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Dynamical two electron states in a Hubbard-Davydov model

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Abstract. We study a model in which a Hubbard Hamiltonian is coupled to the dispersive phonons in a classical *nonlinear* lattice. Our calculations are restricted to the case where we have only two quasi-particles of opposite spins, and we investigate the dynamics when the second quasi-particle is added to a state corresponding to a minimal energy single quasi-particle state. Depending on the parameter values, we find a number of interesting regimes. In many of these, discrete breathers (DBs) play a prominent role with a localized lattice mode coupled to the quasiparticles. Simulations with a purely *harmonic* lattice show much weaker localization effects. Our results support the possibility that DBs are important in HTSC.

PACS. 71.38.-k Polarons and electron-phonon interactions – 63.20.Pw Localized modes – 63.20.Ry Anharmonic lattice modes

1 Introduction

In spite of the many studies [1–5] made since it was first discovered [6], high temperature superconductivity (HTSC) remains a challenge. The nature of the carriers and the mechanism behind pair formation are still unclear. According to many researchers, HTSC can be explained by a purely electronic model, such as that described by the $t-J$ or the Hubbard Hamiltonians, for which charge and/or spin interactions are paramount. This view is essentially based on the absence of isotope effects seen in some experiments [7] and the apparent d-symmetry of the superconducting wavefunction. However, accumulating experimental evidence exists for electron-lattice effects in high temperature superconductors [8–10], and theories based on electron-phonon interactions have also been proposed [2–5]. Here we follow the idea that both electronic correlations and electron phonon interactions are important [12] and study a model in which a Hubbard Hamiltonian is coupled to dispersive phonons. Our main aim is to explore one extra ingredient, which has generally been ignored until now, the importance of the anharmonic character of lattice vibrations. Whilst our ultimate aim is to understand HTSC, here we propose a specific mechanism for pair formation that involves the interaction of polarons through a nonlinear lattice mode, which will have applications in other areas. We study the stability of such a pair as a function of the electron-electron (or hole-hole) interaction.

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2 The Hubbard-Davydov Hamiltonian

The Hamiltonian $\hat{H}$ we use has three parts:

$$\hat{H} = \hat{H}_{\rm qp} + \hat{H}_{\rm qp-ph} + H_{\rm ph} \tag{1}$$

where $\hat{H}_{\rm qp}$ is the Hamiltonian for a quasiparticle with spin $\frac{1}{2}$, $\hat{H}_{\rm qp-ph}$ describes the interaction of the quasiparticle with the lattice and $H_{\rm ph}$ is the lattice (phonon) Hamiltonian.

The Hamiltonian for the quasiparticle is the 1D Hubbard Hamiltonian:

$$\hat{H}_{\rm qp} = \epsilon \sum_{n,\sigma} \left(\hat{c}^\dagger_{n\sigma}\hat{c}_{n\sigma}\right) + \gamma \sum_n \hat{c}^\dagger_{n\uparrow}\hat{c}_{n\uparrow}\hat{c}^\dagger_{n\downarrow}\hat{c}_{n\downarrow} - t \sum_{n,\sigma}\left(\hat{c}^\dagger_{n\sigma}\hat{c}_{n-1\sigma} + \hat{c}^\dagger_{n\sigma}\hat{c}_{n+1\sigma}\right) \tag{2}$$

where the sums are over the sites n, going from 1 to N, (N is the total number of lattice sites) and σ refers to the spin and can be up or down. $\hat{c}^\dagger_{n\sigma}$ is the creation operator for a quasiparticle of spin σ at site n. ϵ is the self-energy of the quasiparticle, t the transfer term for the quasiparticle to move between neighbouring sites. We depart from the usual notation in that the on-site quasiparticle-quasiparticle coupling is here designated as γ (and not U) to avoid confusion with the variables $\{u_n\}$ used for lattice displacement (see below). Both negative and positive values of γ will be considered, corresponding to the attractive and repulsive Hubbard models, respectively.

As in the Davydov model for energy transfer in proteins [13], $\hat{H}_{\rm qp-ph}$, the Hamiltonian for the interaction of the quasiparticle with the lattice includes the coupling to acoustic (or Debye) phonons:

$$\hat{H}_{\rm qp-ph} = \chi \sum_{n,\sigma} \left[(u_{n+1} - u_{n-1}) \left(\hat{c}^{\dagger}_{n\sigma} \hat{c}_{n\sigma} \right) \right] \quad (3)$$

where χ is a parameter which describes the strength of the quasiparticle-lattice interaction. Many previous publications have included electron-phonon interactions in the framework of the model of Holstein [14], in which only short-range interactions are are considered. As has been pointed out elsewhere [15], when the electron screening is poor, such as in cuprates, electron-phonon interactions are long range, which can be described by acoustic phonons.

The phonon Hamiltonian is as follows:

$$H_{\rm ph} = H^{\rm co}_{\rm ph} + H^{\rm os}_{\rm ph}$$

$$H^{\rm co}_{\rm ph} = \frac{\kappa a^2}{72} \sum_{n=1}^{N} \left[\left(\frac{a}{a + u_n - u_{n-1}} \right)^{12} - 2 \left(\frac{a}{a + u_n - u_{n-1}} \right)^{6} \right]$$

$$H^{\rm os}_{\rm ph} = \kappa' \sum_{n=1}^{N} \left(\frac{1}{2} u_n^2 + \frac{1}{4} u_n^4 \right) + \frac{1}{2M} \sum_{n=1}^{N} p_n^2 \quad (4)$$

where u_n is the displacement from equilibrium position of site n, p_n is the momentum of site n, a is the equilibrium distance between sites, κ is the elasticity of the nonlinear lattice and κ' is a similar constant for the on-site potential. Here, the coupling interactions between sites are described by a Lennard-Jones potential, $H^{\rm co}_{\rm ph}$, a potential commonly used to describe interactions between atoms. In a high temperature cuprate, this potential describes the interactions of the copper and oxygen atoms in one Cu-O layer. The on-site potential $H^{\rm os}_{\rm ph}$ is as used in many breather studies [16]. It can be considered to represent the effect, in a mean field approach, of the rest of the crystal on the one dimensional chain whose states are studied explicitly. In a cuprate, this models the effect of the neighbouring layers on the Cu-O layer.

Our Hamiltonian (1–4) includes two sources of nonlinear effects. The first comes from the intrinsic nonlinearity of the Lennard-Jones potential, $H^{\rm co}_{\rm ph}$ and the on-site potential, $H^{\rm os}_{\rm ph}$. The second source of nonlinearity is extrinsic and comes from the interaction of the quasiparticle with the lattice (cf. Eq. (3)). The former is the source of nonlinearity in the studies of discrete breathers [16] and the latter is the cause of localization in polaron theory.

We adopt a mixed quantum-classical approach in which the lattice is treated classically, while the quasiparticle is treated quantum mechanically. Accordingly, the displacements u_n and momenta p_n are real variables. The quasiparticle variables are operators, a distinction which is marked by the hats above the operators. The importance of quantum effects of the lattice can be assessed by considering the full quantum model at finite temperature, which has already been done for the Davydov Hamiltonian. It was found that, at 0.7 K, the lattice displacement correlated with the position of the quantum particle in exact semiclassical Monte Carlo simulations differed by 15% from the corresponding variable in exact simulations in the fully quantum system. At 11.2 K, the two approximations lead to virtually the same value [17]. We would like to emphasize that the approximation we consider here is *not* an adiabatic approximation. In an adiabatic approximation the kinetic energy of the phonons is neglected with respect to the kinetic energy of the quantum particle. We do not do that here, as our dynamical equations, equations (6) and (7) below, include the time derivative of the momenta of the lattice sites. What we do is to consider that the dynamics of the lattice can be treated classically. Both the semiclassical (or quantum/classical, as we prefer to call it to differentiate from other use in the literature) approach we apply here and the adiabatic approximation lead to similar results when we consider the ground states of the system (because the corresponding solutions have zero kinetic energy), but they are different when we deal with dynamics, as we do in this work.

The arguments above suggest that our mixed quantum/classical approach results may give a good approximation to the full quantum solution, but we stress that our results are only strictly valid in this approximation, and require confirmation by a full quantum simulation. In addition, the need for a full quantum treatment comes from comparison with experimental results, since isotopic effects can only be described in a fully quantum framework. Our main aim here is to explore the importance of anharmonicity in the lattice for the dynamics of paired states, something which is much more complicated to do within a fully quantum formalism. Thus, as a first approximation, we restrict ourselves to the mixed quantum-classical regime and study the behaviour of a pair of quasiparticles, coupled to a nonlinear lattice.

With these assumptions, the exact two quasiparticle wavefunction for the Hamiltonian (1–4) is:

$$|\psi(t)\rangle = \sum_{n,m=1,N} \phi_{nm}(\{u_n\}, \{p_n\}, t)\, \hat{c}^{\dagger}_{n\uparrow}\, \hat{c}^{\dagger}_{m\downarrow} |0\rangle \quad (5)$$

where ϕ_{nm} is the probability amplitude for a quasiparticle with spin up to be at site n and a quasiparticle with spin down to be at site m. The probability amplitude is dependent on the lattice displacements and momenta in a way that is not specified a priori and is determined by the equations of motion. Similarly to other systems [18], the equations of motion for probability amplitudes ϕ_{nm} are derived by inserting the wavefunction (5) in the Schrödinger equation for the Hamiltonian (2–4), and the equations for the displacements and momenta are derived from the Hamilton equations for the classical functional $\mathcal{E}^2 = \langle \psi | \hat{H} | \psi \rangle$. They are:

$$\imath\hbar \frac{d\phi_{jl}}{dt} = -t\left(\phi_{j-1l} + \phi_{j+1l} + \phi_{jl-1} + \phi_{jl+1}\right) + \gamma \phi_{jl} \delta_{jl} + \chi\left(u_{j+1} - u_{j-1} + u_{l+1} - u_{l-1}\right)\phi_{jl} \quad (6)$$

$$\frac{dp_j}{dt} = -\frac{\partial H_{\rm ph}}{\partial u_j} - \chi\left(|\varphi^{\uparrow}_{j-1}|^2 - |\varphi^{\uparrow}_{j+1}|^2 + |\varphi^{\downarrow}_{j-1}|^2 - |\varphi^{\downarrow}_{j+1}|^2 \right) \quad (7)$$

where $|\varphi_j^{\uparrow}|^2$, the probability for the quasiparticle with spin up to be in site j and $|\varphi_j^{\downarrow}|^2$, the probability for the quasiparticle with spin down to be in the same site. These are given by:

$$|\varphi_j^{\uparrow}|^2 = \langle\psi|\hat{c}_{j\uparrow}^{\dagger}\hat{c}_{j\uparrow}|\psi\rangle = \sum_{l=1}^{N}|\phi_{jl}|^2,$$

$$|\varphi_j^{\downarrow}|^2 = \langle\psi|\hat{c}_{j\downarrow}^{\dagger}\hat{c}_{j\downarrow}|\psi\rangle = \sum_{l=1}^{N}|\phi_{lj}|^2.$$

3 Dynamical states

We consider the case in which the quasiparticle density is low and the starting point is that of an isolated quasiparticle interacting with the lattice. We wish to find if the addition of a second quasiparticle with opposite spin to that state can lead to pairing of the two quasiparticles, and how the relative stability of the paired state depends on the quasiparticle-quasiparticle interaction γ.

We start from the state of a single quasiparticle. The wavefunction is

$$|\psi_{\sigma}^{1}\rangle = \sum_{n}\phi_n^1\hat{c}_{n|\sigma}^{\dagger}|0\rangle. \tag{8}$$

Minimum energy states for this one quasiparticle can be found by numerical minimization of the energy functional $\mathcal{E}^1 = \langle\psi^1|\hat{H}|\psi^1\rangle$ with respect to the probability amplitude for a single quasiparticle in site n, ϕ_n^1, and to the displacements u_n [19]. Two kinds of minimum energy states are found. For sufficiently large quasiparticle-lattice interaction χ, the quasiparticle states are localized and there is an associated lattice distortion. We call this the single particle polaron, or simply polaron. Below a threshold value for χ, the states are delocalized, as in the usual Bloch states, and the lattice is undistorted. We have considered a value of χ and other parameters such that the initial one quasiparticle polaron state is neither too weak nor too stable when compared with delocalized, Bloch states for the same values. While it is important to find the behaviour of the two quasiparticle states considered here for different values of the parameters, our choice ensures that the results here are not the consequence of extreme values.

The dynamical states we study are the perturbations of the single polaron state, induced by the presence of a second quasiparticle with opposite spin. Because the number of variables ϕ_{nm} that characterize the wavefunction (5) increases with the square of the lattice size, in order to be able to integrate the equations of motion for a sufficiently long time, the size of the lattice was kept relatively short, i.e. the number of sites is $N = 20$. The aim is to investigate the influence of the strength and sign of the quasiparticle-quasiparticle interaction γ on the dynamics of the paired quasiparticle states.

The parameters of the simulations in the figures are the same, except for the quasiparticle-quasiparticle interaction γ. In Figure 1 we set $\gamma/t = -10$ in an *attractive* Hubbard model. The addition of a second quasiparticle leads to a localized state for the pair, with a very slight

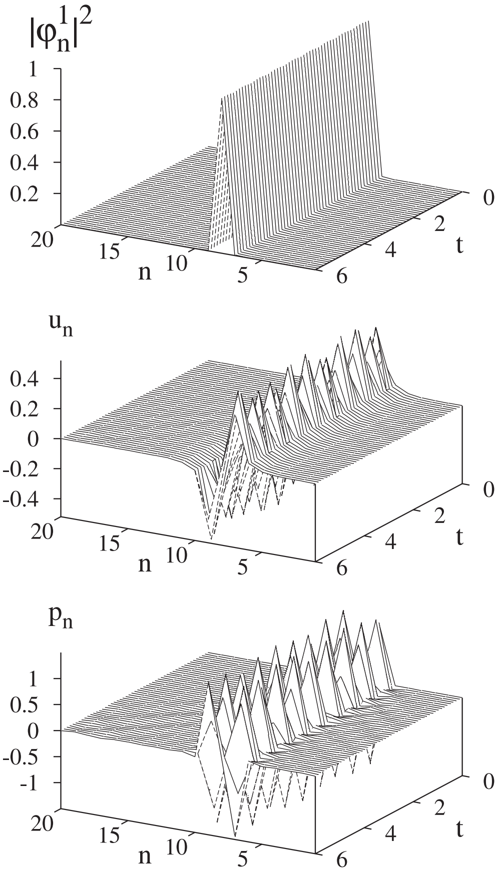

Fig. 1. Time dependence for (a) the probability for one quasiparticle to be in site n, ($n = 1 \cdots N$, $N = 20$), (b) the lattice displacement and (c) the momentum of site n. Time is in picoseconds. The parameters are $t = 10 \times 10^{-22}$ J, $\chi = 100$ pN, $\kappa = 1$ N/m, $\kappa' = 2\kappa$, $a = 4.5$ Å and $\gamma = -100 \times 10^{-22}$ J.

peak oscillation, that is hardly visible in the figure. (The probability for the second quasiparticle is the same as that shown and is not displayed.) The lattice, however, sets into a breather-like oscillation [16], i.e., a localized excitation with an internal oscillation. Indeed, at the site of the initial lattice distortion, oscillations are clearly visible in the lattice displacements and momenta. A striking observation is that the amount of radiation generated is very small, and most of the energy of the lattice is associated with the breather. Figure 2, which displays another 6 ps period of the dynamics at a later time, demonstrates the stability of this solution.

A Hubbard Hamiltonian with a much weaker attraction, corresponding to a ratio of $\gamma/t = -0.5$, is considered in Figure 3, where the last 6 picoseconds of a 42 picosecond simulation are displayed. A modulation of the peak of the probability distribution is now clearly seen, which has the same frequency as the main modulation of the lattice breather. The modulation of the quasiparticle probability is associated with a periodic change of shape in which a lower peak with a slight tail appears. Even at this comparatively much weaker interaction, the amount of radiation is very small and most of the lattice energy is in the

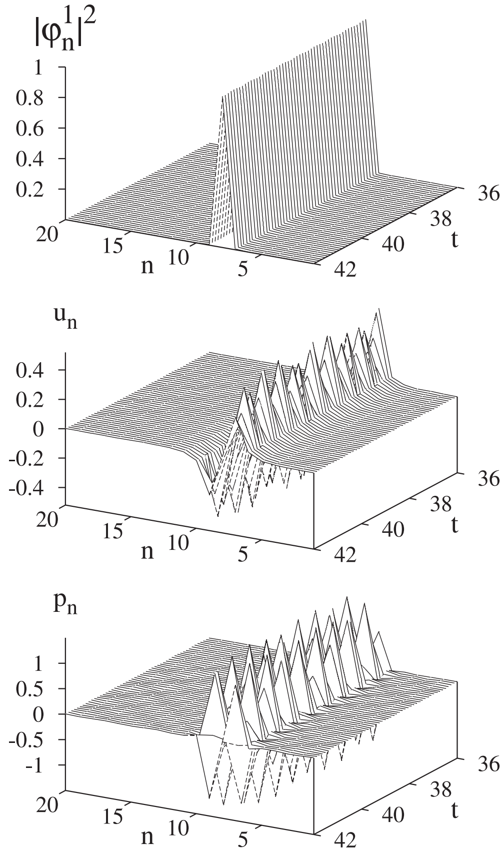

Fig. 2. Same as Figure 1, at a later time.

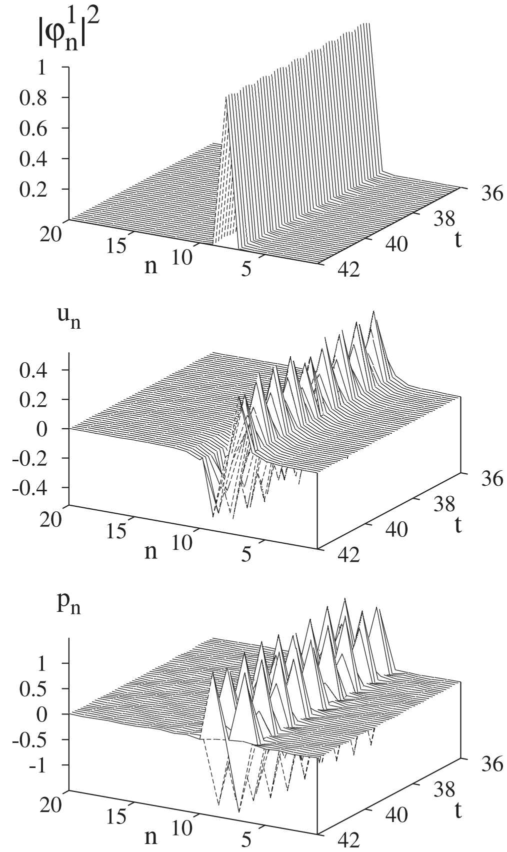

Fig. 3. Same as Figure 1, but with $\gamma = -5 \times 10^{-22}$ J.

breather. The frequency of the main modulation of the breather is as for $\gamma/t = -10$.

In Figure 4 a *repulsive* Hubbard Hamiltonian is considered, with $\gamma/t = +0.5$. The modulations and the associated tails of the probability distribution for the quasiparticle are now more pronounced, but their main frequency is unchanged. Although there is a slight increase in the radiation in the lattice, the stability of the breather and of the quasiparticle solution is apparent.

In Figure 5 the repulsive interaction is increased to $\gamma/t = +1$. The modulations in the probability distribution for the quasiparticles lead to greater periodic changes of shape, still with the same frequency as for the other values of γ. The radiation in the lattice is now more visible, but the breather remains stable.

In Figures 6 and 7, a large repulsive value, corresponding to $\gamma/t = 5$ is taken. This leads to a change in the probability distribution for the quasiparticles, from a single site peak into a two site peak, with periodic oscillations which make one probability at one site larger than the other. The lattice variables show that, concurrently with the appearance of the breather, a considerable amount of radiation is generated. Also noticeable is the fact that the frequency of the modulations has changed. Figure 7 shows that the new quasiparticle probability distribution is stable, as well as the lattice breather, even if the noise which results from successive passes of the radiation through the periodic boundaries, constitutes a significant part of the lattice energy.

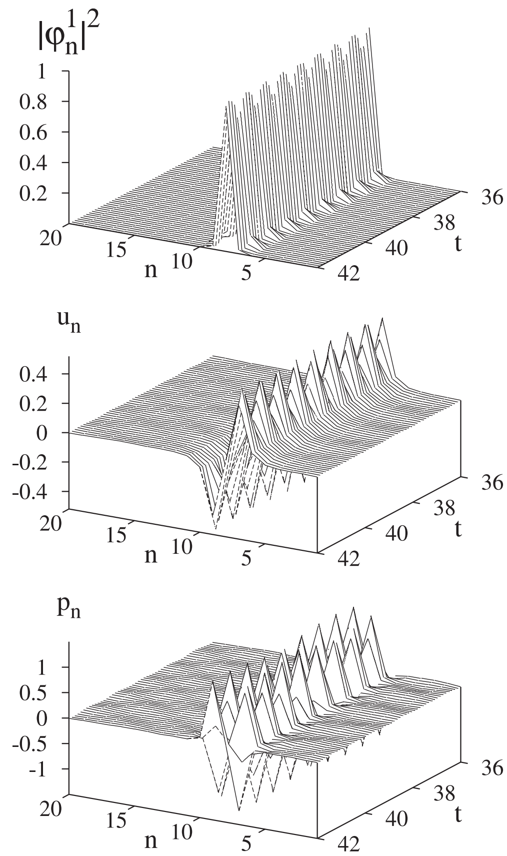

Fig. 4. Same as Figure 1, but with $\gamma = +5 \times 10^{-22}$ J.

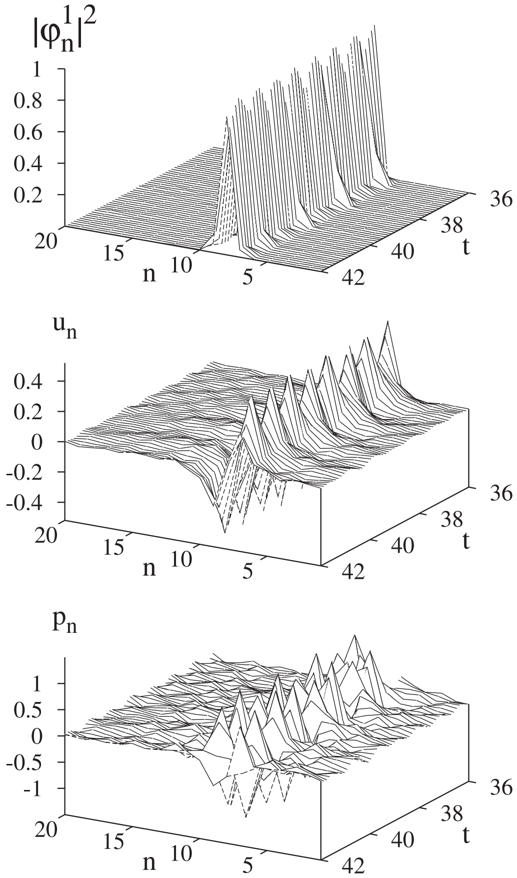

Fig. 5. Same as Figure 1, but with $\gamma = +10 \times 10^{-22}$ J.

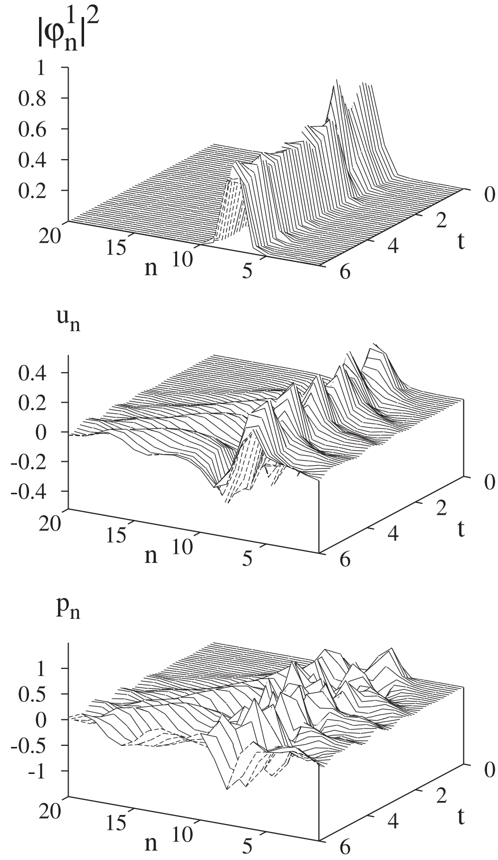

Fig. 6. Same as Figure 1, but with $\gamma = +50 \times 10^{-22}$ J.

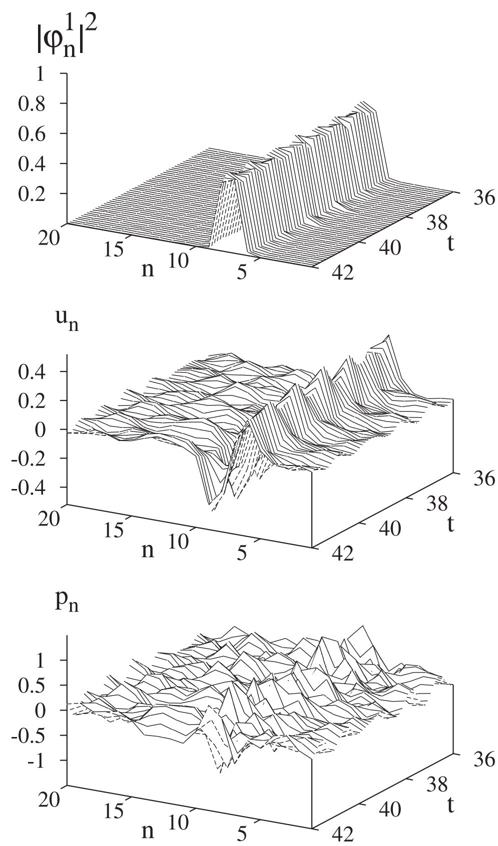

Fig. 7. Same as Figure 6, but at a later time.

In Figures 8 and 9, a repulsive interaction corresponding to $\gamma/t = 10$ is used. Figure 8 shows that a drastic transformation takes place in which the initial distribution changes into a two peak distribution. One of the peaks is located where the initial lattice distortion was and the second peak is as far away from it as it can be in this lattice. Also, while the peak that is located at the original lattice distortion site remains unmodulated in time, as well as its associated lattice distortion, the second peak oscillates with approximately the same frequency as that in Figures 6 and 7. The momenta in Figure 8 show clearly that the second peak has an associated lattice breather, while the first peak is associated with a distortion that is essentially static. After some time, because of the repeated reflection of the radiation from the boundaries, this picture is not so clear. Both peaks show oscillations in the displacements and the momenta of the lattice are rather noisy. However, Figure 9 does illustrate the stability of the two peak solution, even in the presence of such relatively large amount of noise.

4 Dynamical states in the fully harmonic approximation

The early theory of pair formation via interaction with phonons assumed that the lattice motion was harmonic. It

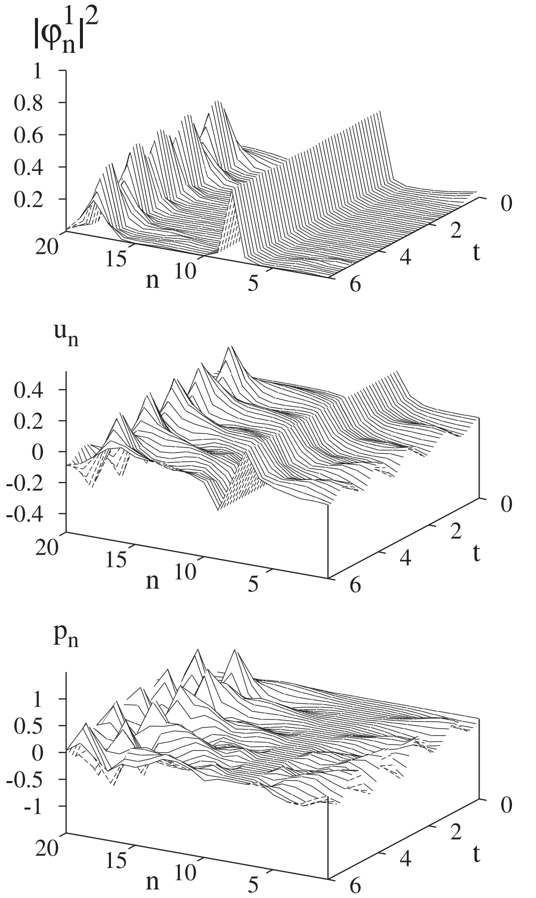

Fig. 8. Same as Figure 1, but with $\gamma = +100 \times 10^{-22}$ J.

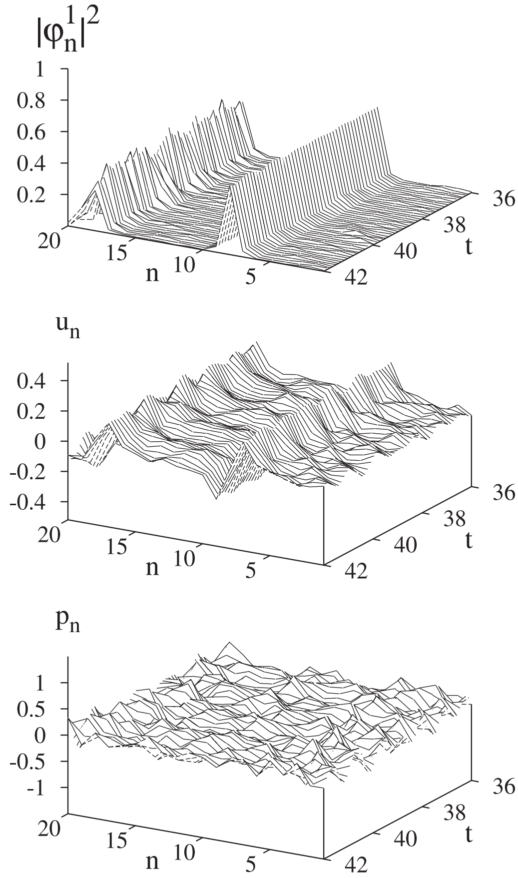

Fig. 9. Same as Figure 6, but at a later time.

is interesting to see how the dynamics of the two electron states would be in this case, and this section is devoted to that question. The first two terms (2), (3) in the Hamiltonian we consider in this section are the same as before, but now the phonon Hamiltonian is given by:

$$H_{\rm ph}^{\rm harm} = H_{\rm ph}^{\rm co-harm} + H_{\rm ph}^{\rm os-harm} \tag{9}$$

$$H_{\rm ph}^{\rm co-harm} = \frac{1}{2}\,\kappa \sum_{n=1}^{N} (u_n - u_{n-1})^2 ,$$

$$H_{\rm ph}^{\rm os-harm} = \kappa' \sum_{n=1}^{N} \left(\frac{1}{2} u_n^2\right) + \frac{1}{2M} \sum_{n=1}^{N} p_n^2 .$$

The phonon Hamiltonian (9) can be obtained from (4) by considering the limit of small displacements, in which only the linear terms remain. In this case, the only nonlinear term left for the total Hamiltonian is that which describes the quasiparticle-lattice interaction. It should be pointed out that, if we disregard the correlation term in (2), the equations of motion for this system are those studied by a number of authors [14,20] for a single single polaron, and for any number of polarons by Alexandrov [21].

Figure 10 shows that when the effective interaction is such that $\gamma/t = -10$, the addition of an extra electron to the minimum energy single polaron leads to a state in which both electrons are in the same site with a strong lattice deformation of breather type associated with their presence. The time evolution of the momenta, however, shows that there is no breather formation, only phonons which travel along the lattice. Because of the periodic boundary conditions, these phonons eventually come back and after they have crossed each other many times the lattice becomes very noisy. The lattice deformation associated with the two electrons oscillates periodically because of the interference of these phonons, but does not move. Also, the state of the two electrons remains localized on one site all the time.

Similar dynamics takes place for $\gamma/t = -0.5$, except that very slight oscillations in the probability distribution for the electron states also takes place (not shown).

When the electron-electron interaction is repulsive and such that $\gamma/t = +5$, the phonon emission leads to fluctuations in the electron probability distribution that are clearly visible in Figure 11. The dynamics is similar to that of Figure 10, with phonons propagating along the lattice and causing oscillations in the otherwise constant distortion induced by the two electrons. Again, the momenta show that there is no breather formation and all the dynamics of the lattice is due to the phonon propagation and interference.

For a repulsive interaction for which $\gamma/t = +10$, the two electrons split up and the probability distribution

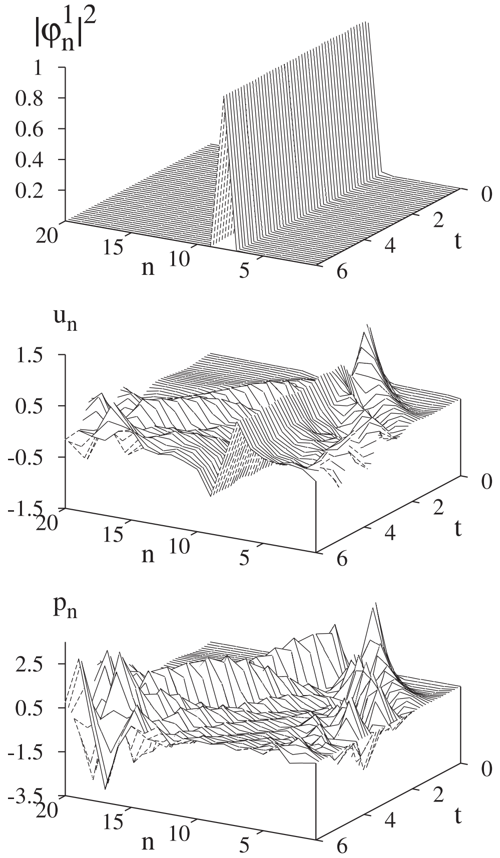

Fig. 10. Same as Figure 1, but with $\gamma = -100 \times 10^{-22}$ J and for the harmonic lattice (9).

shows two peaks, both of which have an associated lattice deformation with the breather profile (see Fig. 12). Phonons are generated from each of these locations and their interference eventually leads to a noisy lattice. The two peaks in the probability distribution for the electrons oscillate in a less regular fashion than in the anharmonic lattice, but remain stable throughout the simulation. It should be noticed that for this harmonic approximation also, the lattice displacements induced by the electrons/holes are not small. Hence, an accurate representation of the dynamics should include the nonlinear terms in the lattice Hamiltonian, as was done in the previous section.

5 Discussion

Our aim was to investigate the relative stability of a correlated pair of quantum quasiparticles with opposite spins with respect to their uncorrelated states. The starting point was thus the state of a single quasiparticle polaron and we studied the dynamic states which arise when a second quasiparticle is added to the first state. The Hamiltonian used includes several physical ingredients. On the one hand, it contains two sources of nonlinearity, one intrinsic to the lattice and another which arises from the quasiparticle lattice interaction. Such nonlinear lattices have been shown to possess generic solutions known

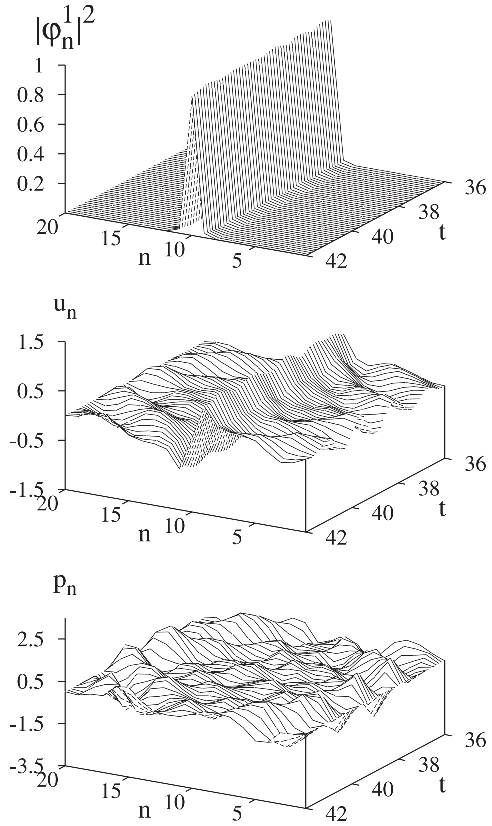

Fig. 11. Same as Figure 1, but with $\gamma = +50 \times 10^{-22}$ J and for the harmonic lattice (9).

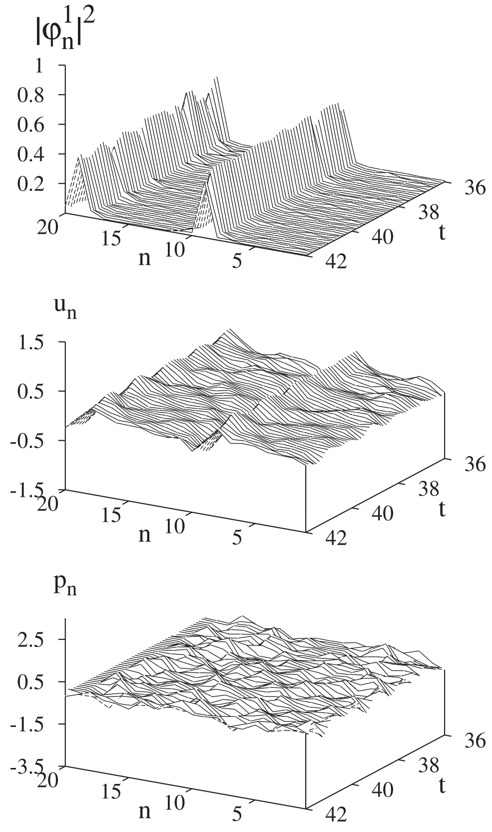

Fig. 12. Same as Figure 1, but with $\gamma = +100 \times 10^{-22}$ J and for the harmonic lattice (9).

as discrete breathers (DBs) [16]. The study of systems in which nonlinear lattices are coupled to one quantum quasiparticle, on the other hand, is just beginning [22,23].

To our knowledge, this is the first time that the coupling of two quantum quasiparticles to a nonlinear lattice has been considered. Indeed, a second ingredient is the inclusion of quasiparticle-quasiparticle interactions, in addition to the quasiparticle-lattice interactions found in the polaron model. The quasiparticle-quasiparticle interactions can represent Coulomb interactions, and/or spin-spin interactions, and be either attractive or repulsive. The dynamical simulations indicate that for these extended systems, DBs are generic solutions also and can be generated by the presence of a second quasiparticle. These lattice breathers can in turn stabilise localized, paired, quasiparticle states, for a large range of γ values. Windows of γ were found for which similar solutions are obtained. Thus, for a ratio of γ/t between -10 and $+1$ (Figs. 1–5), DBs are found in the lattice and in the quasiparticle, with the same main modulation frequencies. For larger values of γ/t, two different solutions were found (see Figs. 6–9). In one solution the quasiparticles distribution is split into equal values in two neighbouring sites and in the second a two peak distribution, with the peaks as far apart as possible in the lattice used, is observed.

This Hamiltonian includes the two main physical causes for quasiparticle pairing that have been considered in HTSC and allows for interpolation between them, by varying the strength of the relevant parameters. According to our results, a greater importance of quasiparticle-lattice interactions in pair formation should arise in systems for which the dynamics of the lattice is fast enough compared to the quasiparticle dynamics, so that the lattice relaxes when the two quasiparticles meet. Conversely, a corresponding greater importance of quasiparticle-quasiparticle interactions should be associated with systems in which the lattice dynamics is much slower than the quasiparticle dynamics.

An implicit assumption in this study is that the nonlinear character of the lattice plays an important role in HTSC. Although the lattice distortions are weak in conventional superconductors, and thus the lattice dynamics can be approximately described by a linear system, we argue that in HTSC these distortions are such that the lattice enters a nonlinear regime. This may be why the sound velocity decreases by a few parts per million in conventional superconductors, whereas in a high T_c material there is an increase which is two or three orders of magnitude larger than in the former case. Our simulations with the harmonic lattice show that the percentage of energy transferred to travelling phonons is much larger than for the anharmonic lattice.

The breather-like solutions found in the dynamical simulations are a signature of the nonlinear dynamics of the lattice. The possibility that breathers are associated with HTSC has been suggested elsewhere [24,25]. Our study indicates that DBs are generic excitations in systems governed by the Hamiltonian used here. Moreover, within a certain range of the parameters, the states in which two quasiparticles are paired and coupled to a DB are energetically more favourable than those of uncorrelated quasiparticles. Hence, this study gives weight to the possibility that DBs are important in HTSC.

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