Density-matrix renormalization group study of pairing when electron-electron and electron-phonon interactions coexist: Effect of the electronic band structure

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(Dated: January 23, 2022)

PACS numbers: 71.10.Hf; 71.38.-k; 74.20.Mn

Introduction — The problem of what happens when the electron-electron interaction coexists with electron-phonon interaction is arousing interests from various viewpoints.1–6 In fact, there are a number of classes of materials where electron-electron (el-el) and electron-phonon (el-ph) interactions are both significant. One example is the superconducting doped fullerenes,6 where the electrons in narrow conduction bands are strongly coupled to intra-molecular, high-frequency phonons. Theoretically, a fundamental question is: can superconductivity arise in the coexistence of the el-el and el-ph interactions? It may seem difficult for them to work constructively, since the effective electron-electron attraction arising from the el-ph coupling favors isotropic pairs, while the (spin-fluctuation mediated) pairing interaction due to the el-el repulsion favors anisotropic pairs. The problem becomes especially nontrivial for a region intermediate between the adiabatic (Migdal’s) and antiadiabatic limits.

There is a theoretical reason why we have to look into the intermediate regime. Superconductivity (SC) has to compete with diagonal orders in general, and SC phases in fact often arise adjacent to density-wave phases on the phase diagram. In the present context, a strong el-ph interaction will favor a charge density wave (CDW), while a strong el-el interaction will favor a spin density wave (SDW). A metallic phase has a chance to appear around the boundary where CDW gives way to SDW, at which the el-el and el-ph interactions are indeed comparable. Takada and coworkers have in fact argued that an off-site pairing arises in a region between CDW and SDW phases, from the enhancement factors in the CDW, SDW and SC response functions in a two-site result by assuming that the two-site system is already close to the infinite system,7, and from an exact diagonalization for two- and four-site Holstein-Hubbard model at half-filling.8 However, a study for larger systems may be desirable to elaborate why and how the pairing occurs when the el-el and el-ph interactions are comparable. This region is physically interesting as the case of interacting fermions and bosons with similar energy scales, but is technically challenging as well, since we are not allowed to adopt the Migdal’s approximation for the phonon energy $\hbar \omega$ assumed to be much smaller than the electron energy scale, $t$, nor can we adopt the antiadiabatic limit ($\hbar \omega \gg t$).

We shall conclude that, (i) while the correlation functions obtained here indicate that superconductivity does not dominate over, but is nearly degenerate with the CDW correlation (a curious similarity with the behavior in purely electronic systems where the two correlations should coincide with each other when the system is electron-hole symmetric), but (ii) pairing becomes dominant when we destroy the electron-hole symmetry in a trefoil lattice. These occur in the region of interest, where the phonon-induced attraction almost cancels the electron-electron repulsion, and intermediate between the adiabatic and antiadiabatic limits. So the message here is that the coexistence of el-el and el-ph interactions can, in a manner dependent on the underlying electronic structure, give rise to pairing.
**Method** — Inclusion of the phonon degrees of freedom makes the DMRG calculation more demanding. However, Jeckelmann and White have introduced the pseudosite method\(^{[13]}\), which makes the application of DMRG to models with on-site (Einstein) phonons feasible, and charge and spin gaps have been calculated for the one-dimensional Holstein-Hubbard model\(^{[11]}\)[12].

\[
H = -t \sum_{i,\sigma} (c_{i+1,\sigma}^\dagger c_{i,\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + g \sum_{i,\sigma} n_{i\sigma} (b_i + b_i^\dagger) + \hbar \omega \sum_i b_i^\dagger b_i. \tag{1}
\]

Here \(c_{i\sigma}^\dagger\) creates an electron of spin \(\sigma\) on the \(i\)th lattice site, \(t\) is the nearest-neighbor hopping (which we take as the unit of energy hereafter), \(U\) is the on-site electron-electron repulsion, \(a_i^\dagger\) creates a phonon at \(i\), \(g\) is the on-site el-ph interaction, and \(\hbar \omega\) is the bare phonon energy. In the pseudo-site method, we consider only finite numbers of phonons at each site \((M = 2^N\) for 0-boson, 1-boson, \ldots, \(2^N - 1\)-boson states) Sites are expressed in terms of fictitious \(N\) phonon “pseudo-sites”, on top of an electron pseudo-site. The pseudo-sites are taken into the system one by one, as in real sites in conventional DMRG. Thus the maximum dimension of the Hilbert space considered in the DMRG depends only on the maximum number of retained states \(m\) and not on \(M\). We have here retained up to \(m = 600\) states in each block of the DMRG calculation for each chain with \(L = 40\) sites with \(M = 2^4\) states considered for each site.

In calculating the correlation functions, we have noticed a flaw in the conventional infinite-size DMRG algorithm, in which two new sites are inserted between two symmetrical blocks. For the Holstein-Hubbard model, the retained states when the electron pseudo-site is added tend to significantly deviate from those describing the system at later stages. This is because the electrons on the added pseudo-sites feel the bare repulsion there, while the repulsion on other sites is reduced due to the electron-phonon coupling, and this degrades the convergence. So we propose\(^{[14]}\) to remedy this by modifying the chemical potential for the electrons for the added electron pseudosites in the calculation for the ground states, so that the expectation value of the number of electrons at each of the new pseudo-sites equals those in the target state, which is unity for the half-filled band assumed here. This method, which we call the compensation method, has indeed given lower ground state energies and hence more accurate ground states and correlation functions.

**Results** — We have calculated the correlation function \(\langle O_{i}^\dagger O_j \rangle\) for \(O_i = n_{i\uparrow} + n_{i\downarrow}\) (charge), \((n_{i\uparrow} - n_{i\downarrow})/2\) (spin), \(c_i^\dagger c_j\) (on-site pair), \(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\) (nearest-neighbor spin-singlet), and \(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\) (nearest-neighbor triplet). Typical result is displayed, on double-logarithmic scales, in Fig. 1 for the cases where (A) \(U > \lambda\), (B) \(U = \lambda\), and (C) \(U < \lambda\). After the infinite-algorithm DMRG calculation is performed with the compensation method, at least three sweeps of the finite-algorithm are done.

We immediately notice the following: if we concentrate on power-law correlations, they are the charge and on-site pair correlations for \(U \lesssim \lambda\), or the spin correlation for \(U \gtrsim \lambda\), while all of the charge, spin and on-site pair correlations decay with power laws for \(U \simeq \lambda\). This is our first key result. It is interesting to compare the present correlation functions with an estimation of spin and charge gaps in the same system by Fehske et al.\(^{[12]}\). They suggested that a charge gap opens and spin gapless when \(U \gg \lambda\), both gapless when \(U \simeq \lambda\), both gapful when \(U \ll \lambda\). The former two agree with the present result. As for the latter, we can interpret that

![FIG. 1: Various correlation functions versus real-space distance in the Holstein-Hubbard model at half-filling calculated for \((\lambda, \omega) = (3.6, 5.0)\) (in units where \(t = 1, \hbar = 1\) with three values of \(U\), indicated as A,B,C in a schematic parameter space (top inset). Error bars are smaller than the size of each symbol. Only the data for \(i - j \equiv \text{odd}\) are plotted, because of an even-odd effect in correlation functions in open-boundary condition. Vertical arrows with (a),(b) correspond to the scans in Fig. 2(a)(b).](image)
Here we are looking at a region where $U$ is only moderately smaller than $\lambda$ and a spin-gapped metal can exist, for which CDW and on-site SC have power-law correlations as far as the Tomonaga-Luttinger physics \cite{12} goes.

So a next key issue is whether the exponents are solely determined by $U - \lambda$, which would be the case if the TL picture somehow holds everywhere. We have looked at its systematic dependence, and Fig. 2 plots typical behaviors. For a smaller $\lambda (\propto g^2$) the dominant correlation in Fig. 2(a) changes from the CDW/on-site SC to SDW almost exactly at the point where $U > \lambda$.

To be more precise, it is difficult, for finite systems, to distinguish whether the decay of a correlation function is power or exponential. So we have checked how the result compares with the exponent, calculated in the same way, for a purely electronic (i.e., the Hubbard) model for the same system size in Fig. 2(d). In the one-dimensional Hubbard model, the correlations that decay with a power law ($\sim 1/r$) are on-site SC and CDW for $U < 0$ (SDW for repulsive $U > 0$). In Fig. 2(d), this appears as a crossing of two, continuous curves (one of which are doubly-degenerate) at $U = 0$, and the result resembles Fig. 2(a). For finite systems we have also to be careful about the effect of discreteness of the levels (against spin and charge gaps) on the correlation function \cite{16}. We have checked that the spin gap for the levels (against spin and charge gaps) on the correlation is power or exponential. So we have checked how the systematic dependence, and Fig. 2 plots typical behaviors. For a smaller $\lambda$, as shown in Fig. 2(c) for $\omega = 2.5$. There again, CDW and on-site SC correlations both have power-decay, but they start to decay exponentially when $U$ is further decreased, signalling an opening of the charge gap $\Delta_c$ as well as spin gap $\Delta_s$. This should correspond to the region of $\Delta_c \sim \Delta_s \gg 0$ for $U \ll \lambda$ in Ref. \cite{12}. So, as we move away from the $\omega \to \infty$ limit where the spin-gapped metallic region appears for $U < \lambda$, the region becomes bounded from both below (opening of $\Delta_c$) and above (CDW-SDW crossing point). The decrease in $U - \lambda$ at the CDW-SDW crossing may be related to the effective repulsion enhanced from $U - \lambda$ as studied in \cite{17} with the dynamical mean field theory (DMFT).

If we assume, as in \cite{13}, that the Tomonaga-Luttinger (TL) theory \cite{11} applies to the present system, in a spin-gapped metal the CDW correlation should behave as $r^{-\kappa}$, while the pairing correlation $r^{1/\kappa}$, so that $\kappa > 1$ corresponds to dominant SC correlation. While the behavior of the CDW correlation with a power greater than unity is consistent with the results in \cite{18}, we also note that the power for the on-site SC is larger than that for CDW, which would not occur if the TL description persisted. Since this is observed over the entire range of $U - \lambda$, this should not be due to a finite-size effect from the above argument. So, while a deviation from the TL does exist (which is not surprising since the coupling to phonons should make the el-el interaction effectively energy-dependent), the on-site SC does not become the most dominant correlation in the region studied here. We note that this robustness of CDW against SC at half-filled Holstein-Hubbard chain, where $U$ is varied along the dashed arrows in inset of Fig. 1. Gray shadow indicates $U < 0$. (d) The result for the Hubbard model (with $\lambda = 0$), where the curves for charge and on-site SC are degenerate.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2}
\caption{Calculated powers ($\eta$) for the correlation functions ($\propto r^{-\eta}$) against $U - \lambda$ for (a) $(\lambda, \omega) = (0.4, 5.0)$, (b) $(\lambda, \omega) = (3.6, 5.0)$ and (c) $(\lambda, \omega) = (3.6, 2.5)$ in an $L = 40$, half-filled Holstein-Hubbard chain, where $U$ is varied along the dashed arrows in inset of Fig. 1. Gray shadow indicates $U < 0$. (d) The result for the Hubbard model (with $\lambda = 0$), where the curves for charge and on-site SC are degenerate.}
\end{figure}

About the curious near-degeneracy between the CDW and on-site SC correlations, we can say the following. If the system were purely electronic, then an electron-hole transformation (for down spins) maps, when the lattice is bipartite, the CDW correlation onto the SDW correlation ($\langle S^z S^z \rangle$) and the on-site SC correlation onto the SDW correlation ($\langle S^z \rangle$), which should be identical with $\langle S^z S^z \rangle$ due to the SU(2) symmetry). When the Hamiltonian is the (half-filled) Hubbard model, the electron-hole transformation is the well-known attraction-repulsion ($U \leftrightarrow -U$) transformation, \cite{13} and the CDW and on-site pairing correlations are genuinely degenerate (as displayed in Fig 2(c)). Now, the system at hand is a coupled electron-phonon system, which can be mapped to the Hubbard model only in the limit of $\omega \to \infty$. So the present result amounts that the degeneracy curiously
persists approximately for the Holstein-Hubbard model for finite values of $\omega$.

_Destruction of the electron-hole symmetry_ — This leads us to the following idea: a destruction of the electron-hole symmetry in the (one-electron) band structure with e.g. an introduction of the second-neighbor hopping $t''$ may possibly be a way to make the pairing correlation the single, most dominant correlation, as in the on-site pair correlation in the half-filled attractive $t$-$t'$-$U$ model. So we introduce the second-neighbor hopping term, $-t'' \sum_{i,\sigma} \langle c^\dagger_{i+2,\sigma} c^\dagger_{i,\sigma} + H.c. \rangle \equiv \text{trestle lattice; see inset of Fig. 3},$ in the Holstein-Hubbard model.

![Figure 3](image)

**FIG. 3:** (a) Correlation functions when the electron-hole symmetry is destroyed with $t' = -0.5$ for $(U, \lambda, \omega) = (2.0, 3.6, 5.0)$. (b) Exponents against $-t'$ for various correlation functions for $(U, \lambda, \omega) = (2.0, 3.6, 5.0)$, and (c) a similar plot for the attractive Hubbard model with $U = -1.6$. The inset in (b) depicts the trestle lattice.

The result in Fig. 3(a), for the same $(U, \lambda, \omega) = (2.0, 3.6, 5.0)$ as in Fig. 2(b), shows that the introduction of $t'$ makes the CDW correlation suppressed (i.e., the power increases), while the power for the on-site SC correlation does not significantly change. This persists, as shown in Fig. 3(b) plotting various exponents against $t'$, up to $t' = -0.5$, at which the number of Fermi points in the non-interacting band increases from two. So in the region $0.25 \lesssim t' \lesssim 0.5$ the on-site SC becomes the single, most dominant correlation. We also note that the nearest-neighbor singlet pair correlation, too, becomes dominant (i.e., decays more slowly than the charge, spin or nearest-neighbor triplet pair correlations), and becomes nearly as dominant as the on-site pair when $-t'$ approaches 0.5. Here again, the calculated exponents for the Holstein-Hubbard model violates the TL relation, $\eta_{\text{CDW}} \eta_{\text{SC}} = 1$, for a spin-gapped metal.

**Discussion** — We have obtained an instance where superconductivity appears in a manner dependent on the lattice structure, while one might think that the electronic band structure should be irrelevant for the on-site (an s-wave) pairing arising from the on-site $U$ and on-site phonon. The result, if extensible to general dimensions, is suggestive for superconducting alkali-fullerides $A_2C_60$ having an fcc (i.e., electron-hole asymmetric) array of fullerenes, while DMFT studies for superconductivity primarily assume a symmetric (semilelliptic) electron density of states. Non-half-filled bands are also interesting, and the study is under way.

This work is in part supported by a Grant-in-Aid for Science Research on Priority Area from the Japanese Ministry of Education.

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