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Abstract. We analyse the validity ranges of the adiabatic and anti-adiabatic approximations for a model with electron–electron and electron–phonon interactions for a three-site cluster. This model describes the motion of apical oxygen atoms in $YBa_2Cu_3O_7$. We show that the adiabatic approximation still applies for critical infrared coupling where the gap between the ground state and first excited electronic state becomes nearly equal to the double-well potential barrier. For this high coupling value, the motion of holes and ions is already highly correlated. We arrive at the non trivial conclusion that in this model the adiabatic approximation is valid even in a parameter region where the electronic energy scale is not much larger than the phononic energy scale. This approximation is able to describe polaronic effects which have been shown to appear in the infrared absorption spectrum in previous exact numerical calculations. We also investigate the range of validity of the anti-adiabatic approximation. We find that the window where none of the above-mentioned approximations is valid shrinks with decreasing on-site repulsion U until it closes at $U = 0$ in agreement with other work in the literature.

Results from recent EXAFS [1, 2] and Raman [3] experiments on the compound $YBa_2Cu_3O_7$ have been interpreted in terms of a highly anharmonic potential for the apex oxygen motion along the c axis, although this interpretation has been debated lately [4, 5]. On the other hand, a model that ascribes this behaviour to strong electron–phonon interactions has been proposed [6]. We have shown [7] (for the response to this comment see [8]) that the adiabatic approximation can account for the anharmonicity and the optical response of the proposed model system [6]. Regardless of the physical motivations, the model considered provides a non-trivial testing ground for the validity of adiabatic as well as anti-adiabatic approximations in systems with both strong electron–electron and electron–phonon interactions. The purpose of this work is to analyse the criterion for the validity of the above-mentioned approximations and to determine the ranges where these approximations are valid. We consider the Holstein–Hubbard model of [6] for two apex oxygen atoms O(4) and a chain copper atom Cu(1) in $YBa_2Cu_3O_7$:

$$H = H_{el} + H_{ph} + H_{el-ph} \tag{1}$$

where

$$H_{el} = \sum_{\sigma} \sum_{i=1}^{3} \epsilon_i n_{i\sigma} + U \sum_{i=1}^{3} n_{i\uparrow} n_{i\downarrow} + t \sum_{\sigma} [(c_{1\sigma}^{\dagger} c_{2\sigma} + c_{3\sigma}^{\dagger} c_{2\sigma}) + \text{HC}] \tag{2}$$

$$H_{ph} = \hbar\omega_{ir}^0 b_{ir}^{\dagger} b_{ir} + \hbar\omega_{R}^0 b_{R}^{\dagger} b_{R} \tag{3}$$

$$H_{el-ph} = -\lambda_R (b_R^{\dagger} + b_R) \sum_{\sigma} 2(n_{1\sigma} - 2n_{2\sigma} + n_{3\sigma}) - \lambda_{ir}(b_{ir}^{\dagger} + b_{ir}) \sum_{\sigma} (n_{3\sigma} - n_{1\sigma}). \tag{4}$$

Here, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ denotes the number operator for holes of spin σ at site i; $i = 1, 3$ indicates the lower and upper O(4) sites, and $i = 2$ the Cu(1) site, with site energies ϵ_i ($\epsilon_1 = \epsilon_3 \neq \epsilon_2$), hopping amplitude t and on-site repulsion U. The ionic charges are taken to be -2 for oxygen atoms and $+1$ for the copper atom, and there are two holes added to the cluster. In the phonon part we include only harmonic Raman- and infrared-active modes, with creation operators $b_R^\dagger$ and $b_{ir}^\dagger$ and frequencies ω_R^0 and ω_{ir}^0, respectively. These operators are related to the Raman and infrared coordinates by

$$u_\alpha = \sqrt{\frac{\hbar}{2m_O\omega_\alpha^0}}(b_\alpha^\dagger + b_\alpha) \tag{5}$$

where $\alpha = \text{ir, R}$.

This model was exactly diagonalized by Mustre de Leon *et al* [6] using a Lanczos algorithm, with a basis of 40 Raman and 40 infrared phonons and the nine states of two holes in the three-site cluster. This corresponds to $40\times40\times9 = 14\,400$ states. They used the following values of the parameters in (1): $\epsilon_{1,3} = -\epsilon_2 = 0.5$ eV, $t = 0.5$ eV, $U = 7.0$ eV, $\omega_R^0 = 500$ cm^{-1}, and $\omega_{ir}^0 = 600$ cm^{-1}. These workers found that the squared many-body ground-state wavefunction develops a double-peak structure in the infrared coordinate for $\lambda_{ir} \simeq 0.12$ eV. In the Raman coordinate there is only a single-peak shift from the bare equilibrium position $u_R = 0$ as λ_R increases, but no double-well structure develops even for $\lambda_R = 0.2$ eV. In addition, they computed the absorption spectrum and obtained peculiar features that were ascribed to non-adiabatic effects.

It is unusual to have exact solutions of physically interesting electron–phonon models where approximate treatments can be checked. Taking advantage of the existence of exact results for (1), we reinvestigate this model for the purpose that we have already mentioned.

In the adiabatic approximation the phononic coordinates are treated classically, and the electronic ground state is computed exactly in terms of these quantities. The corresponding ground-state energy $E_0(u_{ir}, u_R)$ is later used as the potential function in a Schrödinger equation for the ionic dynamics. To solve this equation we use a basis of 15 Hermite polynomials for each coordinate. On the other hand, in the anti-adiabatic approximation, for arbitrarily fixed electronic configuration we first determine the equilibrium phonon coordinates and its corresponding total (phononic plus electronic) energy. Then we construct a 9×9 matrix containing these energies in the diagonal and the hopping energies as off-diagonal elements. The diagonalization of this matrix produces finally the groundstate and first excited state of the cluster.

The criterion used in the literature for the validity of the adiabatic approximation is that the electronic excitation energies are much higher than the phonon energies [9–11]. We shall see in the following that, even when this criterion is not satisfied for the parameters used in the present model, the adiabatic treatment is able to reproduce the energies and wavefunctions of the many-body states well. The validity of the wavefunctions is verified for an integral physical property, namely the infrared absorption spectra. On the other hand, the anti-adiabatic approximation is expected to hold as long as the electronic excitation energies are negligible compared with the phonon energies [10]. This is satisfied at very large electron-phonon couplings.

The result of the adiabatic calculation of $E_0(u_{ir}, u_R)$ as a function of λ_{ir} shows a double-well structure in the infrared coordinate for $\lambda_{ir} \geqslant 0.11$ eV, while in terms of u_R it presents a single minimum whose position depends on λ_R (in the following, we shall always consider the Raman coupling $\lambda_R = \lambda_{ir}$ for $\lambda_{ir} \leqslant 0.10$ eV, and $\lambda_R = 0.10$ eV for $\lambda_{ir} \geqslant 0.10$ eV, as was done in [6]). This is in fairly good quantitative agreement with the probability distribution obtained in [6] using the exact wavefunction, which develops two peaks for $\lambda_{ir} \geqslant 0.12$ eV.
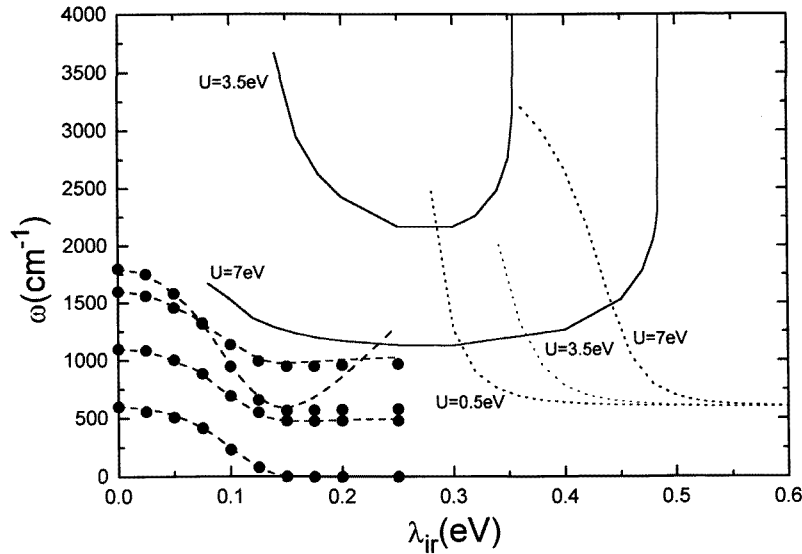
Figure 1. Energies of the first four allowed dipolar transitions from the many-body ground state for $U = 7$ eV in the adiabatic approximation (- - - -), and exact results from [6] (●), together with the energies of the dipolar transitions in the anti-adiabatic approximation for different values of U (······). We also show the electronic energy difference between the first excited state and ground state with the ions at their equilibrium positions (——), for different values of U.

The splitting between peaks in the exact calculation reaches 0.125 Å for $\lambda_{ir} \simeq 0.13$ eV, in agreement with the experimental value of 0.13 Å from EXAFS [1]. We obtain this separation between the two minima of $E_0(u_{ir}, u_R)$ for a slightly smaller $\lambda_{ir} \simeq 0.12$ eV. We wish to point out that a double-well structure in the infrared coordinate is also obtained in a model for the chains of $YBa_2Cu_3O_7$ where the electron–phonon interaction is introduced as a modulation of the hopping integral [12]. In our calculation, the dimensionless infrared coupling where the double well develops is approximately $\lambda = 0.7$ (as defined in [12]), close to the value of 1.1 found in the above-mentioned work. It is important to note that these values of the coupling constants are much larger than the values obtained by analysing experimental data through strong-coupling calculations for several phonons in $YBa_2Cu_3O_7$ ($\lambda \sim 0.01$) [13, 14]. We also note that the infrared coupling neccesary for the existence of the double-well structure in our calculation is of the order of the total electron–phonon coupling obtained by first-principles calculations for the sum over all modes in $YBa_2Cu_3O_7$ [15]. We wish to point out that a systematic study of the validity of the adiabatic approximation is important in that it allows the analysis of larger systems. For example, it may be useful to give more support to some conclusions arrived at in [12]. One of them is that there is a strong interaction between chains and basal planes in $YBa_2Cu_3O_7$, a fact that should explain structural parameter changes with doping.

We solve the Schrödinger equation for the ionic movement using the obtained $E_0(u_{ir}, u_R)$ as the potential energy. The lowest infrared allowed transitions are shown in figure 1, where they are compared with the exact values. As can be seen, the agreement is excellent up to $\lambda_{ir} \simeq 0.16$ eV . Note also that the first excited electronic level for both $U = 7$ eV and 3.5 eV lies not far above the highest vibrational level considered. As we have already mentioned, this means that the usual criterion for the validity of the adiabatic approximation
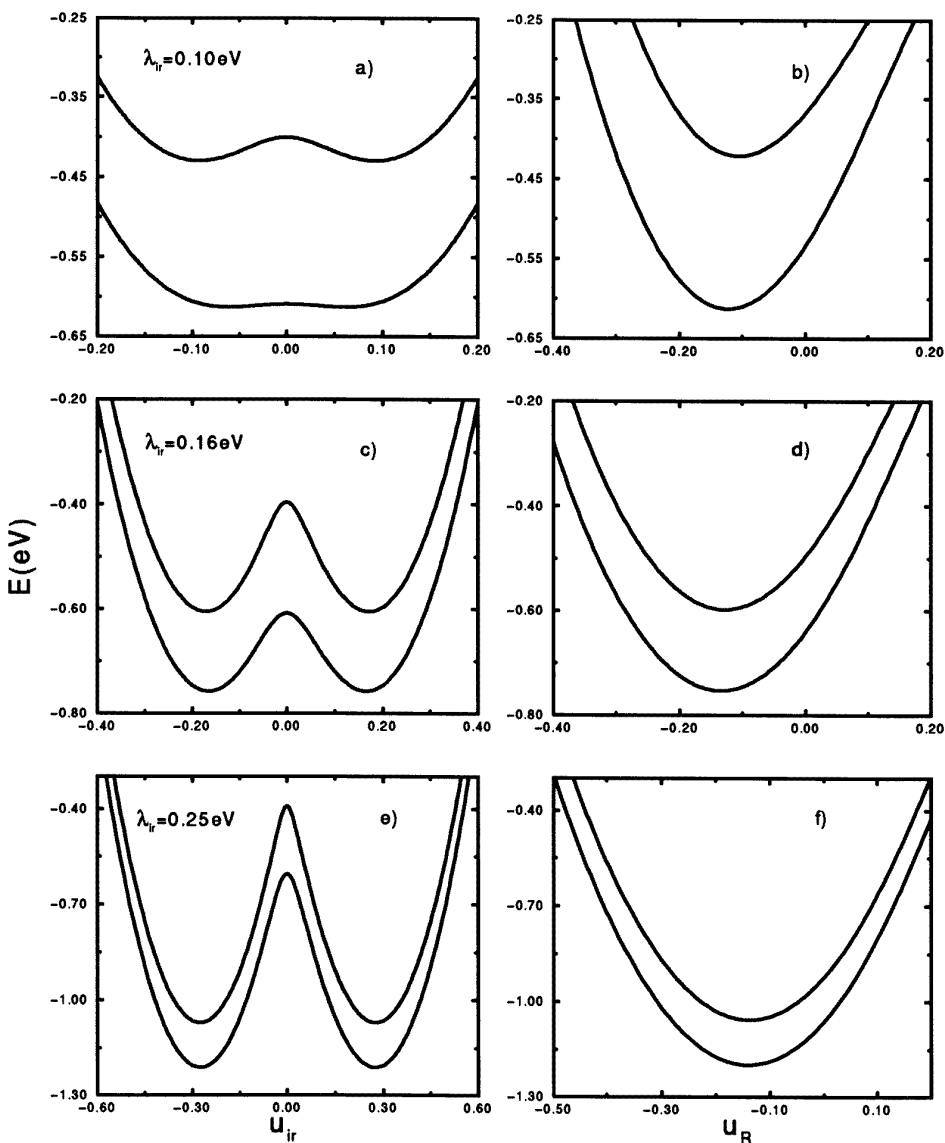
Figure 2. Energies of the two lowest electronic levels as a function of (a), (c), (e) the infrared and (b), (d), (f) the Raman coordinates: (a), (b) $\lambda_{ir} = 0.10$ eV; (c), (d) $\lambda_{ir} = 0.16$ eV; (e), (f) $\lambda_{ir} = 0.25$ eV. The units of the infrared and Raman coordinates are angströms.

is not fulfilled; yet this approximation is still valid. For $\lambda_{ir} > 0.16$ eV, the adiabatic approximation fails at least to reproduce the energies of one band, which corresponds to three infrared phonons at $\lambda_{ir} = 0$. This band should tend to the bare infrared frequency of 600 cm^{-1}, as we can see for the exact results, but at $\lambda_{ir} \simeq 0.16$ eV it begins to increase steadily in energy. The other low-energy bands depicted are well reproduced also at very strong couplings ($\lambda_{ir} \simeq 0.25$ eV) where they approach constant values. Note that the energy of the lowest band (which is the tunnelling frequency when the double well develops)

tends to zero because of the increasingly large barrier of the double-well potential at high couplings. The limits for the other bands are the frequencies of one Raman mode and two Raman modes. To understand this picture, and therefore the regime of validity of the adiabatic approximation, we plot in figure 2 the electronic energies of the ground states and first excited states for different values of λ_{ir}. Figures 2(a), 2(c) and 2(e) show these energies as functions of u_{ir}, where u_R was fixed at the minimum of the ground-state energy. Conversely, in figures 2(b), 2(d) and 2(f) we see the same energies as a function of u_R, having set u_{ir} at one of the degenerate ground-state minima. The adiabatic approximation works well as long as the ions oscillate around the minimum of the ground-state energy and no transition to the first excited electronic level occurs. For $\lambda_{ir} = 0.1$ eV, we observe in figure 2(a) and 2(b) a nearly constant energy gap between the two lowest electronic levels. Thus the ionic motion along the infrared (figure 2(a)) or Raman (figure 2(b)) coordinates would hardly produce an electronic transition to the higher level since this implies a higher energy cost than the energy increase due to their oscillations around the electronic ground state minimum. Note that this argument is valid in spite of the fact that the gap is only 2.5 times larger than the bare infrared frequency! On the other hand, we can see in figure 2(c) for $\lambda_{ir} = 0.16$ eV that, in order to jump across the barrier between the two minima of the double-well ground-state potential, the ions have to lose an energy of the order of the gap between the two lowest electronic levels. In consequence, there is a large chance of an electronic transition, a fact that breaks the validity of the adiabatic approximation. Moreover, for $\lambda_{ir} = 0.25$ eV we can see in figure 2(e) that the gap between the lowest electronic levels is much smaller than the double-well barrier. Then, the probability of an electronic transition becomes high as λ_{ir} increases beyond the critical value $\lambda_{ir} = 0.16$ eV. This produces the deviation from the exact results of the band with infrared character for $\lambda_{ir} > 0.16$ eV (see figure 1). According to the exact results this band approaches the energy of one infrared mode for large coupling.

In the Raman mode, the ions oscillate around a single minimum, and the gap between the two electronic levels is considerably larger than the energies involved in the oscillatory motion, even for large values of λ_{ir} (see figures 2(d) and 2(f)). Note that the gap in figure 2(f) is about 0.14 eV, only 30% smaller than the corresponding value in figure 2(b)). Then, the adiabatic approximation holds for the bands with Raman character, as is seen in figure 1 (see the bands at 500 and 1000 cm^{-1} from $\lambda_{ir} = 0.16$ eV up to values of $\lambda_{ir} = 0.25$ eV).

Below the range of existence of the double-well structure ($\lambda_{ir} < 0.11$ eV) the electronic ground state is the antisymmetric combination of the states with both oxygen sites occupied by holes. When the double well develops, the ground state becomes the antisymmetric combination of states with holes at the copper and oxygen sites. At a certain large value of the infrared coupling, the electronic ground state changes abruptly, becoming the symmetric combination of states with both holes sitting at the oxygen site (see the nearly infinite slope of the difference energy between the first excited state and the ground state at $\lambda_{ir} \simeq 0.48$ eV for $U = 7$ eV, one of the full lines in figure 1). This behaviour is interpreted by the fact that the large infrared distortion favours the occupation of both holes at the same oxygen site in spite of the on-site repulsion U. For smaller values of U, this change in the electronic ground state occurs at smaller values of the infrared coupling (see also the full line for $U = 3.5$ eV in figure 1).

In order to check the anti-adiabatic approximation we perform calculations starting with very large values of λ_{ir}. We obtain in this case a nearly degenerate ground state with both holes sitting almost entirely in one of the two oxygen sites. This is in accordance with the exact results obtained in [6], namely that at large values of λ_{ir} there is a freezing of holes at the oxygen sites which results in harmonic oscillations with the bare infrared

frequency around the new equilibrium positions of the ions. As λ_{ir} decreases, the two nearly degenerate levels start to split. For $U = 7$ eV their separation becomes about 10% of the infrared mode energy for $\lambda_{ir} \simeq 0.48$ eV. The last value is just the critical coupling where there is an abrupt change in the electronic ground state as we have already mentioned (note that, in figure 1, the region where the levels start to split for $U = 7$ eV nearly coincides with that where the electronic energy slope tends to infinity). For smaller values of this coupling, the holes are no longer frozen at the oxygen site and they have a non-zero probability of jumping to the copper ion. Therefore, we consider this critical coupling (which produces the above-mentioned level separation) as roughly the limit of validity of the approximation. For smaller values of U the anti-adiabatic approximation continues to be valid for smaller values of λ_{ir}, as shown in figure 1. Since in the adiabatic region the first excited electronic state energy increases with decreasing U, this approximation also extends its range of validity. This conclusion is also reinforced by the fact that, for smaller U, the infrared coupling where the double well develops is larger (for $U = 3.5$ eV, the double well appears at $\lambda_{ir} = 0.16$ eV). Therefore, the window where none of the approximations is valid shrinks with decreasing U. According to [10], this window closes at $U = 0$.

A stringent test on the validity of the adiabatic approximation is reproducing the main features of the exact optical absorption spectrum found in [6]. We have evaluated the imaginary part of the dielectric function

$$\epsilon(\omega) = \sum_j \frac{S_j \omega_j^2}{\omega_j^2 - \omega^2 - i\omega\gamma} \tag{6}$$

where the oscillator strengths S_j and the dipole-moment operator p are as follows:

$$S_j = |\langle j|p|0\rangle|^2 \tag{7}$$

and

$$p = -\left[8\left(1 + \frac{2m_O}{m_{Cu}}\right)\right]^{1/2} u_{ir} + \sum_\sigma \left(R_0 - \frac{u_R}{\sqrt{2}}\right)(n_{3\sigma} - n_{1\sigma})$$

$$+ \sum_\sigma \left(1 + \frac{2m_O}{m_{Cu}}\right)^{1/2} \frac{u_{ir}}{\sqrt{2}}(n_{3\sigma} + n_{1\sigma}). \tag{8}$$

In this equation, $R_0 = 1.87$ Å is the equilibrium Cu–O distance, and we take for the full width the value $\gamma = 0.34$ cm^{-1}. In order to evaluate S_j we used our approximated $\Psi_j(u_{ir}, u_R)$, with j restricted to the first four allowed dipolar transitions. This is enough to compare with the reported exact results. In the integration on u_{ir}, u_R it is important to take into account properly the dependences of $n_{3\sigma}$ and $n_{1\sigma}$ on these variables. This requires calculation of the electronic ground state at every integration step. The spectrum obtained is shown in figure 3(a) for $\lambda_{ir} = 0.13$ eV, together with the exact results from [6]. The more subtle feature of the spectrum is peak B (well defined in our case) which Mustre de Leon *et al* assigned to non-adiabatic effects. In our calculations it arises owing to both the dependence of the electronic wavefunction on phononic coordinates, and the non-separability of the effective potential $E_0(u_{ir}, u_R)$. Using a rigid double-well potential [1, 2], peak B does not appear [6]. Peak A is centred at the tunnelling frequency between the two minima of the double well in the infrared coordinate. We found $\omega_A = 53$ cm^{-1}, which should be compared with the exact value of 52 cm^{-1}. It is worth mentioning that, for $\lambda_{ir} = 0.15$ eV near the critical infrared coupling where the adiabatic approximation begins to fail, we have $\omega_A = 9.5$ cm^{-1} which is still fairly close to the exact value of 8 cm^{-1} [6]. In our case the peak A intensity is about six times larger than that of peak C. In the
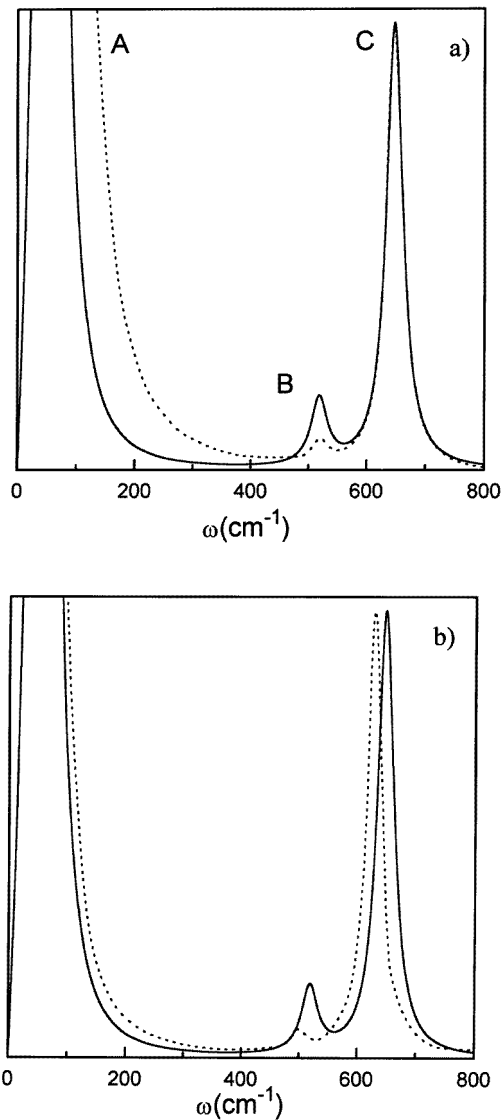
Figure 3. Infrared absorption spectrum in arbitrary units for $U = 7$ eV, $\lambda_R = 0.1$ eV, and $\lambda_{ir} = 0.13$ eV: ———, adiabatic approximation; - - - -, exact results for (a) $\lambda_{ir} = 0.13$ eV from [6], and (b) $\lambda_{ir} = 0.133$ eV from [16].

caption to figure 2 in [6] it is mentioned that this ratio is about 10. Nevertheless, with a small change in λ_{ir} (from 0.130 to 0.127 eV) we obtained the same ratio and very small changes in the rest of the spectrum: shifts of less than 3% in the frequencies at which peaks B and C are centred, and a 7% of increase in peak B intensity. Conversely, our results for $\lambda_{ir} \simeq 0.130$ eV have even better agreement with the exact results for $\lambda_{ir} \simeq 0.133$ eV of [16] (see figure 3(b)). Then, for a slightly different λ_{ir} all the features of the exact spectrum are reproduced qualitatively and, to a reasonable extent, also quantitatively. Note also that a decrease in λ_{ir} leads to an enhancement of peaks A and B, which reinforces the idea that
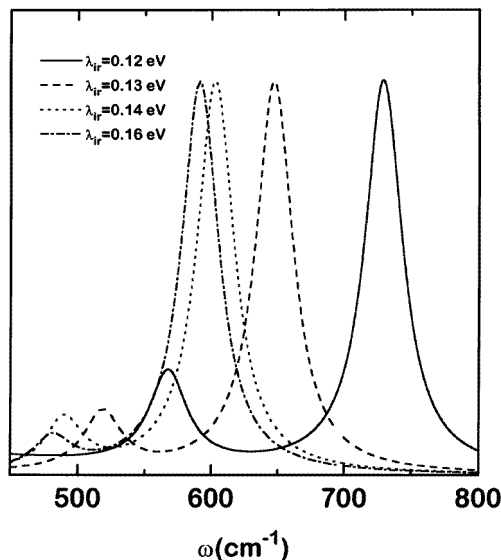
Figure 4. Infrared absorption spectrum in arbitrary units for $U = 7$ eV, showing only peaks C and B in the adiabatic approximation for different values of λ_{ir}.

non-adiabatic effects are not relevant to the appearance of peak B. We show in figure 4 how the intensity of peak B decreases in the adiabatic approximation, tending to zero as λ_{ir} is increased (the intensities of peak C were fixed to be all equal for all the couplings showed, owing to the arbitrary nature of the units). This feature shows at least qualitatively that the wavefunction of peak B tends correctly to the region where it has Raman character and zero oscillator strength. The same occurs for the mode whose frequency tends to $2\omega_R^0$, but its intensity is smaller than that of peak B. We also see the correct tendency of the frequencies for the modes C and B (the centre of the peaks) which nearly approach ω_{ir}^0 and ω_R^0 respectively, as λ_{ir} increases to $\lambda_{ir} \simeq 0.16$ eV (see also figure 1). The intensity of peak A at $\lambda_{ir} = 0.13$ eV is ten times the value corresponding to $\lambda_{ir} = 0.14$ eV, showing also the correct qualitative tendency as λ_{ir} increases. Note that we can only suggest the above-mentioned tendencies because at $\lambda_{ir} = 0.16$ eV the adiabatic approximation begins to fail. Nevertheless, these tendencies are in accordance with the exact results, where for large enough values of λ_{ir} the absorption spectrum converges to a single peak at ω_{ir}^0 [6].

In conclusion, the adiabatic approximation is valid for the system considered in a context where the electronic energy scale is not much larger than the phononic energy scale. This approximation fails for an infrared coupling regime where the gap between the ground state and first excited electronic level becomes smaller than the double-well potential barrier. As for the low-energy infrared absorption spectrum, this failure affects only a band which has infrared character and should approach ω_{ir}^0 for large λ_{ir}. On the other hand, the approximation reproduces the bands which tend to ω_R^0 and $2\omega_R^0$ at large λ_{ir}. This is explained by the fact that the gap between the ground state and first excited electronic level is larger than the energy variations associated with the Raman mode. We have also determined the validity range of the anti-adiabatic approximation, which holds at very large couplings where the holes are nearly frozen at the oxygen site. The window where none of the approximations is valid shrinks with decreasing U. The validity of the many-body wavefunction is verified

for the infrared absorption spectrum, where we can also reproduce a peculiar feature that arises as a small peak in the exact results. This peak is due to a mixing of the Raman and infrared modes through the electron–phonon correlations. It is worth mentioning that the infrared reflectivity of La_2CuO_4 shows a low-frequency shoulder for the peak of the stretching mode [17]. In previous work, we conclude that this feature should be ascribed to a polaronic excitation [18]. Photoinduced carrier experiments [19] show a bleaching for the stretching mode that supports this interpretation. Infrared reflectivity measurements on chemically doped samples also detect with increasing oxidation the above-mentioned low-frequency shoulder of the stretching mode [20]. It would be interesting to analyse in future work with an electron–phonon model and within the adiabatic approximation the possibility of finding such a feature in the absorption spectra and therefore in the reflectivity bands. Note that this feature may be analogous to the small peak B found, but considering the possibility of polaron formation through the mixing of the stretching and other phononic modes with carriers due to the strong electron–phonon interaction.

Finally, we have shown that the proper use of the adiabatic and anti-adiabatic approximations reproduces the exact results in a model with strong electron–electron and electron–phonon interactions, for most of the parameter range. Moreover, all the relevant features of the physics involved are correctly described by these approximations.

Acknowledgments

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