Polaronic Band Structure of Holstein Model *

WAN Shao-Long (完绍龙)[1,2], WANG Ke-Lin (汪克林)[2]
[1]CCAST (World Laboratory), P.O. Box 8730, Beijing 100080
[2]Department of Astronomy and Applied Physics, University of Science and Technology of China, Hefei 230026

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A new concise approach is presented for analytic study of the properties of the Holstein model. New analytic results for the polaronic band structure and phonon distribution, of the Holstein molecular crystal model, are given in one dimension. And all analytic results given are in accordance with the known numerical research results.

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Research on polarons has recently gained renewed interest[1-6] on account of the observation of the polaronic effects in several important classes of materials.[7] It is well known that the very fundamental problem of a single tight-binding electron coupled locally to a set of noninteracting Einstein oscillators (Holstein model[8]) has not been solved exactly, i.e., no satisfactory description of the full spectral properties has been obtained so far. Furthermore, as yet none of the various analytical treatment, based on variational approaches[9] or on weak-coupling[10] and strong-coupling adiabatic[8] and nonadiabatic[11-13] perturbation expansions, is suitable for the investigation of the physically most interesting transition region. For this reason, many numerical researches, such as the (quantum) Monte Carlo simulation,[14,15] the exact diagonalization,[1,2,16] and the global-local variational method,[4] have been completed in the Holstein model. In this letter, the polaronic band structure and phonon distribution of the Holstein model are studied by using a concise approach.

The Holstein model has been studied extensively as paradigmatic model for polaron formation in systems with dominant short-range electron-lattice interactions. The Hamiltonian of the Holstein model reads

$$H = -t\sum_{ij}\left(c_i^\dagger c_j + c_j^\dagger c_i\right) + \omega\sum_i b_i^\dagger b_i + g\sum_i c_i^\dagger c_i\left(b_i^\dagger + b_i\right), \tag{1}$$

where $c_i(c_i^\dagger)$ and $b_i(b_i^\dagger)$ are the annihilation (creation) operators of a (spinless) fermion and a boson (phonon) at Wannier site i, respectively. And $g = -\sqrt{\epsilon_p\omega}$, ϵ_p denotes the electron–phonon coupling constant and ω is the bare phonon frequency. When the free electron transfer is restricted to the nearest-neighbour pairs, the Hamiltonian (1) can be rewritten as

$$H = -t\sum_i\left(c_{i+1}^\dagger c_i + c_{i-1}^\dagger c_i\right) + \omega\sum_i b_i^\dagger b_i + g\sum_i c_i^\dagger c_i\left(b_i^\dagger + b_i\right). \tag{2}$$

In order to study the Holstein model, we assume that the wave functions of the system take the following form

$$|\psi_n\rangle = \sum_l \varphi_l c_l^\dagger |A_l\rangle, \tag{3}$$

where, considering periodic boundary conditions on a one-dimension lattice of N sites, the phase factor φ_l is expressed as

$$\varphi_l = \frac{1}{\sqrt{N}}\exp(\mathrm{i}k_n l), \qquad k_n = \frac{2\pi n}{N}, \quad (n = 0, 1, \cdots, N), \tag{4}$$

and while, the wave function of the phonons is assumed as

$$|A_l\rangle = \exp\left[\sum_i\left(-\frac{1}{2}\mid\alpha_{l,i}\mid^2 + \alpha_{l,i}b_i^\dagger\right)\right]|0\rangle, \tag{5}$$

where $\alpha_{l,i}$ is the function of the wave vector k_n.

If this state is really a solution of the Holstein model, it should obey the Schrödinger equation

$$H|\psi_n\rangle = E_n|\psi_n\rangle. \tag{6}$$

Substituting Eqs. (2) and (3) into the Schrödinger equation (6), we obtain

$$-t\sum_l \varphi_{l-1}c_l^\dagger|A_{l-1}\rangle - t\sum_l \varphi_{l+1}c_l^\dagger|A_{l+1}\rangle + \omega\sum_{l,i}\varphi_l\alpha_{l,i}b_i^\dagger c_l^\dagger|A_l\rangle + g\sum_l\varphi_l\left(b_l^\dagger + \alpha_{l,l}\right)c_l^\dagger|A_l\rangle = E_n\sum_l\varphi_l c_l^\dagger|A_l\rangle. \tag{7}$$

In addition, based on the wave function of the phonons, Eq. (5), we get

$$|A_{l\pm1}\rangle = \exp\left[\sum_i\left(\alpha_{l\pm1,i} - \alpha_{l,i}\right)b_i^\dagger\right]|A_l\rangle. \tag{8}$$

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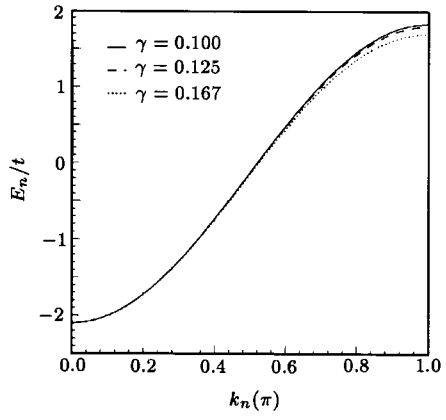

Fig. 1. Polaronic band dispersion E_n given by Eq.(13) at $\epsilon_p = 0.1$ for various phonon frequencies $\gamma = 0.1, 0.125$, and 0.167 in the case of the weak-coupling.

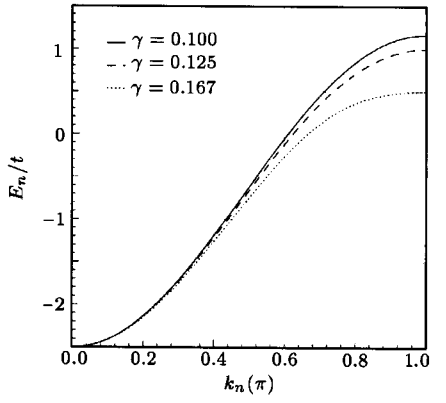

Fig. 2. Polaronic band dispersion E_n is given by Eq.(13) at $\epsilon_p = 0.5$ for various phonon frequencies $\gamma = 0.1, 0.125$, and 0.167 in the case of the intermediate-coupling.

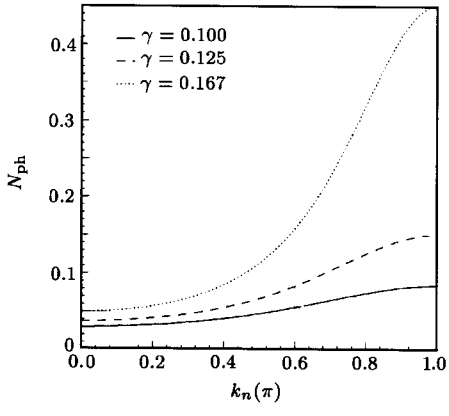

Fig. 3. Phonon distribution given by Eq. (14) at $\epsilon_p = 0.1$ for various phonon frequencies $\gamma = 0.1, 0.125$, and 0.167 which respond to Fig. 1.

Inserting Eq. (8) into Eq. (7), then comparing the terms of $c_l^\dagger|A_l\rangle$ and $b_i^\dagger c_l^\dagger|A_l\rangle$ respectively, we obtain that the energy of the system and $\alpha_{l,i}$ satisfy the following equations

$$E_n = g\alpha_{l,l} - t\left(\frac{\varphi_{l-1}}{\varphi_l} + \frac{\varphi_{l+1}}{\varphi_l}\right) = g\alpha_{l,l} - 2t\cos k_n, \quad (9)$$

$$-\frac{\varphi_{l-1}}{\varphi_l}t\left(\alpha_{l-1,l} - \alpha_{l,l}\right) - \frac{\varphi_{l+1}}{\varphi_l}t\left(\alpha_{l+1,l} - \alpha_{l,l}\right) + \omega\alpha_{l,l} + g = 0. \quad (10)$$

If we assume the relations

$$\alpha_{l\pm j,l} = \alpha_{l,l}\exp\left(\mp jik\right) = \alpha\exp\left(\mp jik\right), \quad (11)$$

we obtain

$$\alpha = -\frac{g_0}{1 - 2\gamma\left(1 - \cos k_n\right)}, \quad (12)$$

where $\gamma = t/\omega$ and $g_0 = g/\omega$.

Put Eq. (12) into Eq. (9), we obtain the polaron energy band

$$E_n = -\left[\frac{g_0^2}{1 - 2\gamma\left(1 - \cos k_n\right)} - 2\gamma\cos k_n\right]\omega, \quad (13)$$

the energy formula is analytic when $\gamma < 1/4$. According to Eq. (13), we start with the study of the weak-coupling case and give the energy band dispersion at $\epsilon_p = 0.1$ for phonon frequencies $\gamma = 0.1, 0.125$, and 0.167 in the non-adiabatic regime in Fig. 1.

For the intermediate-coupling case, we give the energy band structures of the electron-phonon couplings $\epsilon_p = 0.5$ for phonon frequencies $\gamma = 0.1, 0.125$, and 0.167 in the non-adiabatic regime in Fig. 2.

According to the wave function, the phonons distribution can be obtained with the form

$$N_{ph} = \langle\psi_n|\sum_j b_j^\dagger b_j|\psi_n\rangle = \sum_j\left(\alpha_{l,l+j}^*\alpha_{l,l+j}\right), \quad (j = 0, \pm1, \pm2, \cdots),$$

where $\alpha_{l,l\pm j}$ was given from above. The phonons distributions of the system, which respond to Figs. 1 and 2, are shown, by Eq. (14), in Figs. 3 and 4, respectively.

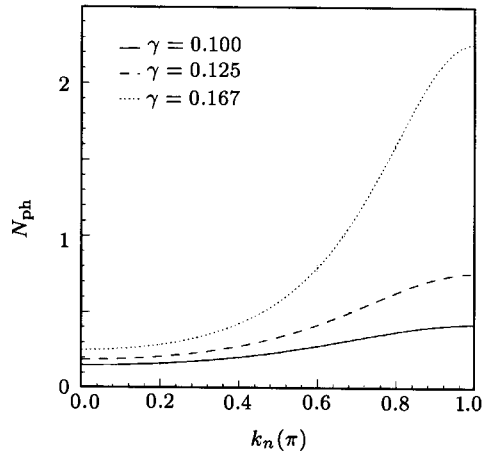

Fig. 4. Phonon distribution given by Eq. (14) at $\epsilon_p = 0.5$ for various phonon frequencies $\gamma = 0.1, 0.125$, and 0.167 which respond to Fig. 2.

In this letter, a new concise approach has been presented for analytic study of the properties of the Holstein model. Analytic results for the polaronic band structure and phonon distribution of the Holstein molecular crystal model are given. All of our results are compared with the numerical research results obtained recently. The comparisons show that they are in accordance with the numerical research results obtained recently,[1] as shown in Figs. 1 and 2, and our analytic formula of the energy band structure is valid from weak-coupling to intermediate-coupling in the non-adiabatic regimes. The phonon distributions of the Holstein model, which respond to Figs. 1 and 2, are shown in Figs. 3 and 4, respectively. Particularly, N can be any integral number ($N \geq 4$) in our analytic results. In all figures, N is chosen as 40 as an example.

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