Optimized phonon approach for the diagonalization of electron-phonon problems

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We propose a new optimized phonon approach for the numerical diagonalization of interacting electron-phonon systems combining density-matrix and Lanczos algorithms. We demonstrate the reliability of this approach by calculating the phase diagram for bi-polaron formation in the one-dimensional Holstein-Hubbard model, and the Luttinger parameters for the metallic phase of the half-filled one-dimensional Holstein model of spinless fermions.

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Problems of electrons or spins interacting with lattice degrees of freedom play an important role in condensed matter physics. To name only a few, consider for instance polaron and bi-polaron formation in various transition metal oxides such as tungsten oxide or high-$T_c$ cuprates [1], Jahn-Teller effects in colossal magnetoresistance manganites [2], or Peierls and spin-Peierls instabilities in quasi one-dimensional materials [3].

As a generic model for such systems the Holstein-Hubbard model,

$$ H = -t \sum_{i,\sigma} (c_{i,\sigma}^{\dagger}c_{i+1,\sigma} + H.c.) + U \sum_i n_{i,\sigma} n_{i,\sigma} + g \omega \sum_{i,\sigma} (b_i^{\dagger} + b_i) c_{i,\sigma}^{\dagger}c_{i,\sigma} + \omega \sum_i b_i^{\dagger} b_i, $$

is frequently considered, where $c_i^{(1)}$ and $b_i^{(1)}$ describe fermions and bosons on a site $i$, respectively. In many physically relevant situations the energy scales of all the subsystems – electrons ($t$, $U$), phonons ($\omega$) and their interaction ($g\omega$) – are of the same order of magnitude, causing analytic methods, and especially adiabatic techniques, to fail in most of these cases. Even for numerical methods strong interactions are a demanding task, since they require some cut-off in the phonon Hilbert space. Starting with the work of White [4] in 1993, during the last years a class of algorithms became very popular, which based on the use of a so called density matrix for the reduction of large Hilbert spaces to manageable dimensions. Considerable focus has been placed on renormalization methods for one-dimensional systems in the thermodynamic limit. However, exact diagonalization of finite clusters also benefit substantially from these ideas, as we will demonstrate in the present paper.

**Optimized phonon approach:** First we recapitulate the connection between density matrices and optimized basis states. Starting with an arbitrary normalized quantum state

$$ |\psi\rangle = \sum_{r=0}^{D_r-1} \sum_{\nu=0}^{D_\nu-1} \gamma_{\nu r} |\nu\rangle |r\rangle $$

expressed in terms of the basis $\{|\nu\rangle |r\rangle\}$ of the direct product space $H = H_\nu \otimes H_r$, we wish to reduce the dimension $D_\nu$ of the space $H_\nu$ by introducing a new basis,

$$ |\tilde{\psi}\rangle = \sum_{\nu=0}^{D_\nu-1} \alpha_{\nu r} |\nu\rangle, $$

with $\tilde{\nu} = 0 \ldots (D_\nu - 1)$ and $D_\nu < D_\nu$. We call $\{|\tilde{\psi}\rangle\}$ an optimized basis, if the projection of $|\psi\rangle$ on the corresponding subspace $\tilde{H} = H_\nu \otimes H_r \subset H$ is as close as possible to the original state. Therefore we minimize $|||\psi\rangle - |\tilde{\psi}\rangle||_2^2$ with respect to the $\alpha_{\nu r}$, under the condition $\langle \tilde{\nu} | \tilde{\nu} \rangle = \delta_{\nu \nu}$, where

$$ \tilde{\psi} = \sum_{r=0}^{D_r-1} \sum_{\nu=0}^{D_\nu-1} \sum_{\nu' r'=0} \alpha_{\nu r} \alpha_{\nu' r'}^* \gamma_{\nu r}^* |\nu\rangle |r\rangle $$

is the projected state. Since we find

$$ |||\psi\rangle - |\tilde{\psi}\rangle||_2^2 = 1 - \sum_{r=0}^{D_r-1} \sum_{\nu=0}^{D_\nu-1} \sum_{\nu' r'=0} \alpha_{\nu r} \gamma_{\nu r}^* \gamma_{\nu' r'}^* \alpha_{\nu' r'}^* $$

$$ = 1 - \text{Tr}(\rho_{\rho \rho}^\dagger), $$

where $\rho = \sum_{r=0}^{D_r-1} \gamma_{\nu r}^* \gamma_{\nu r}$ is called the density matrix of the state $|\psi\rangle$, we observe immediately that the states $\{|\tilde{\psi}\rangle\}$ are optimal if they are elements of the eigenspace of $\rho$ corresponding to its $D_\nu$ largest eigenvalues $w_\nu$. Following Zhang et al. [5], we apply these features to construct an optimized phonon basis for the eigenstates of an interacting electron/spin-phonon system. Consider a system composed of $N$ sites, each contributing a phonon degree of freedom $|\nu\rangle$, $\nu = 0 \ldots \infty$, and some other (spin or electronic) states $|r\rangle$. Hence, the Hilbert space of the model under consideration is spanned by
For weakly interacting systems already a small number of our previous numerical work (see e.g. Ref. [6]).

uses the same optimized basis 

number of small sites. Each site except the large one automatically.

some cases one can avoid these problems by choosing an optimized state including the above 'bare' phonons, thus allowing the optimized states to become

condition 

This is reminiscent of the energy cut-off discussed above, and we therefore propose the following choice of phonon basis states at each site,

\[ \langle \tilde{\nu} | \tilde{v} \rangle \approx \xi^{\nu} \]

where \( \xi \) is the energy cutoff discussed above.

FIG. 1.: Eigenvalues \( \omega_\nu \) of \( \mathbf{\rho} \) calculated with the ground state of the Holstein model of spinless fermions for weak and strong coupling. For larger \( \tilde{\nu} \) the eigenvalues are close to the numerical precision \( \approx 10^{-14} \), explaining the flattening.

The first problem is solved by including all those states into the phonon basis that can be created by symmetry operations, and by calculating the density matrix in a symmetric way, i.e. by adding the density matrices generated with respect to every site, not just site \( i = 0 \).

Concerning the second problem we note that the eigenvalues \( \omega_\nu \) of the density matrix \( \mathbf{\rho} \) decrease approximately exponentially, see Figure 1. If we interpret \( \omega_\nu \sim \xi^{\nu} \) as the probability of the system to occupy the corresponding optimized state \( \tilde{\nu} \), we immediately find that the probability for the complete phonon basis state \( \bigotimes_{i=0}^{N-1} \tilde{\nu}_i \) is proportional to \( \xi^{\sum_{i=0}^{N-1} \tilde{\nu}_i} \). This is reminiscent of the energy cut-off discussed above, and we therefore propose the following choice of phonon basis states at each site,

\[ \forall i : \{|\mu_i\} = \text{ON}(\{|\mu\}) \]

\[ |\mu\rangle = \begin{cases} \text{opt. state } \tilde{\nu} \rangle, & 0 \leq \mu < m \\ \text{bare state } |\nu\rangle, & m \leq \mu < M \end{cases} \]

and for the complete phonon basis 

\[ \bigotimes_{\sum_{i=0}^{N-1} \nu_i < M} |\nu_i\rangle \],

yielding \( D_{\text{ph}} = \binom{N+M-1}{N} \). Implementation of this optimization procedure together with our existing Lanczos diagonalization code [6] allows the study of interacting electron/spin-phonon systems in a much larger parameter space without reaching the limits of available supercomputers.
To demonstrate the power of the method, in the following we address two frequently discussed problems: bi-polaron formation in the Holstein-Hubbard model, and Luttinger liquid characteristics of a 1D polaronic metal. (a) Bi-polarons in the Holstein-Hubbard model have been the subject of numerous studies over the last decades, stimulated for instance by the discovery of high-$T_c$ cuprates, and the belief that the interplay between strong electron-phonon and electron-electron interactions plays a significant role in these highly correlated materials [7]. Nevertheless the influence of the Hubbard interaction $U$ on bi-polaron formation is still not completely understood. Beside bi-polaron formation itself, an interesting open question is the transition between two bi-polaronic regimes, namely the inter-site and the on-site bi-polaron. Since the Hubbard interaction $U$ and the electron-phonon interaction compete, we usually need to consider intermediate to strong electron-phonon coupling $g$, or $\lambda := g^2\omega/(2t)$, making the problem a good testing ground for our optimized phonon algorithm.

In a recent work Bonća et al. [8] studied mobile bi-polarons in the Hubbard model with the aid of a variational technique. Their focus is mainly on the $U$ dependence of the transition from unbound polarons to inter-site bi-polarons and from inter-site to on-site bi-polarons at intermediate frequencies. These transitions also show a significant $\omega$ dependence. Here the adiabatic frequency range is of special interest, since there are no appropriate analytic methods for small but finite frequencies.

Using the optimized phonon approach on lattices sizes up to $N = 12$, we calculated the phase diagram for the transition from unbound polarons to inter-site bi-polarons at fixed $U$. The critical coupling $\lambda_c$ was determined by the condition $\Delta = 0$, where $\Delta$ is the energy difference between the two-particle ground state and twice the one-particle ground state, i.e. $\Delta = E_b - 2E_p$. As indicated in Figure 2, the critical interaction $\lambda_c$ increases with frequency, reaching $U/(4t)$ as the limiting value. The density-density correlation (see inset) signals a second transition from inter-site to on-site bi-polarons, which also causes a distinct feature in the kinetic energy [9], shown in Figure 3 for different frequencies and system sizes. For $\omega = 0.4t$ there is a sharp drop in $E_{\text{kin}}$ at about $\lambda = 1.6$. Near this critical coupling we observe another striking effect if we study the bi-polaron band dispersion: Namely, it is almost a perfect cosine at the critical coupling, but deviates from this simple tight-binding dispersion for other couplings. That means in the vicinity of $\lambda_c$ the residual bi-polaron-phonon interaction vanishes. At present we have no clear explanation for this free-particle like behaviour. As an example we plot the rescaled dispersion for different system sizes and diagonalization methods in the inset of Figure 3.

(b) Luttinger liquid behaviour. The Holstein model of spinless fermions is defined by omitting the electron spin $\sigma$ and consequently the Coulomb interaction $U$ in Hamiltonian (1). In one dimension and at half filling, depending on the coupling strength $g$, this model undergoes a transition from a gapless metallic phase to a Peierls distorted phase with a gap between the ground-state and lowest excitations. Details of this transition and the properties of the different phases were studied with several methods over the last years (see Refs. [10–14]). One interesting aspect is the description of the metallic phase in terms of an effective Luttinger model, which, according to the ‘Luttinger liquid hypothesis’ of Haldane [15], should be an universal picture for the low temperature properties of all one-dimensional metals. The two parameters of the Luttinger model, the renormalized Fermi velocity $u_\rho$ and effective coupling constant $K_\rho$, can be determined through the scaling behaviour of the ground-state energy $E_0$ and the energy of charge excitations $E_{\pm 1}$ with respect to the system size $N$:
In a recent work [14] we used a variational method to calculate eigenstates and the resulting Luttinger parameters for the Holstein model at half filling. Unfortunately the method failed to give consistent results especially for \( K_p \) in the anti-adiabatic regime of large frequencies \( \omega \gg t \) where the Holstein model can be well described by second order perturbation theory, leading to an effective XXZ spin model [10] with known Luttinger parameters. For large frequencies the XXZ model, as well as Monte Carlo [12] and DMRG [13] calculations for the Holstein model, yield \( K_p < 1 \) corresponding to a repulsive interaction. If \( K_p \), starting with the value 1 for the noninteracting case, reaches \( \frac{1}{2} \) with increasing coupling strength, the model undergoes a Kosterlitz-Thouless transition to a gapped phase. In contrast, with our variational technique we found \( K_p > 1 \), corresponding to an attractive interaction, for all frequencies. Since it was not possible to calculate the required eigenstates with sufficient precision for the various system sizes needed for finite size scaling, this unsatisfying situation could not be resolved with our ‘traditional’ Lanczos diagonalization procedure.

In Figure 4 we show the Luttinger parameters we found by scaling the energies for system sizes up to \( N = 10 \). In the anti-adiabatic frequency range the renormalized Fermi velocity \( u_p \) is drastically suppressed within the metallic phase, while for low phonon frequencies it remains almost unchanged up to the phase transition. A very interesting result is the changing character of the interaction below \( \omega \sim t \). For small frequencies the effective fermion-fermion interaction is attractive, while it is repulsive for large frequencies. Possibly there is a transition point, depending on \( g \) and \( \omega \), where the model is free in lowest order. Further analytical studies of this behaviour will be reported elsewhere.

In conclusion, we have proposed an advanced phonon optimization algorithm for application in Lanczos diagonalization, and demonstrated its reliability for two strongly interacting electron-phonon systems.

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\[
\frac{E_0(N)}{N} = \epsilon_{\infty} - \frac{\pi u_p}{6N^2}, \quad E_{\pm 1}(N) - E_0(N) = \frac{\pi u_p}{2K_pN}. \quad (8)
\]

We therefore reconsidered the problem with a more sophisticated variant of the above phonon optimization algorithm, using two different sets of optimized phonon states, one for each possible fermion occupation number (cf. Ref. [5]). Together with the cut-off, this results in a further reduction of the Hilbert space, which is required for the diagonalization of larger systems. It is worth noting that this advantage is gained at the expense of a much more complicated fermionic Hamiltonian, since every hopping is connected with the projection of the actual phonon state onto the other basis set. Hence, for other models with a more difficult structure, like Jahn-Teller problems with two or three phonon modes per site, this procedure is not recommended.

In Figure 4 we show the Luttinger parameters we found

![Figure 4: Luttinger liquid parameters for the Holstein model of spinless fermions at phonon frequencies \( \omega = 0.1, 1.0 \) and 10.](image)

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