Spectral function of the one-dimensional Holstein model at half filling

Hui Zhao, 1 C. Q. Wu, 1,* and H. Q. Lin 2,3

1 Research Center for Theoretical Physics, Fudan University, Shanghai 200433, China
2 Department of Physics, The Chinese University of Hong Kong, Shatin, Hong Kong, China
3 Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China

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The one-electron spectral function of the one-dimensional spin-$1/2$ Holstein model at half filling is computed by use of the cluster perturbation theory. The cluster Green’s function is obtained by the Lanczos exact diagonalization method within an optimized phonon approach. It is shown that the method allows reliable calculations using a relatively small size cluster and a few optimal phonon bases for the system from weak to strong electron-phonon coupling. In the strong-coupling limit, the spectral function shows the excitation behavior of a bipolaron state with a large gap at the Fermi surface. However, the obtained spectral function displays a metallic character in the weak-coupling regime, which is in accord with the suggestion that the Peierls gap is suppressed by quantum fluctuation of the phonons.

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Spectral properties, such as the one-electron spectral function, provide valuable insight into the usually complex physics of electron-electron ($e-e$) and/or electron-phonon ($e-p$) interacting systems, such as high-temperature superconductors, cuprate ladder compounds, and organic conductors. There has been much effort on calculations of the spectral function both by analytical and numerical methods. Analytical methods are often restricted to very limited cases and general results are hard to obtain. Numerical methods, such as exact diagonalization (ED) and quantum Monte Carlo (QMC), have received much attention in recent decades since they are applied to more general systems. Though the ED methods 1–5 based on the Lanczos algorithm allow very accurate calculations of the spectral function, the size of a cluster is usually restricted to be quite small due to the limitation of computing facilities. QMC (Refs. 6–10) can be used for much larger systems, but the maximum entropy method used for carrying out the analytic continuation required to obtain the spectral properties may not get all interesting features. Moreover, computation time increases rapidly as temperature is lowered.

A recent developed cluster perturbation theory 11,12 (CPT) has brought new hope to improve the situation. The CPT is based on a combination of exact diagonalization of finite clusters with strong-coupling perturbation theory 13,14 and its result is reduced to be exact for systems both at the noninteracting and the atomic limits. The method has been successfully applied to the Hubbard models for calculating spectral functions as well as other quantities of interest at zero 11,12,15,16 and finite temperatures. 17 Very recently, it has also been successfully applied to compute the one-electron spectral function of the Holstein polaron, 18 i.e., the one electron in the electron-phonon model with a local coupling of the Holstein type. 19

For electron-phonon interacting systems with many electrons, such as the Holstein model at half filling, it becomes increasingly difficult to include enough phonon states in the calculation, as done in the Holstein polaron case, 18 so as to obtain converged results even for a small cluster. In this work, we show that by adopting the optimized phonon approaches 20,21 together with the CPT, one could compute the one-electron spectral function of the one-dimensional spin-$1/2$ Holstein model at half filling with very good results.

Using the bosonization technique, Meden, Schönhammer, and Gunnarsson 22 investigated one-electron spectral properties for a one-dimensional continuum model including electron-phonon interaction. They showed that spin-$1/2$ electrons coupled with phonon represent a Luttinger liquid with a prominent feature of spin-charge separation. Very recently, by applying the exact diagonalization method to the Holstein-Hubbard model for finite lattices, Fehske et al. 23 obtained the spectral function which exhibits Mott-insulator to Peierls-insulator quantum phase transition at a compatible ratio of the $e-e$ and $e-p$ interaction parameters. Bindloss and Kivelson 24 computed finite temperature single-particle spectral function of a spinful, interacting one-dimensional Luttinger liquid coupled to an optical-phonon band, which is remarkably similar to the angle-resolved photoelectron spectra of high-temperature superconductors.

In this paper, the one-electron spectral function of the one-dimensional spin-$1/2$ Holstein model at half filling is computed by use of the CPT with an optimized phonon approach. We obtain the spectral function in the full frequency region which shows rich satellite structures. The spectral functions at strong- and weak-coupling limits seem to be consistent with the picture that there is a metal-insulator phase transition in the model, which was pointed out by one of the authors and his co-workers 25 in 1995 and later confirmed by a study using the density matrix renormalization group (DMRG) method. 20

The one-dimensional Holstein model with spin-$1/2$ electrons is defined by the Hamiltonian

$H = \sum_i (t c_i^{\dagger} c_i + U n_i n_i - 4J \sum_{i,j} c_i^{\dagger} c_j^{\dagger} c_j c_i)$

where $c_i^{\dagger}$ and $c_i$ are the creation and annihilation operators of an electron on site $i$, $n_i = c_i^{\dagger} c_i$ is the number of electrons on site $i$, $t$ is the hopping integral, $U$ is the on-site correlation energy, and $J$ is the electron-phonon coupling constant. The Hamiltonian is written in the form of a Hamiltonian with a local electron-phonon coupling, which is the Holstein type. The electron-phonon coupling is described by an interaction term $4J \sum_{i,j} c_i^{\dagger} c_j^{\dagger} c_j c_i$, which represents the interaction between the electron and the phonon. The electron-phonon coupling constant $J$ is a measure of the strength of the electron-phonon interaction. The Hamiltonian is typically solved using the density matrix renormalization group (DMRG) method, which is a powerful numerical method for solving quantum many-body systems. The DMRG method allows one to accurately compute the ground state and excited states of the system, and the spectral function can be obtained from the density matrix. The DMRG method is particularly well-suited for systems with a strong electron-phonon coupling, such as the Holstein model.
\[
H = -t \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.}) + \Omega \sum_i b_i^\dagger b_i - \gamma \sum_i (b_i^\dagger + b_i) \\
\times \left(c_{i,\sigma}^\dagger c_{i,\sigma} - \frac{1}{2}\right),
\]
(1)
where \(c_{i,\sigma}^\dagger\) (\(c_{i,\sigma}\)) creates (annihilates) an electron with \(\sigma\) on site \(i\), and \(b_i^\dagger\) and \(b_i\) are creation and annihilation operators of the local phonon mode at site \(i\), respectively. \(t\) is the electron hopping integral for nearest-neighboring sites, \(\Omega\) the bare phonon frequency, and \(\gamma\) the electron-phonon coupling constant. Within the mean-field theory, the ground state of this model is an insulating state for any nonzero electron-phonon coupling due to Peierls dimerization.20 The situation will be different if quantum fluctuations associated with phonons are taken into account. In the strong-coupling limit, the ground state for a half-filling system will be a biplaron state,27 which corresponds to the situation that each site is either empty or doubly occupied due to the attraction induced by phonons. In the weak-coupling limit, the Peierls gap is suppressed by phonon quantum fluctuation and the ground state is metallic.20,25

For the calculation of the spectral properties, the CPT (Refs. 11 and 12) requires that the lattice be divided into fully equivalent clusters of finite sites, the Green’s function for these clusters can be calculated by the ED. Specifically, we rewrite the Holstein Hamiltonian Eq. (1) as
\[
H = \sum_m H^0_m + \sum_{m,n,i,j} T^{m,n}_{i,j} c_{m,i,\sigma}^\dagger c_{n,j,\sigma},
\]
where \(H^0_m\) is the Hamiltonian of the \(m\)th cluster and \(T^{m,n}_{i,j}\) is the hopping integral between nearest-neighbor sites \((i,j)\) of adjacent clusters \((m,n)\). For the Holstein model (1), we have \(T^{m,n}_{i,j} = -t(\delta m \equiv \delta_{m,n} + \delta_{m,n+1} + \delta_{m,n-1} + \delta_{m,n-1} + \delta_{m,n+1})\), where \(N\) is the total number of sites in the cluster.

For each cluster, we calculate the Green’s function \(G_{i,j}(z) = \{G^r_{i,j}(z) + G^\ast_{i,j}(z)\}\) with \(G^r_{i,j}(z)\) defined as
\[
G^r_{i,j}(z) = \langle \phi_0 | c_{i,\sigma}^\dagger \frac{1}{z-H_E^{\sigma}} c_{j,\sigma} | \phi_0 \rangle,
\]
where \(c_i^\dagger = c_i^\dagger, c_i = c_i\), and \(|\phi_0\rangle\) is the ground state of the cluster, which can be obtained by using the ED method with open boundary conditions. Two terms in \(G_{i,j}\) corresponding to electron and hole propagation can be calculated separately.

The CPT treats intercluster hopping terms in Eq. (2) by a strong-coupling perturbation expansion to the first order in \(t\), then the Green’s function \(G_{i,j}(Q,z)\) of the full system is
\[
\tilde{G}_{i,j}(Q,z) = G(z) \frac{1}{1 - T(Q) G(z)},
\]
where \(G(z)\) is an \(N \times N\) matrix with the Green’s function \(G_{i,j}(z)\) as its elements, \(T(Q)\) is a matrix with elements being the reciprocal superlattice representation of the hopping \(T^{m,n}_{i,j}\), and \(Q\) is a superlattice wave vector. The Green’s function \(\tilde{G}_{i,j}(Q,z)\) is in a mixed representation: real space within the cluster and Fourier space between clusters. In order to calculate the spectral function, we take a true Fourier transformation in terms of the original reciprocal lattice of the system.

The lowest-order CPT approximation to the Green’s function gives
\[
G_{CPT}(k,z) = \frac{1}{N} \sum_{i,j} e^{-ik(j-i)} \tilde{G}_{i,j}(Nk,z).
\]
The spectral function \(A(k,\omega)\) is related to the Green’s function \(A(k,\omega)\) via the Fourier transform, where \(\omega\) being a small positive number to give delta peak a finite width.

In order to perform an exact diagonalization of the Holstein Hamiltonian for a cluster at half filling, one needs to introduce a finite basis to describe phonon degrees of freedom. If one uses a bare phonon basis as done for the Holstein polaron case,18 the number of bases needed for an accurate result will be extremely large, especially in the strong-coupling regime. However, the number of phonon bases can be significantly reduced if we use the optimized phonon approach.20,21 The spirit of this approach is similar to that of the DMRG which transforms the basis to that of eigenvectors of reduced density matrix and then discards states with low probabilities. To be specific, consider any wave function \(|\phi\rangle\) in the Hilbert space of the Holstein model. Let \(\alpha\) label the four possible electronic states of a particular site, \(n\) the bare phonon levels of this site, and \(j\) the combined states of all other sites. Then \(|\phi\rangle\) can be written as \(|\phi\rangle = \sum_{n,m} \phi_{n,m,j} |\alpha\rangle |n\rangle\). The reduced density matrix \(\rho\) of the state \(|\phi\rangle\) for this site is
\[
\rho = \sum_{\alpha} \langle \alpha | \rho | \alpha \rangle \sum_{n,m} |\alpha\rangle |n\rangle |\alpha\rangle |m\rangle,
\]
where \(m\) is also a bare phonon index. This density matrix is always diagonal for electronic states because of the conservation of electron numbers. The phonon density matrix of the site for electronic state \(\alpha\) has elements \(\rho_{n,m}^{\alpha} = \sum_j \phi_{n,m,j} \phi_{n,m,j}^\ast\). Let \(\omega_{nk}\) be the eigenvalues and \(|\xi_{nk}(n)\rangle\) the eigenvectors of \(\rho^{\alpha}\), where \(k\) labels different eigenstates for a given electronic state of the site. The set of states
\[
|\xi_{nk}(n)\rangle = \sum_n |\xi_{nk}(n)\rangle |n\rangle, \quad k = 1, 2, \ldots
\]
forms a new basis of the phonon Hilbert space for each electronic state \(\alpha\) of the site. If \(\omega_{nk}\) is negligible, then the corresponding state \(|\xi_{nk}(n)\rangle\) can be discarded from the basis for the site, without affecting the state \(|\phi\rangle\). In the Holstein model, keeping \(m = 3–5\) optimal states, \(|\xi_{nk}(n)\rangle\) for each electronic state of the site gives results as accurate as that with hundred or more bare phonon states per site for a wide range of model parameters.

Now, we describe the algorithm that we have used in this work. First, we calculate a large optimal phonon basis in a two-site Holstein system with appropriate parameters. In such a small system we can carry out calculations with enough bare phonon levels to render completely negligible errors due to the truncation of the phonon Hilbert space. Thus, target states can be obtained directly by diagonalization in the bare phonon basis. Then, the optimal phonon states of the two-site systems are used as the initial basis states for calculations on larger lattices. A single site (called
the big site) contains a large number of optimal phonon states obtained from the two-site systems. Each other site of the lattice is allowed to have a much smaller number of optimal phonon states, \( m \sim 3 \sim 5 \), for each electronic state of the site. Initially these states are also optimal phonon states of the two-site system. The ground state of the Hamiltonian is calculated in this reduced Hilbert space by exact diagonalization. Then, the density matrix of the big site is diagonalized. The most probable \( m \) eigenstates for each electronic state of the big site form new optimal states which are used on all of the other sites for the next diagonalization. These new phonon states are now optimized for the cluster and thus they are different from the optimal states of the two-site system. After the first diagonalization, the new optimal states of the cluster are not very accurate. Then, diagonalizations of the Hamiltonian and the density matrix are repeated until the optimal states converge. In each diagonalization, the big site always has a large number of phonon states so that it can generate improved optimal states for the next iteration. After full convergence of the optimal phonon basis, the error made by using three to five optimal states instead of hundreds of bare levels is negligible. Typically, the error is smaller than \( 10^{-5} \) with three or more optimal states.

First of all, in Fig. 1, we show the dependence of the spectral function \( A(\pi/2, \omega) \) on the number of optimal phonon bases we took and on the cluster size \( N \) we used in the calculations for an intermediate electron-phonon interaction \( \gamma = 1.0 \). By setting Fermi energy as zero, the spectral function has the symmetry \( A(k, \omega) = A(\pi - k, -\omega) \) because of electron-hole symmetry in the model. From Fig. 1(a), we can see that...
there is not any visible difference between the number of optimal phonon states being taken as $m=3$ and $m=5$ both in the ED and the CPT calculations of the spectra. The convergence for the spectra here is similar to that of the total energies. In the following calculations, we will take the number of optimal states $m=3$ without losing accuracy. In Figs. 1 and 1(c), the dependence of the spectra on the cluster size $N$ is shown for $N=2$, 4, and 6. It is clear that for the position of main peaks the ED spectra are quite different while the CPT spectra give almost the same value even for the smallest cluster size $N=2$. The satellite structures in the CPT spectra for $N=4$ and $N=6$ are also almost the same but they are different for the ED spectra for $N=2–6$.

In Fig. 2, we show the full spectral function of the system at half filling with the intermediate electron-phonon coupling $\gamma=1.0$. As is well known, due to Peierls instability, a gap should appear at the Fermi surface. In Fig. 2, though the phonon quantum fluctuation has smeared out the square root divergence in the mean-field approximation, a gap is still clearly observed. At the same time, we observe rich structures in the spectra due to electron-phonon interaction. At a stronger electron-phonon coupling, such as $\gamma=2.0$, we will observe the dispersionless peaks at almost equal distance $\Delta \omega=1$, which is the character of bipolarons for the bare phonon energy $\Omega=1$, since it is known that the sites will be either empty or doubly occupied in the ground state in the strong electron-phonon coupling limit. The spectra in Fig. 2 show that structures away from the Fermi surface have similar characteristics as that in the strong-coupling limit.

When the electron-phonon coupling decreases, the phonon quantum fluctuation increases. In Fig. 3, we show the spectral function for the system at a relatively weak electron-phonon coupling, $\gamma=0.7$, where the gap at the Fermi surface seems to be smeared out even with a very small (nonzero) Lorentzian broadening parameter, which is in accord with the suggestion that the Peierls gap is suppressed by the phonon quantum fluctuations in the weak-coupling regime. Nevertheless, numerical studies done on small lattices should never be used as a proof. Furthermore, a prominent feature of the spin-charge separation indicated earlier is also clearly shown in the obtained spectra, which will be discussed in detail elsewhere.

In summary, by combining the cluster perturbation theory with Lanczos exact diagonalization method and the optimized phonon approach, we have studied the spectral function of the one-dimensional Holstein model at half filling. We show that even with a very small cluster size our method gives a reliable result. The obtained spectral functions at strong- and weak-coupling limits are in accord with the suggestion that there is a metal-insulator phase transition in the model.

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