A new perspective on the Holstein polaron problem

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The single-polaron band structure of the Holstein model in one and two dimensions is studied using a new form of resummed strong-coupling perturbation theory. Well converged results are obtained for phonon frequencies of the order of the hopping integral and strong to intermediate electron-phonon coupling. The polaron band structure at intermediate coupling is shown to deviate markedly from that of a nearest-neighbor tight-binding model, and is in fact similar in shape to the prediction of weak-coupling self-consistent perturbation theory.

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Despite many years of research, our understanding of the nature of the transition from a quasi-free electron state with small mass renormalization at weak electron-phonon (EP) coupling to the small polaronic state with very narrow band width at strong coupling is still incomplete. In particular, the region of intermediate coupling and phonon frequency is difficult to handle theoretically due to the absence of a small parameter on which to base a perturbation theory. It is known rigorously that the character of the ground state changes significantly at a rather well-defined crossover coupling.

In this paper we concern ourselves with the evolution of the polaron quasiparticle (QP) band structure as a function of EP coupling. We present the results of a study of the Holstein model using a new numerical scheme, which is equivalent to a selected resummation of some terms in strong-coupling perturbation theory (SCPT) to all orders. Our resummed SCPT, denoted FC for “finite cluster”, since the method is a form of cluster expansion, converges well down to quite weak coupling also for phonon frequencies of the order of the electronic hopping integral, where we are able to obtain good agreement with the weak-coupling self-consistent Migdal (SCM) perturbation theory and exact results for small clusters of up to six sites. We present a simple physical picture which clarifies the continuous evolution of the QP band structure from weak to strong coupling.

The Holstein model\[1\] is defined by

\[
H = -t \sum_{<i,j>} (c_i^\dagger c_j + c_j^\dagger c_i) + \omega_0 \sum_i a_i^\dagger a_i + g \sum_i n_i (a_i^\dagger + a_i) \tag{1}
\]

where \(c_i^\dagger\) is the creation operator for a spinless electron on site \(i\), \(n_i = c_i^\dagger c_i\), and \(a_i^\dagger\) is the creation operator for the local oscillator of frequency \(\omega_0\). Although the formalism presented may also be applied to the many-electron case, we treat only the single carrier case here.

We recall first some well known results for the strong-coupling limit: if the EP coupling is large it is natural to treat the coupling term in \(\omega_0\) exactly, and to consider the hopping as a perturbation. Performing the Lang-Firsov canonical transformation leads to

\[
H_0 = -\alpha^2 \omega_0 \sum_i n_i + \omega_0 \sum_i a_i^\dagger a_i \tag{2}
\]

which is diagonalized by the transformation, and the kinetic energy term becomes

\[
H_t = -t \sum_{<i,j>} \left( c_i^\dagger c_j X_i^\dagger X_j + h.c. \right) \tag{3}
\]

with \(X_i = \exp \left[ \alpha (a_i - a_i^\dagger) \right] \) and \(\alpha = g/\omega_0\).

One now chooses as the model space states with no excited phonons, and upon taking the expectation value of \(H\) in the transformed phonon vacuum (first order SCPT) arrives at an effective polaron Hamiltonian consisting of a nearest-neighbor (n.n.) tight-binding model with the hopping integral \(t \rightarrow t^* = t \exp(-\alpha^2)\) together with a constant energy shift (binding energy) of \(-E_B = -\alpha^2 \omega_0\). Continuing with degenerate Rayleigh-Schrödinger perturbation theory, the second order correction involves the application of \(\hat{a}_i\) onto an initial state with no excited phonons, leading to an intermediate state with the electron on a n.n. of the initial site and some excited phonons as well. The second application of \(\hat{a}_i\) must annihilate the phonons and either a) return the electron to the initial site, leading to a renormalization of the binding energy or b), move the electron to a next-nearest-neighbor (n.n.n.) of the initial site, giving rise to an effective n.n.n. hopping. Making use of translational symmetry one finds in one-dimension (1D) the band structure

\[
E(k) = -E_B + E^{(2)} - 2 t^* \cos(k) - 2 t_2 \cos(2k) \tag{4}
\]

where

\[
E^{(2)} = \frac{-2(t^*)^2}{\omega_0} \left[ \text{Ei}(2\alpha^2) - \gamma - \ln(2\alpha^2) \right], \tag{5}
\]
with \[ E_i(x) = \frac{\text{Ei}(x^2) - \gamma - \ln(x^2)}{x^2} \], \[ t_2 = \frac{\left( t_1 \right)^2}{\omega_0} \left[ \text{Ei}(\alpha^2) - \gamma - \ln(\alpha^2) \right] \], \[ \omega_0 = \frac{\hbar}{\tau} \text{Ei}(x) \text{Ei}(x^2) \],

where \( \text{Ei}(x) \) is the exponential integral and \( \gamma \) is Euler's constant.

Note once more that the initial tight-binding model contains only n.n. hopping terms, but due to the strong coupling to the lattice degrees of freedom the polaron dispersion develops n.n.n. terms. At higher order in perturbation theory one generates further longer range hopping terms as well as renormalizations of the previously obtained contributions. If one considers \( \omega_0 \approx t \) the convergence of this series is poor, even for quite strong coupling. One option for a systematic and controlled approach to a description of this intermediate regime is to continue as we have started and to generate further terms in the Rayleigh-Schrödinger perturbation expansion. While this is clearly feasible, it may be necessary to go to quite high order to achieve converged results for a wide range of parameters. We choose instead an alternative approach: it has been shown that it is possible to resum to infinite order some of the terms of a strong-coupling perturbation expansion by making appropriate use of some exact information obtained from the numerical diagonalization of a sequence of finite clusters. This method has been shown to allow the low-lying states of the Hubbard model to be quantitatively well described by a generalized \( t - J \) model also for \( U/t \) not very large.

The general form of the result obtained is a series of terms involving connected clusters of increasing numbers of sites, \( h = h^{(1)} + h^{(2)} + h^{(3)} + \ldots \), where \( h^{(n)} \) is an operator which acts on all connected clusters of exactly \( n \) sites. By construction, the eigenvalues of \( h \) will be exact eigenvalues of the original full Hamiltonian on this same cluster if terms up to \( h^{(n)} \) are applied to a cluster of \( n \) sites.

The terms of \( h \) are constructed recursively: given the series up to \( h^{(n)} \) one may extract a “total” \( h \) for an \( n+1 \) site cluster of a particular topology as \( h = U E U^{-1} \), where \( E \) is a matrix containing a subset of the exact eigenvalues of the full original Hamiltonian for this given cluster on the diagonal, and the transformation matrix is \( U = \left( S^{-1} S^{-1} \right)^{1/2} S \). Here \( S \) is the matrix whose columns are the projections of the relevant eigenvectors of the full Hamiltonian onto the model space (in the present case the zero phonon subspace). The factor of \( \left( S^{-1} S^{-1} \right)^{1/2} \) in \( U \) ensures that \( h \) is Hermitian (for further details and explanation see Ref. 4).

The exact information for \( E \) and \( S \) is obtained in the present case by numerical diagonalization after first rendering the problem finite by introducing a cutoff in the phonon occupation. The matrix elements of \( h^{(n+1)} \) are now found from those of this “total” \( h \) on the \( (n+1) \)-site cluster by subtracting the contributions from all embedded subgraphs of up to \( n \) sites which have previously been calculated. It should be stressed that this procedure is not a fitting or extrapolation of eigenvalues: in general also information from the exact eigenvectors enters in the determination of the matrix elements of \( h^{(n)} \).

For the single carrier case the resulting effective Hamiltonian is a single-particle tight-binding model which may be diagonalized directly for the infinite system. If the same approach is applied to a many-carrier system one may “integrate out” the phonon degrees of freedom just as in the single particle case, but one is then still left with a complicated many-fermion problem to analyze. Work in this direction using numerical diagonalization of the resulting effective Hamiltonians for finite systems is in progress.

The convergence of the SCPT for the Holstein model which is evaluated up to second order in \( h \) depends on two parameters: both the degree of adiabaticity \( \omega_0/t \) and the coupling strength \( \alpha \) are important. For \( \omega_0/t >> 1 \) (anti-adiabatic limit) the expansion is well convergent for all \( \alpha \), but for \( \omega_0/t \approx 1 \) large \( \alpha \) is required. This behavior is also reflected in the resummed FC approximation described above, where it manifests itself in the spatial range of interaction needed to achieve a converged result. In general the smaller the phonon frequency the larger the interaction range needed for a given \( \alpha \).

We compare in Fig. 1 the predictions of various approximations to the polaron dispersion in 1D for an intermediate phonon frequency of \( \omega_0/t = 1 \) and two different coupling strengths.

![Fig. 1](image.png)

Fig. 1. Polaron dispersion for a 1D system with \( \omega_0/t = 1 \) and: (a) \( g/t = 1.75 \); (b) \( g/t = 0.8 \). Solid lines are FC approximation to order \( h^{(5)} \), dotted lines FC to \( h^{(4)} \). Dashed lines are second order strong-coupling perturbation theory, and dot-dashed lines weak-coupling self-consistent Migdal approximation. Data points are exact results for various small clusters with periodic boundary conditions: circles, 6 sites; squares, 5 sites; triangles, 4 sites.

The extremely small difference between the predictions of the 4- and 5-site FC approximations in Fig. 1(a) demonstrates the rapid convergence of this approach.
in strong-coupling even for this “difficult” phonon frequency. These curves are also in very good agreement with the diagonalization results, with the discrepancies being of the same order as the finite-size scatter from one system to the next. The second order strong-coupling perturbation theory on the other hand underestimates the band width by approximately a factor of two even for this relatively strong EP coupling because of the low phonon frequency. The weak-coupling SCM result, which is the lowest pole of the single-particle Green’s function

\[ G(k, \omega + i\delta) = [\omega + i\delta - \epsilon_k - \Sigma(k, \omega)]^{-1} \quad (7) \]

with the self-energy

\[ \Sigma(k, \omega) = \Sigma(\omega) = g^2 / N \sum_{k'} G(k', \omega - \omega_0) \quad (8) \]

is as expected quantitatively very unreliable here as well. Marsiglio has previously compared the ground state energy predicted by this approximation with exact numerical results, and found good agreement only for quite weak coupling. We have furthermore confirmed that adding the first vertex correction to the SCM does not significantly improve the agreement of the band width with the results of the other methods for parameters as in Fig. 1(a).

Turning now to the weaker EP coupling case shown in Fig. 1(b), we see that the FC predictions now agree quite well with the weak-coupling SCM prediction for the QP dispersion, as well as with the small-system data points. In this case the FC approach displays slightly poorer convergence than in Fig. 1(a), with the curves for the two different interaction ranges shown oscillating noticeably about one another. For these parameters the polaron size is slightly larger than the range of interaction included in the present calculations, but nevertheless it is clear that the “limiting” result would not be very different from those shown. One expects predominantly a further smoothing of the oscillations with increasing effective interaction range. Note once more that the FC approach starts from the strong-coupling limit, so that the good agreement with the dispersion predicted by the SCM weak-coupling approximation and the exact finite-system data in Fig. 1(b) is non-trivial. In this case the simple second order SCPT prediction is quite poor, but errs in the opposite direction from the stronger coupling case of Fig. 1(a). This behavior is quite generic: for strong coupling the second order SCPT predicts a narrower band width than the FC approach, with the error of course approaching zero for asymptotically strong coupling or large phonon frequency, whereas for weaker EP coupling, as the convergence of the SCPT deteriorates further the band width is overestimated.

At this point we should discuss the physical content of these results. The basic physics that we are observing was studied already many years ago by Engelsberg and Schrieffer for a continuum rather than tight-binding model. Considering the single-particle spectral function, for weak EP coupling the lowest excitation branch at small momentum is a weakly dressed electron. If the energy to excite one phonon lies inside the electron band, then for arbitrarily weak coupling the electron and phonon mix and repel one another near the point where they would be degenerate (this may still be quite clearly seen in Fig. 1(b), where the dispersion “flattens” at an excitation energy near \( \omega_0 \)). What continues as lowest-energy excitation in the single-particle spectral function for larger momentum is in fact the phonon, with a small admixture of electronic character. The main part of the spectral weight disperses upward following the bare electron band structure, but is strongly broadened. With increasing EP interaction the admixture of electronic character in the lower energy “flat” part of the dispersion at large momentum increases and the peak splits away from the continuum, and it begins to be sensible to denote this the polaronic QP band. An interesting new feature in the present results is the fact that even in cases where the band width of this QP is less than half of the bare phonon energy, the QP dispersion may be nearly flat at large momentum. In this crossover region low order strong-coupling perturbation theory underestimates the coherent band width slightly, but more striking is the fact that longer range effective hopping terms are not negligibly giving rise to a dispersion very different from a n.n. cosine band. The SCM approximation on the other hand generally overestimates the band width, but qualitatively describes the shape of the band quite well. The fact that the dispersion is large at small momentum and weak at large momentum implies that the mass enhancement at the band minimum is generally significantly smaller than the exponential prediction of the first order strong-coupling perturbation theory \( m^*/m = \exp (a^2) \), except at very strong coupling.

We have performed similar calculations also for the 2D square lattice. In this case the application of the FC approach requires separate determination of \( h^{(n)} \) for n-site clusters of all inequivalent topologies, and in the application of \( h \) all possible shapes that topologically equivalent embedded subclusters may have must be allowed for. At the present level of approximation this is still quite simple, however, as there are still only three inequivalent topologies for connected clusters of 5 sites. The limiting factor is the size of system for which sufficiently accurate results can be obtained for the eigenvalues and eigenvectors of the Holstein model, and not yet the number of graphs which need be considered. To a good approximation the results for 2D are similar to those for 1D, after renormalization of parameters to take account of the doubling of the bare electronic band width in 2D when compared to 1D. The convergence of the FC approach in 2D for \( \omega_0/t = 2 \) and a given coupling is similar to that for \( \omega_0/t = 1 \) and the same coupling in 1D. In Fig. 2 we present the QP band structure in 2D for EP coupling \( g/t = 2.75 \) and phonon frequency \( \omega_0/t = 1.5 \) (a) and \( \omega_0/t = 2.0 \) (b). In both cases, from a comparison of
the 4- and 5-site FC approximations it is again clear that the polaron size is still slightly larger than the range of effective interactions presently included, but that further corrections will be quite small. For the larger phonon frequency of Fig. 2(b) the discrepancy between second order SCPT and the FC is quite small, consistent with good convergence of the SCPT for large $\omega_0$. Since the effective coupling $\alpha$ is not very large in this case, also the SCM result is reasonable. For the smaller phonon frequency of Fig. 2(a) however, $\alpha$ is significantly larger, and the band width predicted by the FC approximation is much smaller than the weak-coupling SCM result. Once again the first and second order SCPT err in the opposite direction compared to the SCM result, and underestimate the band width by more than a factor of two.

![Graph showing polaron dispersion for 2D system with $g/t = 2.75$ and $\omega_0/t = 1.5$ (a) and $\omega_0/t = 2.0$ (b).](image)

**Fig. 2.** Polaron dispersion for 2D system with $g/t = 2.75$ and: (a) $\omega_0/t = 1.5$; (b) $\omega_0/t = 2.0$. Solid lines are FC approximation to $h(5)$, dotted lines FC to $h(4)$. Dashed lines are first order strong-coupling perturbation theory, long dashed lines are second order strong-coupling perturbation theory, and dot-dashed lines weak-coupling self-consistent Migdal approximation.

However, already in the second order SCPT correction the tendency for the shape of the dispersion to “flatten” at large momentum when compared with the n.n. cosine (first order SCPT) is apparent. One should again stress that the extended flat region at large momentum for such parameters is not trivial: the FC band width is a factor of three smaller than the weak-coupling SCM prediction $\approx \omega_0$, where the flat region is clearly determined by the “collision” of the bare electronic dispersion with the phonon.

We have presented an approach to the polaron problem in the Holstein model which is equivalent to a resummation of some terms in strong-coupling perturbation theory to all orders. For phonon frequencies $\omega_0/t$ greater than 1 (2) in 1D (2D) this approach is sufficiently convergent that good agreement can be achieved with the SCM weak-coupling perturbation theory in the crossover region. The flat band at large momentum, expected for weak EP coupling due to the hybridization of the electron and phonon degrees of freedom when the phonon frequency lies inside the electron band, has been shown to survive to surprisingly strong EP coupling. For $\omega_0/t \approx 1$ and intermediate coupling the low-order strong-coupling perturbation theory has been shown to underestimate the QP band width, and to overestimate the mass enhancement by an even larger factor due to the importance of longer range hopping terms in the effective polaron model.

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