Excitation Spectrum of the Holstein Model

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In this paper the polaron problem for the Holstein model is studied in the weak coupling limit. We use second order perturbation theory to construct renormalized electron and phonons. Eigenstates of the Hamiltonian are labelled and the excitation spectrum is constructed.

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I. INTRODUCTION

The Holstein model which describes electrons coupled to some local molecular deformations is a simple model to study polaron properties\(^1\). These recent years, accurate numerical investigations of this model on finite systems have given new insights\(^2\)\(^3\) closely linked to some current problems in condensed matter physics\(^4\). A polaron corresponds to an electron renormalized by the interactions between the lattice deformations or phonons\(^5\). From a historical point of view\(^6\)\(^7\) the approach to the polaron problem consists in computing the spectrum of the whole system containing a single electron coupled to some optical phonons. Writing \(k\) the momentum of the electron and \(Q\) the momentum of the phonons, the problem is to compute the lowest energy of the system for a total momentum \(K = k + Q\), since the total momentum operator commute with the Hamiltonian. This minimum eigenenergy of the Hamiltonian for a given total momentum \(K\) gives the polaron relation dispersion, as far as we consider only the low lying excitations of the system –that is as far as no phonon excitations are involved.

In this paper, we consider a different approach to the problem and try to decompose the excitations of the system in term of polaron excitations and renormalized phonons excitations. Due to the difficulty of the problem, we address only the weak coupling limit of the problem and we use mainly second order perturbation theory in the electron phonon coupling. Within this framework, one can block diagonalize the Hamiltonian. Then it is possible to label the eigenstates of the Hamiltonian in term of renormalized electron and phonons. In other words, an eigenstate of the Hamiltonian contains one renormalized electron (a polaron) of momentum \(k\) and some renormalized phonons of momentum \(Q\); the total momentum of the state being \(K = k + Q\).

The Hamiltonian for the Holstein model, in Wannier representation, is given by

\[
H = -t \sum_{j,\delta} c^\dagger_{j+\delta} c_j + \omega_0 \sum_j b_j^\dagger b_j - g \omega_0 \sum_j c^\dagger_j c_j (b_j + b_j^\dagger),
\]

(1)

where \(c_j^\dagger\) and \(c_j\) are electron creation and annihilation operators, \(b_j^\dagger\) and \(b_j\) are phonon creation and annihilation operators. \(t\) is the hopping integral, \(\omega_0\) is the optical phonon frequency and \(g\) is the dimensionless coupling constant. In the strong coupling limit, \(g \gg 1\), the Hamiltonian is approximatively diagonalized by the Lang-Firsov transformation\(^8\). The transformed Hamiltonian is given by \(\tilde{H} = e^{-S} H e^S\), with \(S = \sum_j g c^\dagger_j c_j (b_j - b_j^\dagger)\). It is only when the hopping term is zero that the transformed Hamiltonian is diagonal. In this case one obtains some new fermionic operators, which describe small polarons, or localised polarons. The small polaron creation operator is given by \(p_j^\dagger = e^S c_j e^{-S}\), or \(p_j^\dagger = U_j c_j\), with \(U_j = \exp g (b^\dagger_j - b_j)\) while the renormalized phonons operators are given by \(B_j = b_j - g\). The action of this small polaron creation operator on the vacuum is thus to create an electron and a coherent state for the phonons where the annihilation operator takes the expectation value \(g\). For non zero values of the hopping integral, these small polarons become some quasiparticles more or less well defined depending on the value of the coupling and on the phonon frequency\(^2\)\(^3\)\(^9\). We notice that for \(g = 0\), the small polaron correspond to the bare electron, since there is no coupling and thus no renormalization. We shall use a similar unitary transformation formalism but in we weak coupling limit, \(g \to 0\), and work in momentum space where the Hamiltonian reads

\[
H = \sum_k \varepsilon_k c^\dagger_k c_k + \omega_0 \sum_q b^\dagger_q b_q - \frac{g \omega_0}{\sqrt{M}} \sum_{k,q} c^\dagger_{k+q} c_k (b_q + b^\dagger_{-q})
\]

(2)

where \(M\) is the number of sites of the lattice, and indices of various operators correspond to Bloch momenta. In the next section we consider our approach for a two site system, then we will generalize to a general system.
II. THE TWO SITE SYSTEM

We start our perturbation theory for the two site system. In this case, the momentum takes two values \( k = 0, \pi \) and the bare electron relation dispersion is given by \( \varepsilon_q = -t \) and \( \varepsilon_q = +t \). The \( q = 0 \) mode of the phonons is coupled to the total number of electron which is one in this problem. We drop out this mode after performing the shift corresponding to the displaced oscillator \([3]\). The reduced Hamiltonian is then given by

\[
H_R = -\frac{g^2\omega_0}{2}(c_0^\dagger c_0 + c_\pi^\dagger c_\pi) - t (c_0^\dagger c_0 - c_\pi^\dagger c_\pi) + \omega_0 b^\dagger b - \frac{g\omega_0}{\sqrt{2}}(c_\pi^\dagger c_\pi + c_\pi^\dagger c_0)(b + b^\dagger)
\]  

(3)

We have dropped the index \( \pi \) for the boson operators. The basis states are given by \( |k; n\rangle = c_k(b^\dagger)^n/\sqrt{n!}|0\rangle \) and \( |0\rangle \) is the vacuum. For \( g = 0 \) the corresponding eigenenergies are given by \( \varepsilon_n(k) = n\omega_0 + \varepsilon_k - g^2\omega_0/2 \). Using second order perturbation theory, we obtain the eigenstates and eigenenergies,

\[
E_n(k) = \varepsilon_n(k) + \frac{g^2\omega_0}{2} \left[ n\frac{\omega_0}{2\varepsilon_k + \omega_0} + (n + 1)\frac{\omega_0}{2\varepsilon_k - \omega_0} \right] \]

(4)

\[
|k; n\rangle = \left\{ 1 + \frac{g\omega_0}{\sqrt{2}} \left[ \frac{b}{2t - \omega_0} + \frac{b^\dagger}{2t + \omega_0} \right] c_\pi^\dagger c_0 - \frac{g\omega_0}{\sqrt{2}} \left[ \frac{b}{2t + \omega_0} + \frac{b^\dagger}{2t - \omega_0} \right] c_0^\dagger c_\pi \right\} |k; n\rangle
\]

(5)

We show now that the eigenstate \( |k; n\rangle \) describes a state with one polaron of momentum \( k \) and \( n \) renormalized phonons. The states \( |k, n\rangle \) are eigenstates of the Hamiltonian \( H_R \), thus using \( \hat{H}_R = e^{-\hat{S}} H_R e^\hat{S} \), we obtain \( |k; n\rangle = e^\hat{S} |k; n\rangle \). Up to \( \mathcal{O}(g^2) \), the \( S \)-matrix of the unitary transformation is given by

\[
S = \frac{g\omega_0}{\sqrt{2}} \left[ \frac{b}{2t - \omega_0} + \frac{b^\dagger}{2t + \omega_0} \right] c_\pi^\dagger c_0 - \frac{g\omega_0}{\sqrt{2}} \left[ \frac{b}{2t + \omega_0} + \frac{b^\dagger}{2t - \omega_0} \right] c_0^\dagger c_\pi
\]

(6)

We note that if we set \( t = 0 \) in this expression, we obtain the right transformation which diagonalize the reduced Hamiltonian \( H_R \). We can now construct the corresponding polaron operator \( p_k \) through the transformation \( p_k = e^\hat{S} c_k e^{-\hat{S}} \). We obtain explicitly

\[
p_0 = c_0 + \frac{g\omega_0}{\sqrt{2}} \left[ \frac{b}{2t - \omega_0} + \frac{b^\dagger}{2t + \omega_0} \right] c_\pi
\]

(7)

\[
p_\pi = c_\pi - \frac{g\omega_0}{\sqrt{2}} \left[ \frac{b}{2t - \omega_0} + \frac{b^\dagger}{2t + \omega_0} \right] c_0
\]

(8)

These operators are fermionic (they satisfy the anticommutation relations), with the property \( p_{k,k'}^\dagger p_k |k'; n\rangle = \delta_{k,k'} |k; n\rangle \). This means that the eigenstate \( |k; n\rangle \) contains one polaron of momentum \( k \). As concern the phonons, we can proceed the same way, introducing a new operator \( \mathcal{B} = e^\hat{S} b e^{-\hat{S}} \) which describes a renormalized boson or phonon. Explicitly, one obtains

\[
\mathcal{B}^\dagger \mathcal{B} = b^\dagger b + \frac{g\omega_0}{\sqrt{2}} \left[ \frac{b^\dagger}{2t - \omega_0} - \frac{b}{2t - \omega_0} \right] c_\pi^\dagger c_0 + \frac{g\omega_0}{\sqrt{2}} \left[ \frac{b}{2t - \omega_0} - \frac{b^\dagger}{2t + \omega_0} \right] c_0^\dagger c_\pi
\]

(9)

Again, this operator is diagonal with \( \mathcal{B}^\dagger \mathcal{B} |k; n\rangle = n |k; n\rangle \). We therefore conclude that the state \( |k; n\rangle \) contains one polaron of momentum \( k \) and \( n \) renormalized phonons. The total momentum of the state is \( K = k \) if \( n \) is even and \( K = k + \pi \) if \( n \) is odd. Then we write the eigenenergies as \( E_n(k) = \varepsilon_n^* \pm t_n^* \). One obtains

\[
\varepsilon_n^* = n\omega_0 - \frac{g^2\omega_0}{2} \frac{4t^2 - 2\omega_0^2}{4t^2 - \omega_0^2}
\]

(10)

\[
t_n^* = t \left\{ 1 + \frac{g^2\omega_0^2}{4t^2 - \omega_0^2} (2n + 1) \right\}
\]

(11)

For \( n \) phonons or renormalized phonons in the system \( t_n^* \) corresponds to the fermionic (polaronic) excitation energy. In the polaron problem, we restrict ourselves to the case \( n = 0 \), that is we create a polaron from the vacuum,
\( |k; 0\rangle = p_k^\dagger |0\rangle \). We are left with \( \varepsilon^* = \varepsilon_0^* \) which is the polaron binding energy and \( t^* = t_0^* \) which represents the hopping integral of the polaron. If we take \( g = 0.4 \) and \( \omega_0 = 10/11t \) we obtain \( \varepsilon^* = -0.0538t \) and \( t^* = 1.042t \) while exact diagonalization \( \text{III} \) gives \( \varepsilon^* = -0.0576t \) and \( t^* = 1.038t \). We notice the enhancement of the bandwidth for this two site system.

In term of the renormalized operators, the Hamiltonian can now be written in a block diagonal form,

\[
H = \sum_k E_0(k)p_k^\dagger p_k + \frac{1}{2i} \sum_k [E_1(k) - E_0(k)] B^\dagger B p_k^\dagger p_k
\]

\[
+ \frac{1}{3i} \sum_k [E_2(k) - 2E_1(k) + E_0(k)] B^\dagger B^2 p_k^\dagger p_k + \ldots
\]

(12)

The original electron phonon interaction which contained off diagonal transitions between subspaces with the same number of particle (electron or phonon) has been eliminated: there is no more off diagonal interactions between the polaron and the renormalized phonons.

### III. GENERAL CASE

Next, we consider finite size systems for which numerical results have been obtained \( \text{III} \). Let \( |\tilde{n}\rangle \) be the state with the configuration of phonons \( \{\tilde{n}\} \) such that \( b_{q_i}^\dagger b_{q_i}|n_q\rangle = n_q|\tilde{n}\rangle \). The basis vector are then \( |k; \tilde{n}\rangle = c_{\tilde{n}}^\dagger |\tilde{n}\rangle \). The eigenstates are given by \( |k; \tilde{n}\rangle = \varepsilon^*|k; \tilde{n}\rangle \). Now we use the fact that the state \( |\tilde{n}\rangle \) contains no electron, so that \( \varepsilon^*|\tilde{n}\rangle = |\tilde{n}\rangle \). Using the definition of the polaron operator \( p_k = e^{S_k} c_k e^{-S} \), we obtain the desired relation, \( p_k^\dagger |\tilde{n}\rangle = |k; \tilde{n}\rangle \). In other words, the operator \( p_k^\dagger \) acting on the state \( |\tilde{n}\rangle \) with the configuration \( \{\tilde{n}\} \) of bare phonons, gives the eigenstate \( |k; \tilde{n}\rangle \) which contains one polaron of momentum \( k \) and the configuration \( \{\tilde{n}\} \) of renormalized phonons. Defining \( B_q = e^{S_k} c_k e^{-S} \), we therefore obtain \( B_q^\dagger B_q |k; \tilde{n}\rangle = n_q|k; \tilde{n}\rangle \). This is the straightforward generalization of the results obtained for the two site system.

Using second order perturbation theory the polaron dispersion is given by

\[
E(k) = \varepsilon_k + \frac{g^2 \omega_0^2}{M} \sum_q \frac{1}{\varepsilon_k - \varepsilon_{k+q} - \omega_0}
\]

(13)

This is a well known result obtained by many approaches \( \text{III} \). This dispersion relation corresponds to a state with one polaron of momentum \( k \) and zero renormalized phonons. The next excited states correspond, for example, to states with one polaron of momentum \( k \) and one renormalized phonon of momentum \( q \). The total momentum of these states is therefore \( K = k + q \). The energy of such a state is given by

\[
E(k; q) = E(k) + \omega_0 + \frac{g^2 \omega_0^2}{M} \left[ \frac{1}{\varepsilon_k - \varepsilon_{k+q} + \omega_0} + \frac{1}{\varepsilon_k - \varepsilon_{k-q} - \omega_0} \right]
\]

(14)

As concern the corresponding unitary transformation, it has been discussed by Fröhlich \( \text{III} \) and is given by

\[
S = -\frac{g \omega_0}{\sqrt{M}} \sum_q \left\{ \frac{b_q}{\varepsilon_k + \omega_0 - \varepsilon_{k+q}} + \frac{b_{-q}^\dagger}{\varepsilon_k - \varepsilon_{k+q} - \omega_0} \right\} c_{k+q}^\dagger c_k
\]

(15)

We now discuss the excitation spectrum of the system in the weak coupling limit and consider a one dimensional system for simplicity with the bare electron dispersion \( \varepsilon_k = -2t \cos(k) \).

Our basic assumptions are a) that the dispersion of the polaron \( E(k) \) is slightly renormalized from the bare electron dispersion relation \( \varepsilon_k \) and b) the system is large enough so that the phonon frequencies are slightly renormalized, so that \( E(k; q) \approx E(k) + \omega_0 \). The ground state corresponds to the state with a single polaron of momentum \( k = 0 \), with energy \( E(0) \). The state of momentum \( K \) with the lowest energy can be either the state with one polaron of momentum \( k = K \) and no renormalized phonons or either the state with one polaron of momentum \( k = 0 \) and one renormalized phonon of momentum \( q = K \) such that \( K = k + q \). The corresponding energies are respectively \( E(K) \) and \( E(0) + \omega_0 \). Within our assumptions on \( E(k) \), there exists a threshold \( K^* \) such that \( E(0) + \omega_0 = E(K^*) \). For \( K < K^* \) the lowest energy is \( E(K) \) and the state contains only one polaron of momentum \( k = K \). For \( K > K^* \) the lowest energy is \( E(0) + \omega_0 \) and the state contains one polaron of zero momentum and one renormalized phonon
of momentum \( q = K \). As far as the others excitations are concerned, their construction is straightforward. If we compare this spectrum with the results of Ref. [4], where this spectrum was computed, we find a nice agreement in the case of a weak coupling. The flat part in the spectrum is just the energy \( E(0) + \omega_0 \). We further notice that for \( K < K^* \), these numerical results show that the polaron dispersion \( E(k) \) is slightly renormalized from the bare electron dispersion \( \varepsilon_k \).

**IV. CONCLUSION**

In conclusion, we have shown that for any coupling, one can define a renormalized electron of momentum \( k \) and some renormalized bosons of momentum \( q \), such that the spectrum is made up of these renormalized excitations. The renormalized operators can be obtained via an unitary transformation. This was worked out explicitly in the weak coupling limit using perturbation theory. Recent finite size studies support our approach.

In the crossover regime, where level crossings arise in the spectrum of the Hamiltonian, it is not possible to define the unitary transformation perturbatively and it is not clear how to make some quantitative predictions.

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**FIG. 1.** The dispersion of the polaron for a one dimensional lattice with \( \omega_0 = 0.8 \) and \( g^2 \omega_0 = 0.1 \). Energies are in unit of \( t \), solid line is the bare electron dispersion, dotted line is the slight polaron dispersion and dashed line is the lowest excitation as discussed in the text.
dispersion relation

dispersion relation

$K$