resolution of an $8\times8$ lattice, $S(q)$ is peaked at $q=(\pi,\pi)$ in this region. Further work on larger lattices will be required to determine how the peak in $S(q)$ shifts with doping. Here we will focus on the half-filled case, $\langle n\rangle=1$, where the peak in $S(q)$ is at $(\pi,\pi)$. In Fig. 3(a), $S(\pi,\pi)$ vs $\beta$ is shown for lattices of increasing size ($4\times4$, $6\times6$, $8\times8$). One can clearly see that above a certain value of $\beta$, $S(\pi,\pi)$ increases with system size.

At half filling, the $\mathbf{Q}=(\pi,\pi)$ CDW state breaks the translational invariance of the Hamiltonian by alternately increasing and decreasing the charge density on neighboring sites, leading to two degenerate states. Therefore, the CDW state has a two-state order parameter and is expected to be in the same universality class as the two-dimensional Ising model. Assuming this is the case, $S(\pi,\pi)$ should scale with the linear size of the lattice, $N_x$, and $\beta$ as

$$S(\pi,\pi)=N_x^{2-\eta}f(N_x(\beta-\beta_c)^{\nu})\,, \tag{8}$$

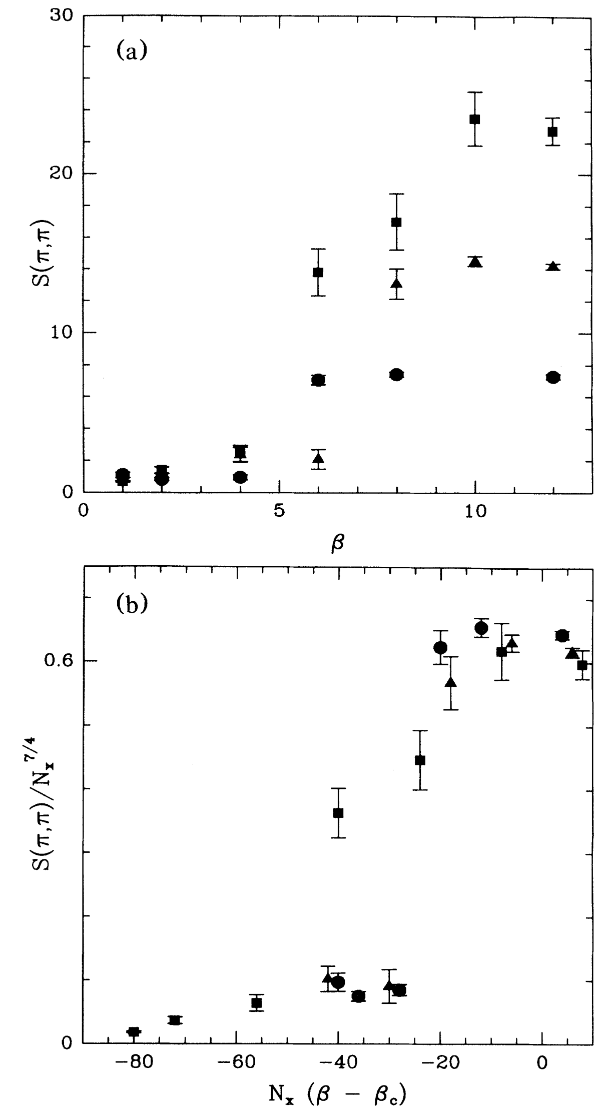


FIG. 3. (a) $S(\pi,\pi)$ as a function of $\beta$ for $g=1$, $\omega_0=1$, $\langle n\rangle=1$ (half filling) for 4×4 (circles), 6×6 (triangles), and 8×8 (squares) lattices, showing scaling with system size. (b) The data of (a) scaled with the two-dimensional Ising-model scaling relation, $S(\pi,\pi)=N_x^{7/4}f(N_x(\beta-\beta_c))$, with $\beta_c=11$.

with $\eta=\frac{1}{4}$ and $\nu=1$. Figure 3(b) shows the data of Fig. 3(a) scaled in this manner with $\beta_c=11$. This corresponds to a significantly lower transition temperature than predicted by the mean-field results, $\beta_c^{\mathrm{MF}}=1.4$, obtained from Eq. (7), reflecting the important role of fluctuations in this two-dimensional system.

As we have seen, when one dopes away from half filling, the charge-density-wave peak in $S(q)$ decreases, as shown in Fig. 2, and pairing correlations, Fig. 1, begin to develop. The superconducting order parameter has a U(1) gauge symmetry, putting the system in the same universality class as the two-dimensional $XY$ model,

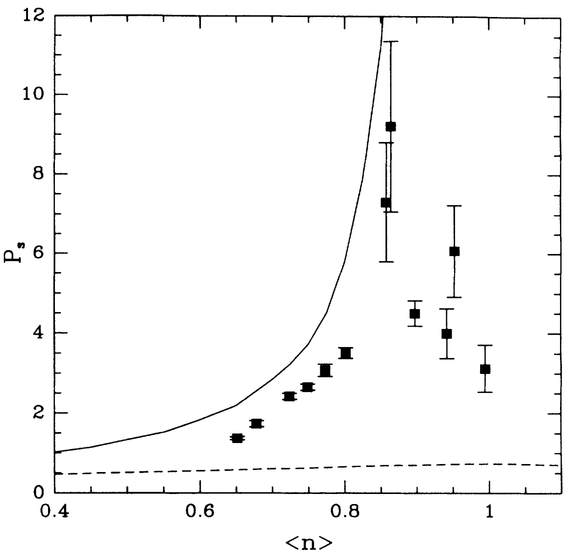


FIG. 4. The $s$-wave pair susceptibility $P_s$ as a function of band filling for $g=2$, $\omega_0=4$, and an 8×8 lattice at $\beta=12$. The squares denote Monte Carlo results, the solid line the results of an Eliashberg calculation, and the dashed line the noninteracting susceptibility.

which has a Kosterlitz-Thouless phase transition.[3] Therefore we expect the superconducting state to have a finite-temperature Kosterlitz-Thouless-like transition.

As is well known from simulations of the classical $XY$ model, such transitions are much more difficult to characterize on small systems. Thus, while we do not at present have sufficient large-lattice and low-temperature data to carry out a scaling analysis of this type of transition,[12] we can calculate the $\langle n\rangle$ dependence of the $s$-wave pair field susceptibility. Figure 4 shows Monte Carlo results for the $s$-wave pair field susceptibility versus the band filling $\langle n\rangle$ for an 8×8 lattice with $g=2$, $\omega_0=4$, at $\beta=12$. The solid line was obtained from the Eliashberg equations and the dashed line is the noninteracting pair field susceptibility. Both of these were computed on a 32×32 lattice which gives essentially the bulk limit. We find that the Eliashberg susceptibility diverges at a filling $\langle n\rangle_c\approx 0.87$. At fillings less than 0.85, the behavior of the Eliashberg susceptibility is qualitatively similar to and bounds the Monte Carlo results.

As shown in Fig. 5 for $g=2$, $\omega_0=4$, as $\langle n\rangle$ increases beyond 0.85, there is again a rapid growth of the CDW correlations. As shown in Fig. 4, these eventually suppress the pairing correlations and $P_s$ decreases. In the region where $P_s$ exhibits a maximum, we find that there is a critical slowing down of both the superconducting and CDW fluctuations, as seen from an increase in the decay time of the autocorrelation functions of the Monte Carlo data. This critical slowing down and the large fluctuations in this region are reflected in the large error bars and scatter in the Monte Carlo data at fillings be-

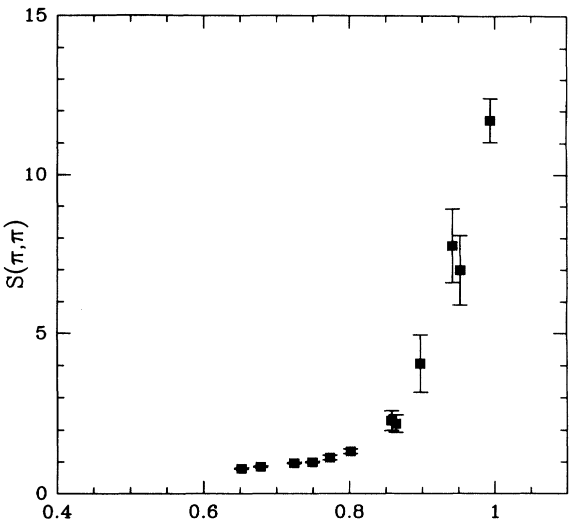


FIG. 5. The CDW structure factor as a function of band filling for $g=2$ and $\omega_0=4$, on an $8\times8$ lattice for $\beta=12$.

tween 0.85 and 0.95, as seen in Figs. 4 and 5. This supports a picture in which the pair susceptibility peaks near the region where there are strong Peierls-CDW fluctuations.

These simulations show that the Holstein model exhibits a metal-insulator transition as a function of doping. Specifically, at half filling, a finite-size scaling analysis shows the existence of a Peierls-CDW state and gives $T_c/t \approx 0.1$ for $g=1$ and $\omega_0=1$. As the system is doped away from half filling, the CDW response becomes weaker and the $s$-wave pair field susceptibility increases. When the system is doped sufficiently far away from half filling, the pair field susceptibility is in reasonable agreement with the Eliashberg result and for the parameters we have studied, the Eliashberg result lies above the Monte Carlo pair field susceptibility at all fillings. From measurements of the structure factor, it appears that the peak in the superconducting pairing response occurs at the onset of strong Peierls-CDW correlations.

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[1]D. G. Hinks, B. Dabrowski, D. R. Richards, J. D. Jorgensen, Shiyou Pei, and J. F. Zasadzinski, Physica (Amsterdam) **162–164C**, 1405 (1989).

[2]T. Holstein, Ann. Phys. (N.Y.) **8**, 325 (1959).

[3]J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).

[4]G. M. Eliashberg, Zh. Eksp. Teor. Fiz. **38**, 966 (1960) [Sov. Phys. JETP **11**, 696 (1960)].

[5]Jorge E. Hirsch and D. J. Scalapino, Phys. Rev. Lett. **56**, 2732 (1986).

[6]It is possible to carry out a coupled CDW-superconducting calculation in which the superconducting transition is suppressed at half filling [F. Marsiglio, Physica (Amsterdam) **162–164C**, 1453 (1989); Phys. Rev. B **42**, 2416 (1990); N. E. Bickers (private communication)]. Here we wanted to see whether a standard Eliashberg calculation would provide a bound on the pair field susceptibility or whether higher-order processes associated with fluctuations near the metal-insulator transition, which are picked up by the Monte Carlo simulation, could lead to a significantly enhanced pairing response.

[7]R. T. Scalettar, N. E. Bickers, and D. J. Scalapino, Phys. Rev. B **40**, 197 (1989).

[8]W. P. Su (to be published).

[9]Marsiglio, Ref. 6.

[10]E. Y. Loh, J. E. Gubernatis, R. T. Scalettar, S. R. White, and R. L. Sugar, in *Workshop on Interacting Electrons in Reduced Dimension,* edited by D. Baeriswyl and D. K. Campbell (Plenum, New York, 1989); S. R. White, D. J. Scalapino, R. L. Sugar, E. Y. Loh, J. E. Gubernatis, and R. T. Scalettar, Phys. Rev. B **40**, 506 (1989).

[11]E. Y. Loh, Jr., J. E. Gubernatis, R. T. Scalettar, S. R. White, D. J. Scalapino, and R. L. Sugar, Phys. Rev. B **41**, 9301 (1990).

[12]In the limit where $\omega_0$ is large compared to the bandwidth, the Holstein model goes over to a negative-$U$ $(U=-2|g|^2/\omega_0)$ Hubbard model. Recent simulations of the pair field susceptibility for this model have been fitted with a Kosterlitz-Thouless scaling form. [A. Moreo and D. J. Scalapino, University of California at Santa Barbara Report No. UCSBTH-90-52 (Phys. Rev. Lett., to be published).]