Dynamical two electron states in a Hubbard-Davydov model

L. Cruzeiro-Hansson,* J.C. Eilbeck,† J.L. Marín, and F.M. Russell
Department of Mathematics, Heriot-Watt University, Edinburgh EH14 4AS, U.K.
(Dated: May 22, 2003)

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 electrons of opposite spins, and we investigate the dynamics when the second electron is added to a single polaron, or solitobreather 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, a state we designate as bipolarobreather. We compare these simulations with those obtained for the corresponding purely harmonic lattice. Our results support the possibility that DBs are important in HTSC.

PACS numbers: PACS: 71.38.-k,63.20.PW,63.20.Ry

I. INTRODUCTION.

In spite of the many studies [1, 2] made since it was first discovered [3], the theory of high temperature superconductivity (HTSC) remains a challenge. The nature of the carriers and the mechanism behind pair formation are still unclear. Some argue that the electron-phonon interaction is the main operating force, as in conventional superconductivity, but others think that charge and/or spin interactions are paramount. The model we study, in which a Hubbard Hamiltonian is coupled to the dispersive phonons, includes both effects. It also includes a third ingredient, that is, intrinsic *nonlinearity in the lattice* which is known to lead to localized modes generally designated as *discrete breathers* (DBs) [5]. Previous studies have shown that the structures that lead to HTSC also support breathers [4, 6]. The motivation for this work is the possibility that breathers are an important element in HTSC.

Other studies have considered the states of *two* electrons coupled to *harmonic* lattices [7, 8] or the state of *one* electron coupled to an *anharmonic* lattice [9]. To our knowledge, this is the first study in which the states of *two* electrons coupled to an *nonlinear* lattice are investigated. Whilst our ultimate aim is to understand HTSC, here we propose a specific mechanism for pair formation that involves the interaction of a bipolaron with a breather, which will have applications in other areas. We study the stability of such a pair as a function of the quasiparticle-quasiparticle interaction.

*Present address CCMAR and FCT, Universidade do Algarve, Campus de Gambelas, 8000 Faro, Portugal.; Electronic address: `lhansson@ualg.pt`
†Electronic address: `J.C.Eilbeck@hw.ac.uk`

II. THE HUBBARD-DAVYDOV HAMILTONIAN.

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

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

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

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

$$\begin{aligned}\hat{H}_{\text{qp}} &= \epsilon \sum_{n,\sigma} \left(\hat{a}^{\dagger}_{n\sigma}\hat{a}_{n\sigma}\right) + \gamma \sum_{n} \hat{a}^{\dagger}_{n\uparrow}\hat{a}_{n\uparrow}\hat{a}^{\dagger}_{n\downarrow}\hat{a}_{n\downarrow} \\ &\quad - t \sum_{n,\sigma} \left(\hat{a}^{\dagger}_{n\sigma}\hat{a}_{n-1\sigma} + \hat{a}^{\dagger}_{n\sigma}\hat{a}_{n+1\sigma}\right)\end{aligned} \tag{2}$$

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. $\hat{a}^{\dagger}_{n\sigma}$ 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 displacements (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 [10], $\hat{H}_{\text{qp-ph}}$, the Hamiltonian for the interaction of the quasiparticle with the lattice includes the coupling to acoustic (or Debye) phonons:

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

where χ is a parameter which describes the strength of the quasiparticle-lattice interaction.

The phonon Hamiltonian is as follows:

$$H_{\rm ph} = H_{\rm ph}^{\rm co} + H_{\rm ph}^{\rm os} \tag{4}$$

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

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

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 $H_{\rm ph}^{\rm co}$, a potential commonly used to describe interactions between atoms. The on-site potential $H_{\rm ph}^{\rm os}$ is as used in many breather studies [5]. 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.

Our Hamiltonian Eqs.(3-4) includes two sources of nonlinear effects. The first comes from the intrinsic nonlinearity of the Lennard-Jones potential, $H_{\rm ph}^{\rm co}$ and the on-site potential, $H_{\rm ph}^{\rm os}$. 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 [5] 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. In a classical system, equilibrium thermodynamic quantities that do not involve velocities do not depend on the mass of its components. A consequence in a classical lattice is that isotopic effects on the transition temperatures do not arise. In some cases, this is a limitation of the mixed quantum-classical approach. The importance of quantum effects of the lattice can be assessed by considering the full quantum model, but such an investigation would make the calculations presented here much more difficult to tackle.

Ultimately, the need for a full quantum treatment comes from comparison with experimental results. Evidence for isotopic effects is as controversial as a mechanism for HTSC, with results for [11] and against [12]. The consensus seems to be that isotopic effects are weak, which constitutes an extra *a priori* justification for a classical treatment of the lattice. An isotopic dependence of magnetic quantities [13], on the other hand, is not necessarily evidence for quantum lattice effects, as magnetic variables are dependent on velocities, and thus on the mass of sites, even in a classical system. 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:

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

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 [14], the equations of motion for probability amplitudes ϕ_{nm} are derived by inserting the wavefunction (5) in the Schrödinger equation for the Hamiltonian (3-4), 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:

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

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

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:

$$|\varphi_j^{\uparrow}|^2 = \langle\psi|\hat{a}_{j\uparrow}^{\dagger}\hat{a}_{j\uparrow}|\psi\rangle = \sum_{l=1}^{N}|\phi_{jl}|^2 \tag{8}$$

$$|\varphi_j^{\downarrow}|^2 = \langle\psi|\hat{a}_{j\downarrow}^{\dagger}\hat{a}_{j\downarrow}|\psi\rangle = \sum_{l=1}^{N}|\phi_{lj}|^2 \tag{9}$$

III. 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

$$|\psi_{\sigma}^{1}\rangle = \sum_{n}\phi_n^1\hat{a}_{n|\sigma}^{\dagger}|0\rangle \tag{10}$$

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 [15]. 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. In the case of an electron in a polarizable lattice this state is known as polaron and, in a previous publication, it was designated as solitobreather, since it shares both soliton and breather characteristics [17]. 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.

As for the parameters, the number of initial conditions we can consider is *a priori* infinite. In order to make a more direct connection to the one electron, polaron, states, the dynamical states we study are perturbations of the single polaron state, induced by the presence of a second electron 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 Fig. 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 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 [5], 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. In analogy with a previous study [7], we may call this state a *bipolarobreather*. We should nevertheless stress that while the polarobreather determined in [7] is an excited state in which the electron and the lattice vibrate with the same frequency, the bipolarobreathers we find in this study do not have that restriction. They do share the stability expected from breathers in that they remain stable after 42 ps of simulations.

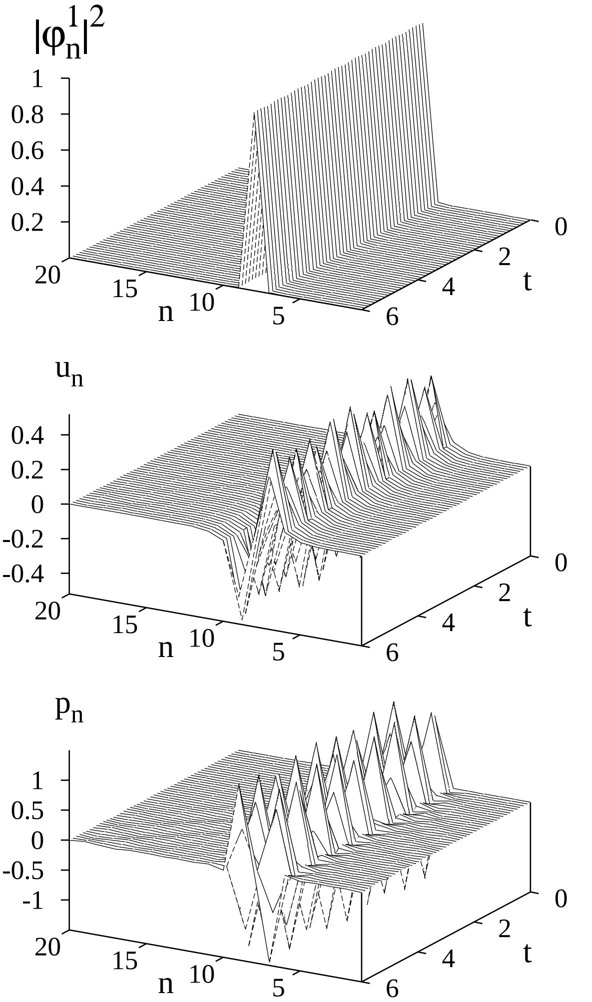


FIG. 1: Time dependence for (a) the probability for one quasiparticle to be in site n, ($n = 1 \cdots N$, $N = 20$), (b) the lattice displacement and (c) the momentum of site n. Time is in picoseconds. The parameters are $t = 10 \times 10^{-22}$J, $\chi = 100$pN, $\kappa = 1$N/m, $\kappa' = 2\kappa$,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

A Hubbard Hamiltonian with a much weaker attraction, corresponding to a ratio of $\gamma/t = -0.5$, is considered in Fig. 2, where the last 6 picoseconds of a 42 pi-

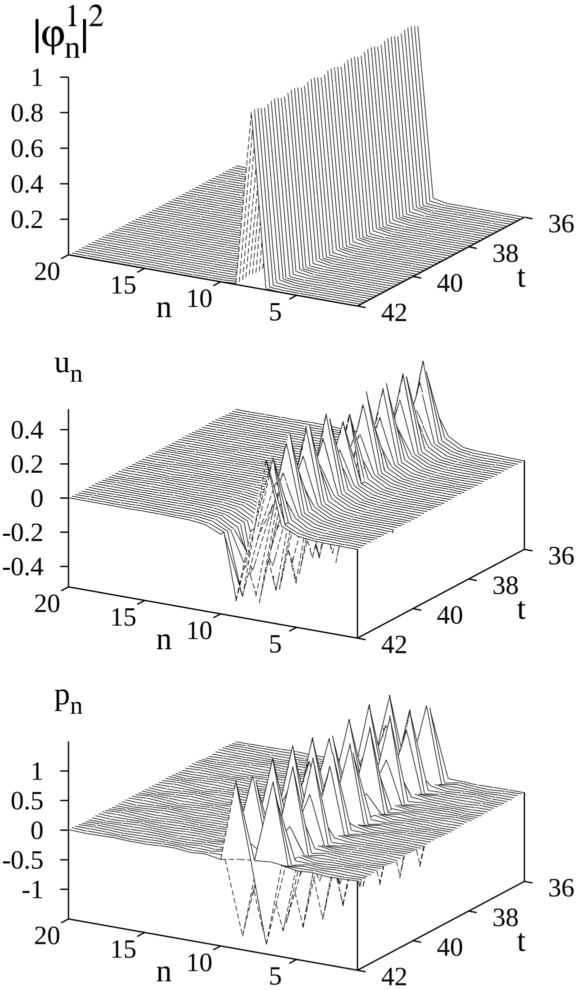


FIG. 2: Same as Fig. 1, but with $\gamma = -5 \times 10^{-22}$J.

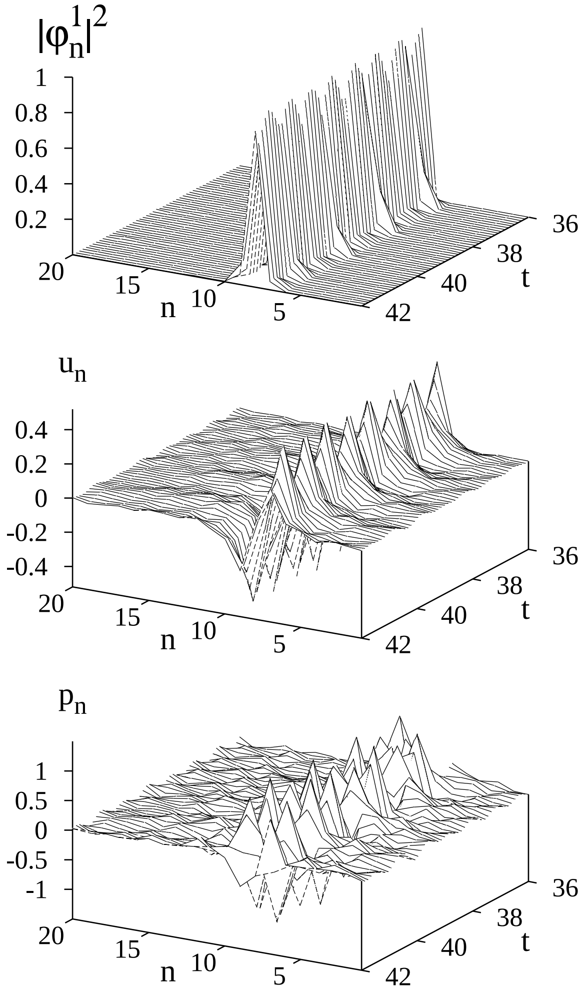


FIG. 3: Same as Fig. 1, but with $\gamma = +10 \times 10^{-22}$J.

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

In Fig. 3 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 Figure 4, 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

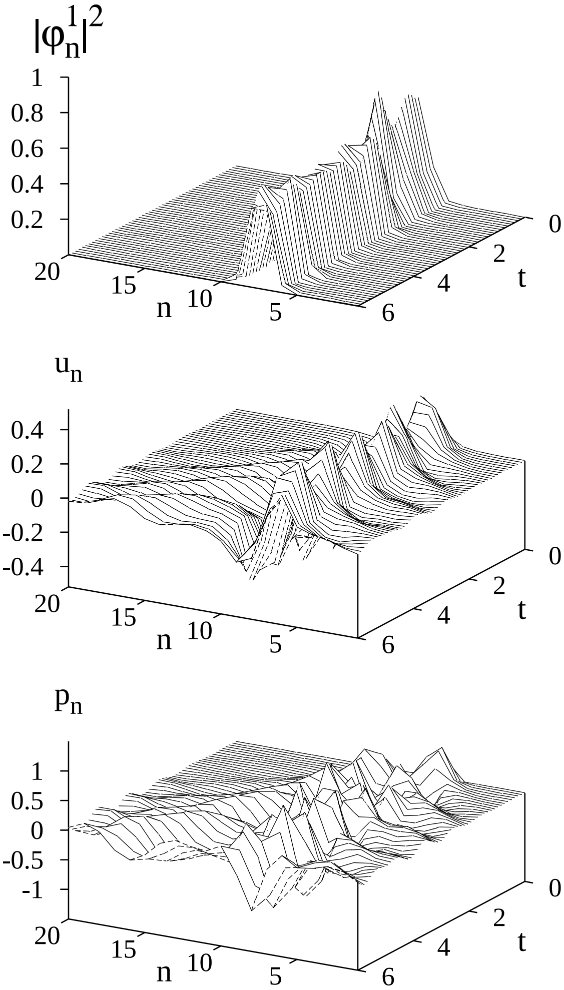


FIG. 4: Same as Fig. 1, but with $\gamma = +50 \times 10^{-22}$J.

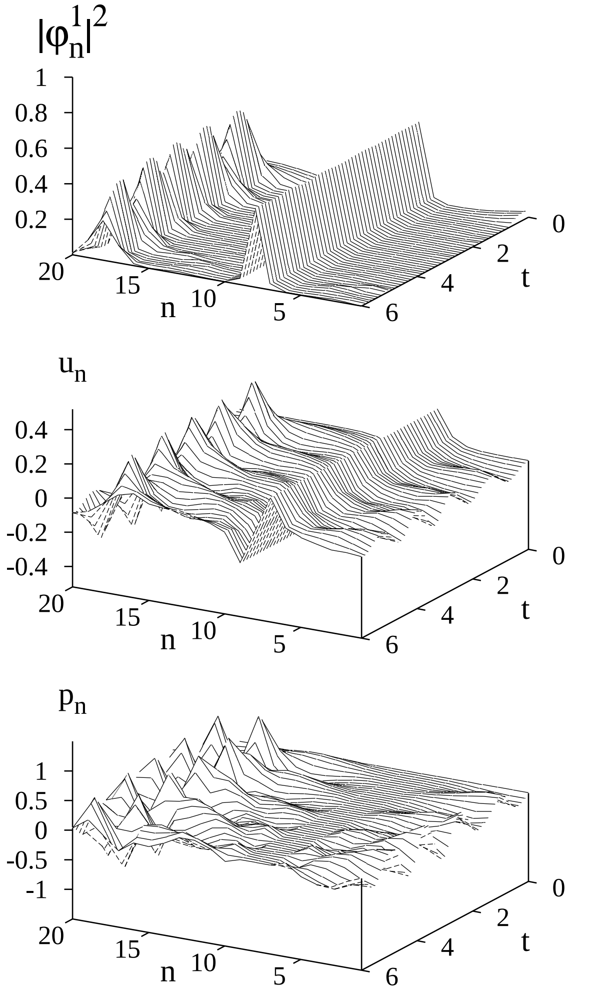


FIG. 5: Same as Fig. 1, but with $\gamma = +100 \times 10^{-22}$J.

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. Continuation of this simulation 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.

In Fig. 5, a repulsive interaction corresponding to $\gamma/t = 10$ is used. It 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

Figs. 4. The momenta in Fig. 5 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, the stability of the two peak solution, even in the presence of such relatively large amount of noise is apparent also after 42 ps (not shown).

IV. 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 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 in the Hamiltonian we consider in this section are the same as before, (see eqs.(3-3)), except that now the phonon Hamiltonian is given by:

$$\begin{aligned}
H_{\rm ph}^{\rm harm} &= H_{\rm ph}^{\rm co\text{-}harm} + H_{\rm ph}^{\rm os\text{-}harm} \qquad (11)\\
H_{\rm ph}^{\rm co\text{-}harm} &= \frac{1}{2}\kappa \sum_{n=1}^{N} (u_n - u_{n-1})^2\\
H_{\rm ph}^{\rm os\text{-}harm} &= \kappa' \sum_{n=1}^{N} \left(\frac{1}{2}u_n^2\right) + \frac{1}{2M}\sum_{n=1}^{N} p_n^2
\end{aligned}$$

In this Hamiltonian the only nonlinear term is that which describes the quasiparticle-lattice interaction. Fig. 6 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. And the state of the two electrons remains localized on one site all the time.

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 Fig. 7. The dynamics is similar to that of fig. 6, 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.

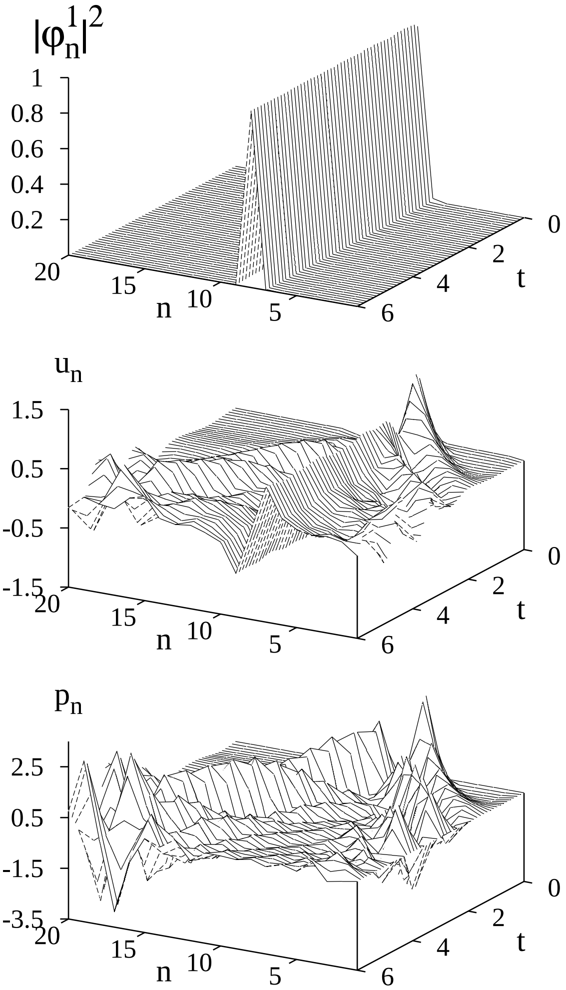
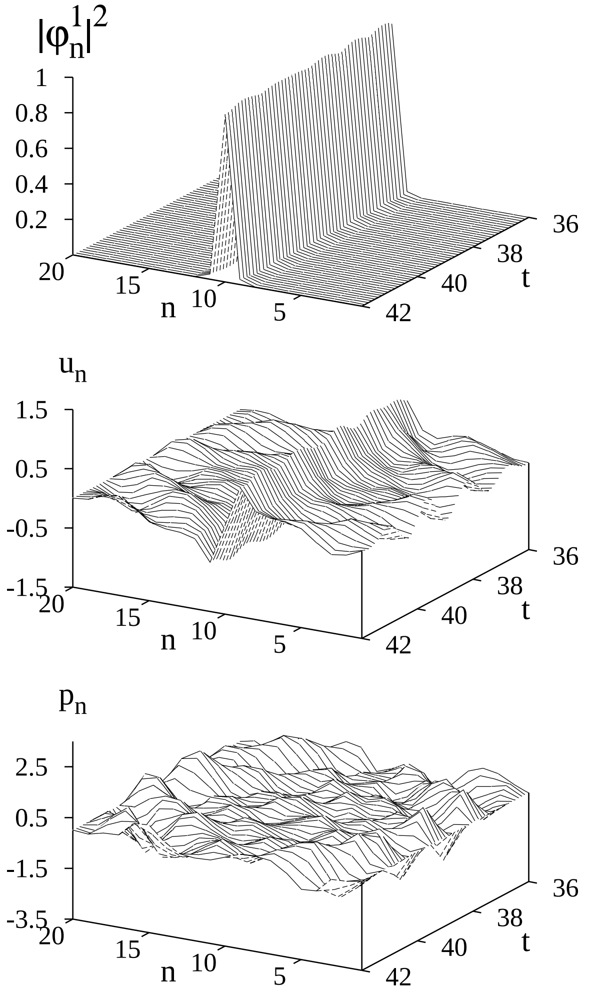


FIG. 6: Same as Fig. 1, but with $\gamma = -100 \times 10^{-22}$J and for the harmonic lattice 11.

For a repulsive interaction for which $\gamma/t = +10$, the two electrons split up and the probability distribution shows two peaks, both of which have an associated lattice deformation with the breather profile (see Fig. 8). 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.



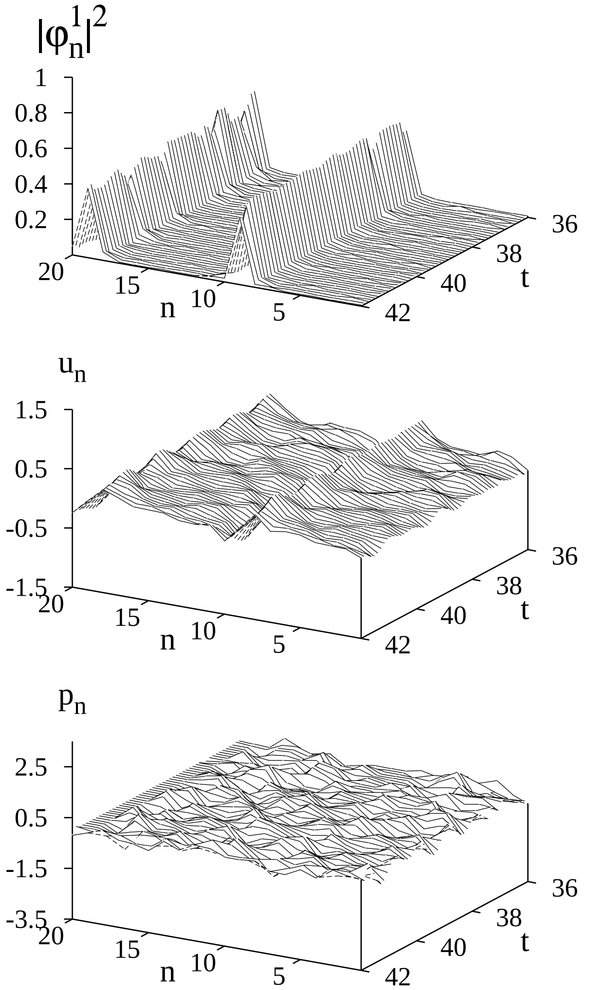


FIG. 7: Same as Fig. 1, but with $\gamma = +50 \times 10^{-22}$J and for the harmonic lattice 11.

FIG. 8: Same as Fig. 1, but with $\gamma = +100 \times 10^{-22}$J and for the harmonic lattice 11.

V. 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. As in a previous study [17], the starting point was a solitobreather, but whilst in [17] we studied higher excited states due to finite momentum, here we considered the dynamic states which arise when a second quasiparticle is added to the solitobreather. 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 as discrete breathers (DBs) [5]. The study of systems in which nonlinear lattices are coupled to quantum quasiparticle, on the other hand, is just beginning [9, 16, 17]. In fact, as far as we know, this is the first time that the coupling of two quantum quasiparticles to a nonlinear lattice has been considered.

A second physical 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 can be either attractive or repulsive. In a previous study we found that DBs can be generated by finite momentum excitations [17]. Here we find that DBs are also generic solutions of this much more complex system 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, leading to bipolarobreathers.

Windows of γ were found for which similar solutions are obtained. Thus, for a ratio of γ/t between -10 and $+1$ (Figs. 1-3), 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. 4-5). 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. Similar dynamical solutions were also determined here in the case of two electrons interacting with a *linear* lattice (see Figs 6-8).

Proville and Aubry [7], who study the minimum energy states of two electrons in interaction with a harmonic lattice, also found these types of solutions, which indicates that they may constitute a general feature of two electron states in extended Hubbard systems. One important difference is, however, that in the case of a nonlinear lattice the lattice states are breathers and these may have a greater stability against thermal fluctuations, something that is particularly important for HTSC. Indeed, the conjecture behind this work is that breathers are an important element in the glue that binds electrons in HTSC making bipolarobreathers more thermally stable than simple bipolarons.

This Hamiltonian also 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 dynamics 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.

As stated above, 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 Tc 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 [4, 6]. 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.

Acknowledgments

JLM. acknowledges a *Marie Curie* TMR fellowship from the EU (no. ERBFMBICT972761). LC-H and JCE are grateful for travel support of a British Council Treaty of Windsor grant. JCE and JLM would also like to acknowledge support from the EU under the LOCNET Research Training Network HPRN-CT-1999-00163.

[1] J. Woods Halley, editor. *Theories of High Temperature Superconductivity.* Addison-Wesley Publishing Company, Inc, Redwood City, California, 1988.

[2] D. Mihailović, G. Ruani, E. Kaldis, and K. A. Müller, editors. *Anharmonic Properties of High-Tc Cuprates.* World Scientific, Singapore, 1995.

[3] J.G. Bednorz and K.A. Müller. *Z. Phys. B*, 64:189–193, 1986.

[4] F.M. Russell and D.R. Collins. Anharmonic excitations in high T_c materials. *Phys. Lett. A*, 216:197–202, 1996.

[5] S. Flach and C. R. Willis. Discrete breathers. *Physics Reports*, 295:181–264, 1998.

[6] J.L. Marín, F.M. Russell, and J.C. Eilbeck. Breathers in cuprate superconductor lattices. *Phys. Lett. A*, :281:21–25, 2001.

[7] L. proville and S. Aubry. Mobile bipolarons in the adiabatic Holstein-Hubbard model in one and two dimensions. *Physica D*, 113: 307–317, 1998.

[8] J. Bonč and S.A. Trugman. Bipolarons in the extended Holstein Hubbard model. *Phys. Rev. B*, 64: 094507, 2001.

[9] G. Kalosakas and S. Aubry. Polarobreathers in a generalized Holstein model. *Physica D*, 113: 228–232, 1998.

[10] A. Scott. Davydov's soliton. *Physics Reports*, 217:1–67, 1992.

[11] H.J. Bornemann and D.E. Morris. Isotope effect in YBA2-XLAXCU3OZ - evidence for phonon-mediated high-temperature superconductivity. *Phys. Rev. B*, 44(10):5322–5325, 1991.

[12] G.V.M. Williams, J.L. Tallon, J.W. Quilty, H.J Trodahl, and N.E. Flower. Absence of an isotope effect in the pseudogap in YBa2Cu4O8 as determined by high-resolution Y-89 NMR. *Phys. Rev. Lett.*, 80(2):377–380, 1998.

[13] Guo-Meng Zhao, M. B. Hunt, H. Keller, and K.A. Müller. Evidence for polaronic supercarriers in the copper oxide superconductors $La_{2-x}Sr_xCuO_4$. *Nature*, 385:236–239, 1997.

[14] Leonor Cruzeiro-Hansson and Shozo Takeno. Davydov model: The quantum, mixed quantum-classical, and full classical systems. *Phys. Rev. E*, 56(1):894–906, 1997.

[15] L. Cruzeiro-Hansson and V.M. Kenkre. Localized versus delocalized ground states of the semiclassical holstein hamiltonian. *Phys. Lett. A*, 190:59–64, 1994.

[16] Serge Aubry. Breathers in nonlinear lattices: existence, linear stability and quantization. *Physica D*, 103:201–250, 1997.

[17] L. Cruzeiro-Hansson, J.C. Eilbeck, J.L. Marín, and F.M. Russell. Breathers in systems with intrinsic and extrinsic nonlinearities. *Physica D*, 142:101–112, 2000.