QUANTUM BREATHERS IN AN ATTRACTIVE FERMIONIC HUBBARD MODEL

Quantum breathers in a Hubbard model

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Abstract In one–dimensional translationally invariant anharmonic lattices, an extended Bloch state with two or more strongly correlated particles is usually called a quantum breather. Here we study an attractive fermionic Hubbard model with two kind of particles of opposite spin. We discuss the existence of breathers, and several effects that break the translational symmetry of the system and localize the breather in the lattice.

Keywords: Anharmonic quantum lattices, Quantum breathers, Quantum lattice solitons

1. Introduction

Recent theoretical developments and improved experimental techniques has led to growing interest in the phenomenon of localization of energy by nonlinearity in anharmonic lattices. The existence and properties of these intrinsic localized modes, known as discrete breathers, have been subject of an much investigation (see, e.g [1] for a number of recent reviews of this topic). At present, discrete breathers in classical systems is a relatively well understood phenomenon, but knowledge of the quantum equivalent of discrete breathers is not very developed. In

particular we restrict ourselves to a study of small lattices and a small number of quanta where some numerically exact solutions can be found. Although of less interest to the study of bulk matter, such studies are relevant to the recent developments in quantum nanotechnology and applications in quantum computing [7].

The quantum equivalent of a discrete breather in a translationally invariant anharmonic lattice is an extended Bloch state with two or more particles in a strongly correlated state. There exist some theoretical results (i.e. [2, 3]), and some experimental observations of these states in different quantum systems, as mixtures of 4–methyl–pyridine [4], in Cu benzoates [5], and in doped alkalihalides [6].

Here we present some results on a quantum one–dimensional lattice problem with a small number of quanta. We study a periodic lattice with f sites containing fermions, described by an attractive fermionic Hubbard model (FH) with two kinds of particles with opposite spins. It is a model of interest in connection with the theory of high-T_c superconductivity [8], and it can be used to describe bound states of electron and holes in some nanostructures as nanorings (excitons) [9]. Many of the results could be extended to a great variety of systems, i.e., we have obtained similar results with a periodic lattice containing bosons and described by the quantum discrete nonlinear Schrödinger equation [10].

This paper is organized as follows: In the next section we present the model, and in Section 3 we study the existence of breathers in the simplest nontrivial case. In Section 4, we consider some modifications that break the translational symmetry of the lattice, and can localize the breather in the lattice. In Section 5 we extend the previous results, obtained in the simplest nontrivial case, to more complicated situations. Finally, in Section 6, we summarize our findings and present our conclusions.

2. The model

We consider an anharmonic lattice with f sites and two kinds of fermions with opposite spins described by an attractive fermionic Hubbard model (FH). The Hamiltonian of the system is given by

$$\hat{H} = -\sum_{j=1}^{f} \gamma_j a_j^\dagger a_j b_j^\dagger b_j + \epsilon_j a_j^\dagger (a_{j-1} + a_{j+1}) + m_e \epsilon_j b_j^\dagger (b_{j-1} + b_{j+1}), \quad (1)$$

where $a_j^\dagger (a_j)$ and $b_j^\dagger (b_j)$ are raising (lowering) operators for different electronic spin states, satisfying the standard fermionic anticommutation relations. The parameter ratio γ_j/ϵ_j represent the ratios of anharmonicity

to nearest–neighbor, hopping energy, and m_e is the ratio of the effective mass of one type of fermion to the other. To eliminate the effects related to the finite size of the chain, we consider periodic boundary conditions and, initially, a translational invariant lattice, $\gamma_j = \gamma$ and $\epsilon_j = \epsilon$, independent of j. In general we consider $\epsilon = 1$.

The Hamiltonian (1) conserves the number of quanta N, and it is possible to apply the number–state–method to calculate the eigenvalues and eigenvectors of the Hamiltonian operator [11]. We use a number–state–basis $|\psi_n\rangle = [n_1^a, n_2^a, ..., n_f^a; n_1^b, n_2^b, ..., n_f^b]$, where n_i^a (n_i^b) represents the number of quanta of fermions a (b) at site i. In this case, $N_a = \sum_i n_i^a$, $N_b = \sum_i n_i^b$, and $N = N_a + N_b$. A general wave function is $|\Psi_n\rangle = \sum_n c_n |\psi_n\rangle$. As a first step, we restrict ourselves to study the simplest nontrivial case $N_a = 1$, $N_b = 1$, and as a second step we consider more complicated situations with a small number of quanta, although many of the results are valid for larger values of N_a and N_b. The bound states correspond to exciton states, localized electron/hole states that may appear in nanorings.

3. Quantum breathers in a translational invariant lattice

In a homogeneous quantum lattice with periodic boundary conditions, it is possible to block–diagonalize the Hamiltonian operator using eigenfunctions of the translation operator $\hat{T}$ defined as $\hat{T} b_j^\dagger = b_{j+1}^\dagger \hat{T}$ ($\hat{T} a_j^\dagger = a_{j+1}^\dagger \hat{T}$). In each block, the eigenfunctions have a fixed value of the momentum k, with $\tau = \exp(ik)$ being an eigenvalue of the translation operator [11]. In this way, it is possible to calculate the dispersion relation $E(k)$ with a minimal computational effort. The corresponding matrix in the case $N_a = N_b = 1$ is

$$H_k = - \begin{bmatrix} \gamma & q^* & 0 & . & . & q \\ q & 0 & q^* & 0 & . & 0 \\ 0 & q & 0 & q^* & . & . \\ . & . & . & . & . & . \\ . & . & . & q & 0 & q^* \\ q^* & . & . & . & q & 0 \end{bmatrix},$$

where $q = (m_e + \tau^*)$.

In this simplest non–trivial case, if the anharmonicity parameter is large enough, as Fig 1 shows, there exists an isolated eigenvalue for each k which corresponds to a localized eigenfunction, in the sense that there is a high probability for finding the two quanta at the same site. But due to the translational invariance of the system, there is an equal probability

for finding these two quanta at any site of the system. In these cases, some analytical expressions can be obtained in some asymptotic limits (for a recent discussion see [2, 11, 12]). Note that, qualitatively, the existence of this localized state is independent of the value of parameter m_e.

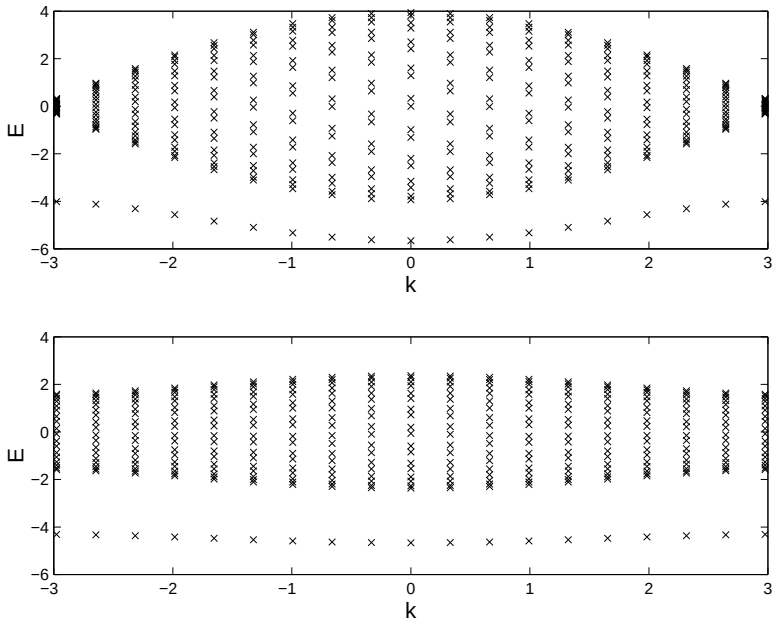

Figure 1. Eigenvalues $E(k)$. $N = 2$, $f = 19$, $\gamma = 4$. $m_e = 1$ (top) and $m_e = 0.2$ (bottom).

If we consider for simplicity the case $k = 0$, the ground state unnormalized eigenfunction is

$$|\Psi\rangle = [10\ldots0;10\ldots0]+[01\ldots0;01\ldots0]+\ldots[0\ldots01;0\ldots01]+O(\gamma^{-1}),$$

i.e. on a lattice of length f, the unnormalized coefficients c_i of the first f terms are equal to unity and the rest are $O(\gamma^{-1})$.

4. Trapping in a lattice with broken translational symmetry

In this section we will consider some modifications that can break the translational invariance of the lattice, changing the coefficients c_i and localize the breather around a particular point of the lattice. In these cases, the Hamiltonian operator cannot be block-diagonalized using eigenvectors of the translation operator. Although the computational

effort increases, it is still possible to calculate its eigenvalues and eigenvectors if f and N are small enough, by using algebraic manipulation methods and numerical eigenvalue solvers. In this section we restrict to the situation $N_a = N_b = 1$.

Perhaps the simplest way to break the translational invariance of the lattice is by considering non–flux boundary conditions to simulate a finite–size chain. In this case, the solution becomes weakly localized around the middle of the lattice. If f is high enough, and we do no take into account boundary effects, this case reduces to the homogeneous lattice case.

A alternative mechanism for breaking the translational invariance can be the existence of local inhomogeneities or impurities. In our model, this can be modeled by making one or more of the γ_j or the ϵ_j dependent on j. This can occur because of localized impurities or long–range interaction between non nearest-neighbors sites due to non–uniform geometries of the lattice chain. The interplay between these two sources of localization, nonlinearity and impurities is important to understand the properties of these bound states.

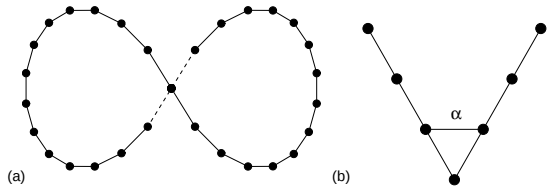

Figure 2. Two non-uniform chain geometries.

Two examples of non–uniform geometries are shown in Fig. 2. In Fig. 2a, a twisted circular geometry causes an interaction between two sites of the chain, which are distant with respect to measurement along the length of the chain. This model has been used in a classical model of a globular protein [13], and it has been shown that moving breathers described by the DNLS equation can be trapped at the cross–over point. Fig. 2b shows another possible geometry, a bent chain, that has been recently studied in the context of the DNLS equation and photonic crystal context [14] and in Klein–Gordon systems [15]. In all these cases, the geometry effects can be modeled by adding a long–range interaction term of the form

$$\alpha_{\ell,m}(b_\ell^\dagger b_m + b_m^\dagger b_\ell), \tag{2}$$

where ℓ and m are the neighbouring sites put brought closer in the twisted–chain case, and $m = m_0 - 1$ and $\ell = m_0 + 1$ in the bent–chain case, where m_0 is the vertex of the chain.

We will analyze in more detail these modifications that break the translational invariance of the system.

4.1 Localization in a chain with impurities

We introduce a local inhomogeneity in the anharmonic parameter in our system and retain periodic boundary conditions, in order to isolate the effect caused by this local inhomogeneity alone. We put $\gamma_\ell = \gamma_{imp}$, and $\gamma_j = \gamma$ for $j \neq l$.

In the homogeneous system, as discussed above, if the anharmonicity parameter is large enough there exists a high probability of finding the two particles at the *same* site of the chain, but with equal probability at *any* site of the chain. If we consider a point impurity, a isolated localized bound state appears, as shown in Fig. 3. This state has minimal energy and corresponds to the ground state.

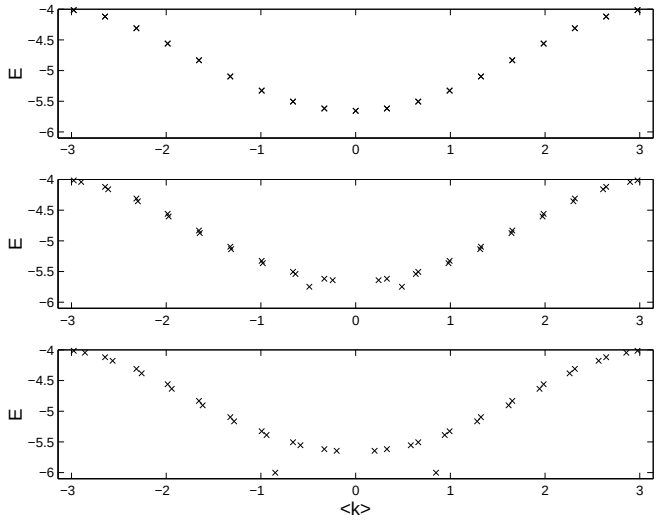

Figure 3. Eigenvalues E as a function of the expected value of k corresponding to the localized eigenfunctions. $N = 2$, $f = 19$, $m_e = 1$ and $\gamma = 4$. Point impurity at the site $\ell = 10$. Homogeneous chain (top). $\gamma_{imp} = 4.5$ (center). $\gamma_{imp} = 5$ (bottom).

If we analyze this ground state, we observe that as γ_{imp} increases, the localization around the impurity increases too, as shown in Fig 4. In particular, the main contribution to the wave function corresponds

to the bound states centered around the impurity. There exists also a small contribution that corresponds to states with particles in adjacent sites around this local inhomogeneity.

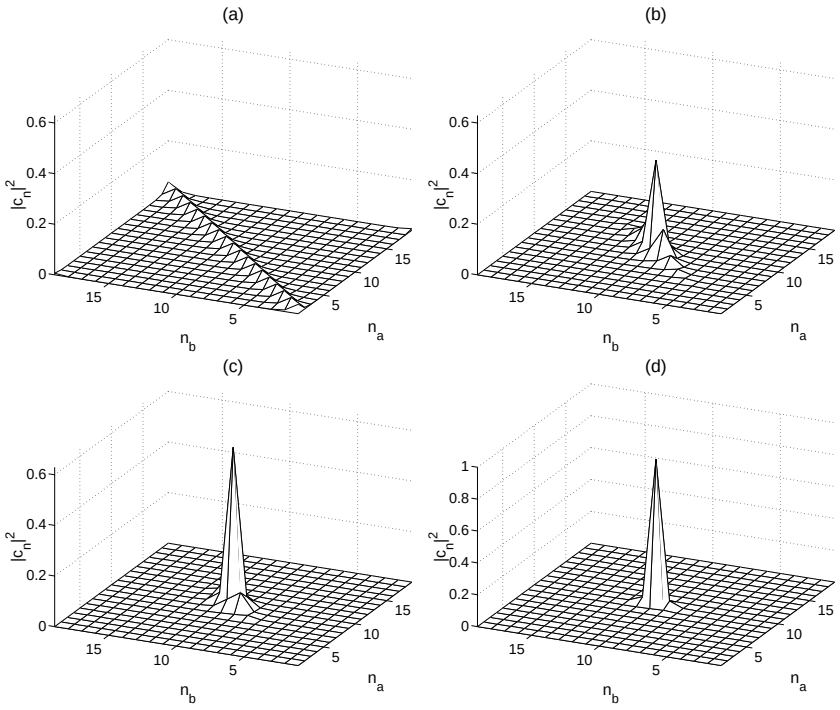

Figure 4. Square wave function amplitudes $|c_n|^2$ corresponding to the ground state as a function of the positions of the two fermions along the chain n_a and n_b. $f = 19$ and $\gamma = 4$. Point impurity at the site $\ell = 10$. (a) Homogeneous chain, $m_e = 1$. (b) $\gamma_{imp} = 4.5$, $m_e = 1$. (c) $\gamma_{imp} = 5$, $m_e = 1$. (d) $\gamma_{imp} = 5$, $m_e = 0.2$.

If we analyze the contribution of the components of the wave function of the ground state corresponding to the two particles centered around the local inhomogeneity in the same site, in adjacent sites, and separated by one site, as shown in Fig 5, we observe that the localization increases very rapidly with the magnitude of the impurity. Varying the value of m_e from unity amplifies this effect even further. We note that, in this case, as harmonic terms are homogeneous (null), there exists no Anderson–like localization.

4.2 Localization in a twisted chain

In order to simulate the twisted chain shown in Fig. 2a, we consider a long–range hopping term between sites m and ℓ given by parameter $\alpha_{m,\ell}$.

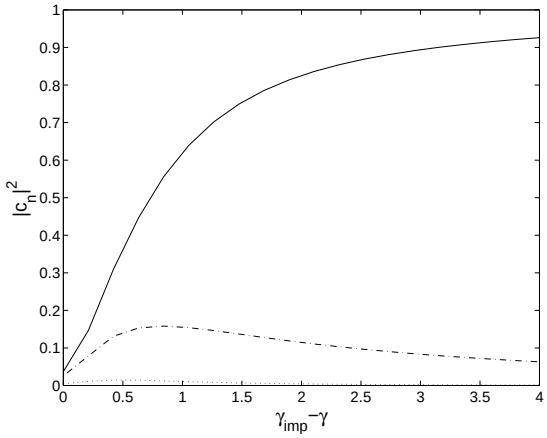

Figure 5. Some components of the wave function corresponding to the ground state. $N = 2$, $f = 19$, $\gamma = 4$ and $m_e = 1$. Two particles centered on the impurity (continuous line). Two particles in adjacent sites with one of them centered on the impurity (dashed–dotted line). Two particles separated by one site and one of them on the impurity (dotted line).

As Fig. 6 shows, this coupling generates a localized bound state around the sites m and ℓ that is a ground state of the system, a phenomenon similar to that shown in Fig 3. Although there exist some degree of localization in the harmonic case ($\gamma = 0$) due to an Anderson–like effect, the existence of bound states due to the anharmonicity parameter γ strongly increases the localization. Similar results have been obtained with different values of the parameter $\alpha_{m\ell}$.

4.3 Localization in a bent chain

To simulate the bend shown in Fig. 2b, we introduce an additional term that takes into account the interaction between the two neighbouring sites of the vertex. In this case, if we suppose that the hopping term varies as the inverse of the square of the distance between sites, the parameter α can be related to the wedge angle θ through $\alpha = \frac{1}{2}/(1-\cos\theta)^{-1}$.

As shown in Fig. 7, due to the existence of this long–range interaction, there exist a localization phenomenon around the vertex of the chain. If the wedge angle is small enough, the ground state is mainly a bound state with the two particles localized in the neighbouring site of the vertex, but when this angle decreases, the contribution of the components corresponding to non–localized states with particles around

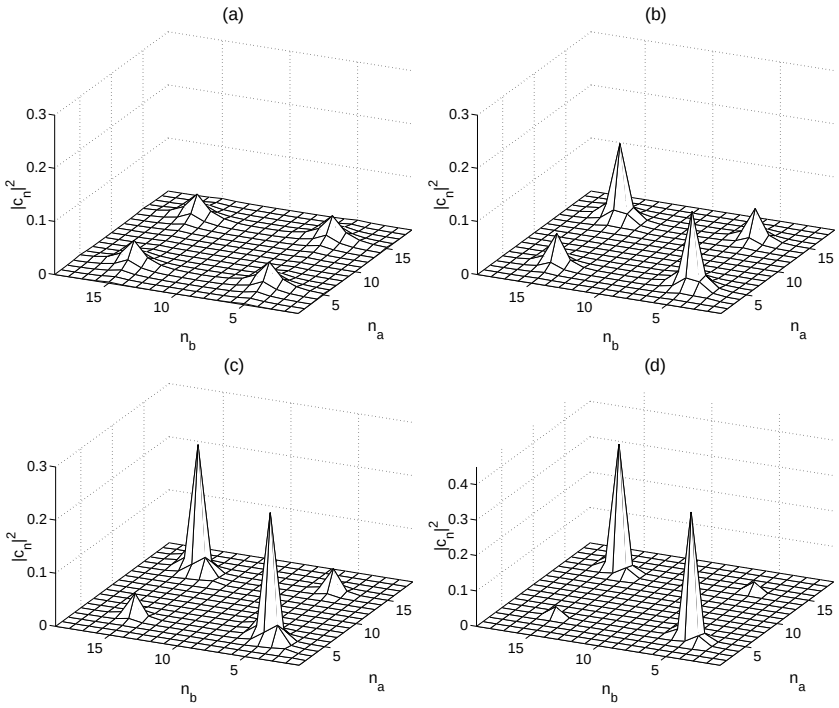

Figure 6. Square wave function amplitudes $|c_n|^2$ corresponding to the ground state as function of the positions of the two fermions n_a and n_b along the twisted chain. Long range interaction between sites $m = 5$ and $\ell = 15$ with $\alpha_{m\ell} = 1$ and $f = 19$. (a) $\gamma = 0$ (harmonic case), $m_e = 1$. (b) $\gamma = 2$, $m_e = 1$. (c) $\gamma = 4$, $m_e = 1$. (d) $\gamma = 4$, $m_e = 0.2$.

the vertex becomes significant. In the limit $\theta \to 0$, the lattice becomes a T-junction. We have found that in this system, the ground state is mainly localized around the junction.

We have compared this localization effect with the Anderson-like localization in the harmonic system ($\gamma = 0$). As shown in Fig. 8, the existence of bound states in the anharmonic case implies that the localization effect due to the curvature of the system increases. This enhancement decreases when θ decreases, although there exists a maximum around $\theta \approx 0.5$.

We note that this model, to give a more realistic approximation of a bent chain, must be improved to take into account the long–range interaction between all sites that becomes significant when the angle θ

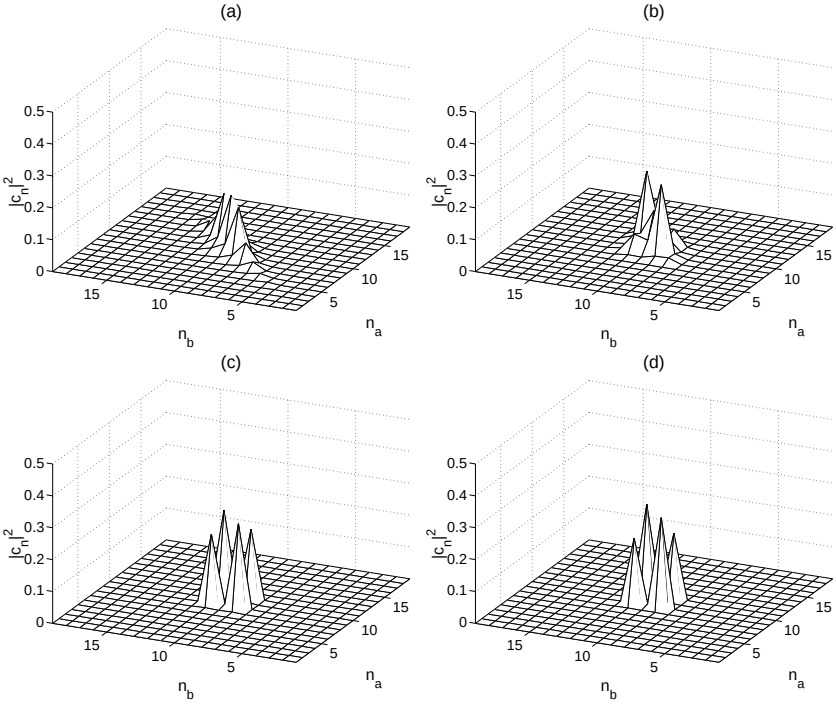

Figure 7. Square wave function amplitudes $|c_n|^2$ corresponding to the ground state as a function of the positions of the two fermions n_a and n_b along the bent chain. $f = 19$ and $\gamma = 4$. (a) $\theta = \pi$, $m_e = 1$. (b) $\theta = \pi/3$, $m_e = 1$. (c) $\theta = \pi/10$, $m_e = 1$. (d) $\theta = \pi/10$, $m_e = 0.2$.

is small enough. We have considered the model given by the Hamiltonian

$$\begin{aligned} \hat{H} &= -\gamma \sum_{j=1}^{f} a_j^\dagger a_j b_j^\dagger b_j - \sum_{j=1}^{f} \sum_{i>j} \frac{1}{d_{ij}^2} (a_i^\dagger a_j + a_j^\dagger a_i) - \\ & \sum_{j=1}^{f} \sum_{i>j} \frac{m_e}{d_{ij}^2} (b_i^\dagger b_j + b_j^\dagger b_i), \end{aligned} \tag{3}$$

where d_{ij} represents the distance between sites i and j. We have found the same qualitative behavior.

5. Higher number of quanta

In previous sections, we have restricted our studies to the case $N_a = N_b = 1$. Proceeding as the same way, it is possible –in principle– to construct the Hamiltonian matrix for any value of the quantum numbers

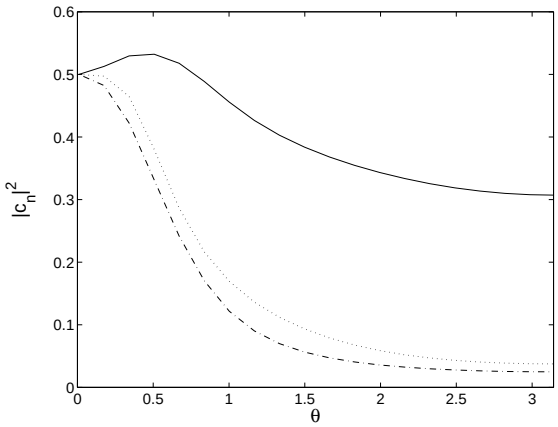

Figure 8. Some components of the wave function corresponding to the ground state. $N = 2$, $f = 19$ and $m_e = 1$. Localized state corresponding to the two particles at the neighbor site of the vertex and $\gamma = 4$ (continuous line). Two particles in a non–localized state at neighbouring sites of the vertex and $\gamma = 4$ (dashed-dotted line). Two particles in a non–localized state at neighbouring sites of the vertex and $\gamma = 0$ (dotted line).

N_a and N_b and to calculate the spectrum. However, the computational effort increases rapidly and can go beyond the limits of computational convenience. Nevertheless, we have studied some cases involving a higher number of fermions. In particular, we have considered the case $N_a = 2$ and $N_b = 1$ and the case $N_a = N_b = 2$.

In general, we have found the same qualitative behavior than in the previous case. In the homogeneous system, if the anharmonic parameter is high enough, the ground state is mainly a localized state, in the sense that there exists a high probability to find two different fermions at the same point of the lattice, but due to the translational invariance of the system, with equal probability of finding these two particles at any site of the system. However, we observe that the main components of the ground state correspond to states where fermions of the same type are as far apart as possible from each other. This is a similar effect as due to the finite–size of the chain where the ground state is weakly localized around the center of the chain. When a fermion is close to other of the same type, the hopping in that direction is limited, as in the case of a finite–size chain.

When we introduce some local inhomogeneities in the system, we have observed similar localization phenomena as noted above. In Fig 9 we show the case $N_a = 2$ and $N_b = 1$ with a point impurity at the

anharmonic parameter. We observe that the ground state is mainly a bound state. The two different fermions are mainly in a localized state centered at the impurity with the other fermion in the other extremum of the chain. We note that there exists a significant contribution of other components corresponding to localized states of the two different fermions in the impurity and the other one in different sites of the chain, this contribution being more significant when it corresponds to states where the two fermions are separated by a large number of sites. This system, in the context of excitons in ring geometries, is usually called ortho–trion, and can be viewed as an exciton plus an additional electron smeared over the ring [16].

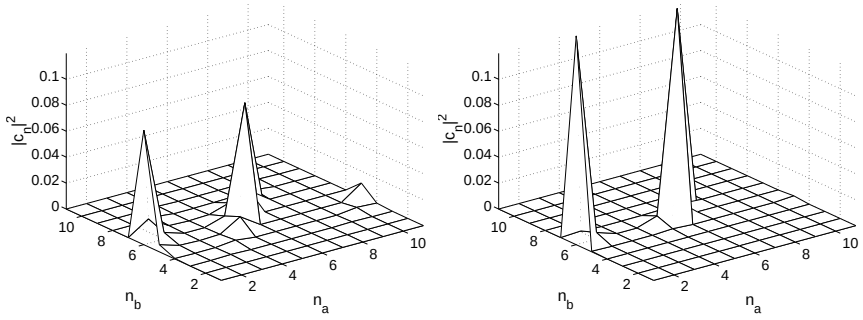

Figure 9. Some components of the wave function of the ground state corresponding to the case $f = 11$, $N_a = 2$, $N_b = 1$, $\gamma = 4$, point impurity at the site $\ell = 6$ and $\gamma_{imp} = 5$. n_a represents the position of one of the fermions of type (a) (the other fermion is located at $n_a + 5$) and n_b the position of the fermion of type (b). $m_e = 1$ (left), $m_e = 0.2$ (right).

In the other cases, when a local inhomogeneity is introduced by means of a long–range interaction term, or $N_a = N_b = 2$ is considered, the behavior is similar. The ground state corresponds to a localized state centered at the local inhomogeneities where different fermions are together and fermions of the same type are located as further apart as possible one from the other.

6. Conclusions

In this work we have shown some results related with the existence and properties of quantum breathers in a fermionic Hubbard model with two kinds of particles of opposite spins. We have studied the existence of localized states due to the nonlinearity and to the influence of local inhomogeneities in these localized states. In particular, we have found

that these local inhomogeneities, due to the geometrical factor and to a long–range interaction or an impurity in the anharmonicity parameter, break the translational invariance of the system and localize the ground state around a particular site of the chain. We expect that these results are rather general, and could be extended to a great variety of systems.

Acknowledgments

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