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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The density-matrix renormalization group is used to study the pairing when both electron-electron and electron-phonon interactions are strong in the Holstein-Hubbard model at half filling in a region intermediate between the adiabatic (Migdal's) and antiadiabatic limits. We have found (i) the pairing correlation obtained for a one-dimensional system is nearly degenerate with the charge density-wave correlation in a region where the phonon-induced attraction is comparable with the electron-electron repulsion, but (ii) pairing becomes dominant when we destroy the electron-hole symmetry in a trestle lattice. This provides an instance in which pairing can arise, in a lattice-structure dependent manner, from coexisting electron-electron and electron-phonon interactions.

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Introduction.—The problem of what happens when the electron-electron interaction coexists with the electron-phonon interaction is arousing interest from various viewpoints [1–5]. In fact, there are a number of classes of materials where electron-electron (e-e) and electron-phonon (e-ph) interactions are both significant. One example is the superconducting doped fullerenes [6], where the electrons in narrow conduction bands are strongly coupled to intramolecular, high-frequency phonons. Theoretically, a fundamental question is this: Can superconductivity arise in the coexistence of the e-e and e-ph interactions? It may seem difficult for them to work constructively, since the effective electron-electron attraction arising from the e-ph coupling favors isotropic pairs, while the (spin-fluctuation mediated) pairing interaction due to the e-e 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 e-ph interaction will favor a charge density wave (CDW), while a strong e-e interaction will favor a spin density wave (SDW). A metallic phase has a chance to appear around the boundary where a CDW gives way to an SDW, at which the e-e and e-ph interactions are indeed comparable. Takada and co-workers 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 a two- and a 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 e-e and e-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 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 ($\hbar\omega \gg t$).

The present Letter focuses on this problem, where we adopt the density-matrix renormalization group (DMRG) [9] for a one-dimensional Holstein-Hubbard model. DMRG can treat interactions nonperturbatively, and various types of correlation functions at $T = 0$ can be obtained from the wave functions. Of crucial interest here is how the system is dissimilar (or similar) to purely electronic systems, so we scan the three parameters (the three axes in the inset of Fig. 1) characterizing the system: U/t (the electron-electron repulsion U divided by t), $\hbar\omega/t$ (ratio of the phonon and electron energy scales), and $\lambda \equiv 2g^2/\hbar\omega$ (the effective attraction between electrons on the same site as defined in the $\omega \to \infty$ limit). As for the electronic band filling, we have concentrated here on the half filling as in [5,10–12], having $A_3C_{60}(A = \mathrm{K}, \mathrm{Rb})$ in mind.

We shall conclude the following. (i) 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 trestle 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 e-e and e-ph interactions can, in a manner dependent on the underlying electronic structure, give rise to pairing.

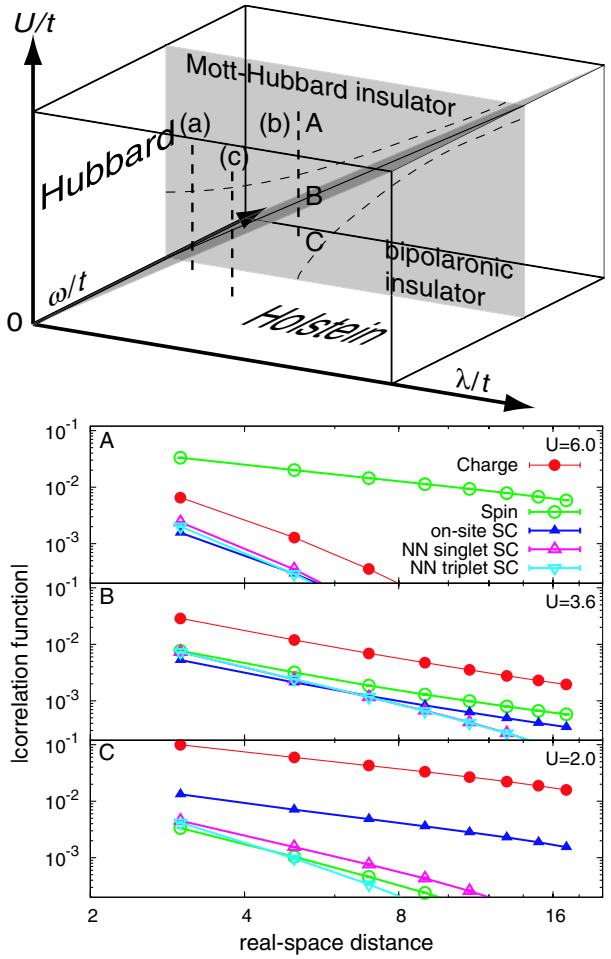

FIG. 1 (color online). Various correlation functions versus real-space distance in the Holstein-Hubbard model at half filling calculated for $(\lambda, \omega) = (3.6, 5.0)$ (in units where $t = 1$, $\hbar = 1$) with three values of U, indicated as A, B, and C in a schematic parameter space (top inset). Error bars are smaller than the size of each symbol. Only the data for $|i - j| =$ 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 Figs. 2(a) and 2(b).

Method.—The inclusion of the phonon degrees of freedom makes the DMRG calculation more demanding. However, Jeckelmann and White have introduced the pseudosite method, 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],

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

Here $c^{\dagger}_{i\sigma}$ creates an electron of spin σ on the ith lattice site, t is the nearest-neighbor (NN) hopping (which we take as the unit of energy hereafter), U is the on-site electron-electron repulsion, $b_i^{\dagger}$ creates a phonon at ith, g is the on-site e-ph interaction, and $\hbar\omega$ is the bare phonon energy. In the pseudosite method, we consider only finite numbers of phonons at each site ($M = 2^N$ for 0-boson, 1-boson, ..., $2^N - 1$-boson states). Sites are expressed in terms of fictitious N phonon "pseudosites," on top of an electron pseudosite. The pseudosites 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 pseudosite is added tend to significantly deviate from those describing the system at later stages. This is because the electrons on the added pseudosites 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 pseudosites 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), $c_{i\uparrow}c_{i\downarrow}$ (on-site pair), $c_{i\uparrow}c_{i+1\downarrow} - c_{i\downarrow}c_{i+1\uparrow}$ (nearest-neighbor spin singlet), and $c_{i\uparrow}c_{i+1\downarrow} + c_{i\downarrow}c_{i+1\uparrow}$ (nearest-neighbor triplet). A 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 is gapless when $U \gg \lambda$, both are gapless when $U \simeq \lambda$, and both are gapful when $U \ll \lambda$. The former two agree with the present result. As for the latter, we can interpret that here we are looking at a region where U is only moderately

smaller than λ and a spin-gapped metal can exist, for which CDW and on-site SC have power-law correlations as far as the Tomonaga-Luttinger (TL) physics [15] goes.

So the 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 λ ($\propto g^2$) the dominant correlation in Fig. 2(a) changes from the CDW/on-site SC to SDW almost exactly at the point where U exceeds λ.

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 attractive $U < 0$ (SDW for repulsive $U > 0$). In Fig. 2(d), this appears as a crossing of two continuous curves (one of which is 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 [16]. We have checked that the spin gap for $(U, \lambda, \omega) = (2.0, 3.6, 5.0)$ extrapolated from the $L \leq 50$ result is about twice as large as the difference between the lowest-unoccupied and highest-occupied one-electron levels. So

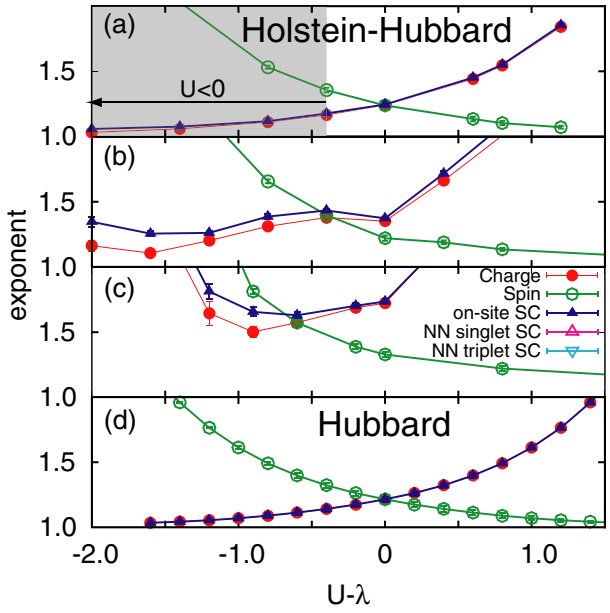

FIG. 2 (color online). Calculated powers (η) for the correlation functions ($\propto r^{-\eta}$) against $U - \lambda$ for (a) $(\lambda, \omega) = (0.4, 5.0)$, (b) $(\lambda, \omega) = (3.6, 5.0)$, and (c) $(\lambda, \omega) = (3.6, 2.5)$ in an $L = 40$, half-filled Holstein-Hubbard chain, where U is varied along the dashed arrows in inset of Fig. 1. The 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.

finite-size effects would not be significant, at least for $|U - \lambda| \gtrsim 1.0$.

However, we have found that, when λ is increased (with a fixed adiabaticity ω/t), the crossing point does deviate from $U - \lambda = 0$ as seen in Fig. 2(b). Also, the degeneracy between CDW and on-site SC is lifted (with the power for the latter slightly larger). This becomes more manifest for smaller ω, 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, signaling an opening of the charge gap Δ_c as well as spin gap Δ_s. This should correspond to the region of $\Delta_c \sim \Delta_s > 0$ for $U \ll \lambda$ in Ref. [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 Δ_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 [17] with the dynamical mean field theory (DMFT).

If we assume, as in [18], that the TL theory [15] applies to the present system, in a spin-gapped metal the CDW correlation should behave as r^{-K_ρ} while the pairing correlation r^{-1/K_ρ}, so that $K_\rho > 1$ corresponds to dominant SC correlation. While the behavior of the CDW correlation with a power greater than unity is consistent with the results in [18], we also notice 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 e-e 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 the half-filled Holstein-Hubbard model has also been observed in a DMFT calculation for the transition temperature [4].

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 [$\langle S^- S^+ \rangle$, 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, [19] 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 approxi-

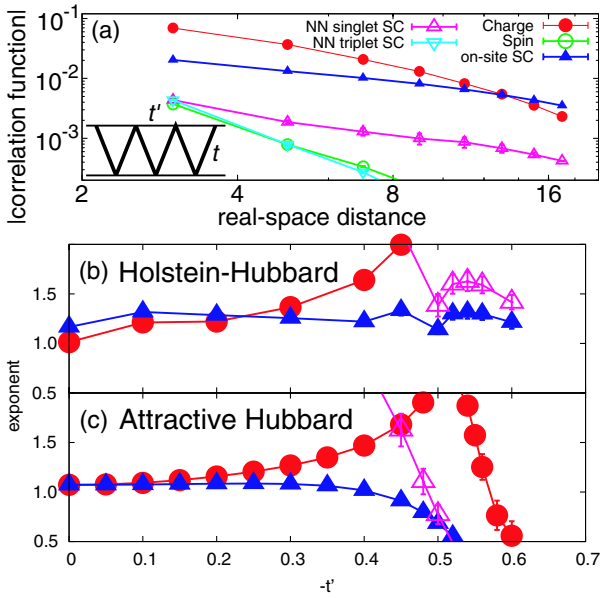

FIG. 3 (color online). (a) Correlation functions when the electron-hole symmetry is destroyed with $t' = -0.5$ for $(U, \lambda, \omega) = (2.0, 3.6, 5.0)$. (b) Exponents against $-t'$ for various correlation functions for $(U, \lambda, \omega) = (2.0, 3.6, 5.0)$, and (c) a similar plot for the attractive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

mately for the Holstein-Hubbard model for finite values of ω.

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, $-t'\sum_{i,\sigma}(c^{\dagger}_{i+2,\sigma}c_{i,\sigma} + \text{H.c.})$ ($\equiv$ trestle lattice; see inset of Fig. 3), in the Holstein-Hubbard model.

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 noninteracting 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, $\eta_{\mathrm{CDW}}\eta_{\mathrm{SC}} = 1$, 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_3C_{60} having an fcc (i.e., electron-hole asymmetric) array of fullerenes, while DMFT studies for superconductivity primarily assume a symmetric (semielliptic) electron density of states. Non-half-filled bands are also interesting, and the study is under way.

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[1] Z. B. Huang, W. Hanke, E. Arrigoni, and D. J. Scalapino, Phys. Rev. B **68**, 220507(R) (2003).
[2] M. Capone, M. Fabrizio, C. Castellani, and E. Tosatti, Science **296**, 2364 (2002).
[3] J. E. Han, E. Koch, and O. Gunnarsson, Phys. Rev. Lett. **84**, 1276 (2000).
[4] J. K. Freericks and M. Jarrell, Phys. Rev. Lett. **75**, 2570 (1995).
[5] G. S. Jeon, T.-H. Park, J. H. Han, H. C. Lee, and H.-Y. Choi, Phys. Rev. B **70**, 125114 (2004).
[6] O. Gunnarsson, Rev. Mod. Phys. **69**, 575 (1997).
[7] Y. Takada, J. Phys. Soc. Jpn. **65**, 1544 (1996).
[8] T. Hotta and Y. Takada, Physica (Amsterdam) **230B–232B**, 1037 (1997).
[9] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
[10] Y. Takada and A. Chatterjee, Phys. Rev. B **67**, 081102(R) (2003).
[11] G. Hager, E. Jeckelmann, H. Fehske, and G. Wellein, J. Comput. Phys. **194**, 795 (2004).
[12] H. Fehske, G. Wellein, G. Hager, A. Weiße, and A. R. Bishop, Phys. Rev. B **69**, 165115 (2004).
[13] E. Jeckelmann and S. R. White, Phys. Rev. B **57**, 6376 (1998).
[14] M. Tezuka, R. Arita, and H. Aoki, Physica (Amsterdam) **359B–361B**, 708 (2005).
[15] J. Sólyom, Adv. Phys. **28**, 201 (1979); V. J. Emery, in *Highly Conducting One-Dimensional Solids*, edited by J. T. Devreese *et al.* (Plenum, New York, 1979), p. 247; H. J. Schulz, in *Mesoscopic Quantum Physics*, edited by E. Akkermans *et al.* (Elsevier, Amsterdam, 1995), p. 533.
[16] K. Kuroki, T. Kimura, and H. Aoki, Phys. Rev. B **54**, R15641 (1996).
[17] G. Sangiovanni, M. Capone, C. Castellani, and M. Grilli, Phys. Rev. Lett. **94**, 026401 (2005).
[18] R. T. Clay and R. P. Hardikar, Phys. Rev. Lett. **95**, 096401 (2005).
[19] Y. Nagaoka, Prog. Theor. Phys. **52**, 1716 (1974).