Strongly correlated hopping and many-body bound states

Julien Vidal
Groupe de Physique des Solides, CNRS UMR 7588, Universités Paris 6 et 7, 2, place Jussieu, 75251 Paris Cedex 05, France

Benoit Douçot
Laboratoire de Physique de la Matière Condensée, CNRS UMR 8551, École Normale Supérieure, 24, rue Lhomond, 75231 Paris Cedex 05, France
Laboratoire de Physique Théorique et Hautes Énergies, CNRS UMR 7589, Universités Paris 6 et 7, 4, place Jussieu, 75252 Paris Cedex 05, France

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We study a system in which the quantum dynamics of electrons depend on the particle density in their neighborhood. For any on-site repulsive interaction, we show that the exact two-body and three-body ground states are bound states. We also discuss the finite density case in a mean-field framework and we show that the system can undergo an unusual transition from an effective attractive interaction to a repulsive one, when varying the electron density.

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I. INTRODUCTION

Correlated hopping models have been the subject of many studies within various contexts. First proposed by Foglio and Falicov to decribe mixed valence solids,[1] they have also been widely used to study the organic conductors[2–5] in order to take into account bond-charge effect.[6] Finally, these models where the probability of an electron to move depends on the particle density, have been proposed to mimick effective attractive interaction between electrons high-T_c superconductivity[7,8] and have provided rich phase diagrams.[9–26]

In a completely different framework, we have recently described a localization phenomenon induced by the magnetic field that occurs for special geometries and for special values of the magnetic flux.[27] This surprising effect has been experimentally observed in superconducting wire networks,[28] and in two-dimensional electron gas.[29] We have also studied the influence of electron-electron interactions on such systems and we have shown that a Hubbard-like term (on-site repulsion) was able to delocalize two particles initially confined in a given so-called Aharonov-Bohm cage.[30,31] These results have led us to formulate the simple toy model presented here in which we introduce this delocalization process directly in the Hamiltonian by imposing that an electron can move only if another electron is in its close neighborhood. Of course, we do not claim to capture all the physics of the interacting Aharonov-Bohm cages with this simple one-dimensional system, but we think that it can help us in understanding the delocalization process induced by (repulsive) interactions.

This paper is organized in two main parts. In the first one, we exactly solve the two-body (Sec. II) and three-body (Sec. III) problems and we show that the ground state is always a bound state for any strength of the on-site repulsion. Therefore, we give a simple picture in terms of a graph in the Hilbert space that makes the physical interpretation clearer. In the second part (Sec. IV), we propose a mean-field like approach for the finite density case by considering the low-energy excitations above the Fermi sea. We show that in the vicinity of a curve in its two parameter space, the initial Hamiltonian can be mapped onto an effective Hubbard model with an interacting term that depends on the particle density and that can be either repulsive or attractive.

We consider interacting spin 1/2 fermions in a one-dimensional chain of linear size $L=Na$ with periodic boundary conditions[32] described by the following Hamiltonian:

$$H=-t\sum_{i,\sigma}\left(c^{\dagger}_{i+1,\sigma}c_{i,\sigma}+c^{\dagger}_{i,\sigma}c_{i+1,\sigma}\right)\left(n_{i,-\sigma}+n_{i+1,-\sigma}\right)+U\sum_{i}n_{i,\uparrow}n_{i,\downarrow}, \tag{1}$$

where $c^{\dagger}_{i,\sigma}$ ($c_{i,\sigma}$) denotes the creation (annihilation) operator of a fermion with spin σ, $n_{i,\sigma}=c^{\dagger}_{i,\sigma}c_{i,\sigma}$ the density of spin $\sigma=\uparrow,\downarrow$ fermion on site i, and $\langle\cdots\rangle$ stands for nearest neighbor pairs. The kinetic part of the Hamiltonian (1) allows a particle of spin σ located on a site i to jump on a neighboring site j only if there is already a particle either on site i or on site j. For simplicity, we restrict our analysis to the repulsive case $U>0$. However, since the structure is bipartite, the spectrum of H is odd under the tranformation $U\rightarrow -U$.[33]

II. THE TWO-BODY PROBLEM

The single-body problem is trivially solvable for this model since the particle can neither move, nor interact. In this case, the spectrum consists in one eigenvalue $\varepsilon=0$ which is N-fold degenerate. So, let us pay attention to the two-body problem. Denoting $|i\rangle$ the orbital localized on the site i, the two-body state space is generated by

$$|i,j\rangle=|i\rangle_{\uparrow}\otimes|j\rangle_{\downarrow}, \quad \forall(i,j)\in[0,N-1]^2. \tag{2}$$

We only consider here the orbital degrees of freedom since for two particles, the spin degrees of freedom are completely determined by the symmetry of the orbital wave function. This problem can be mapped on that of a single particle

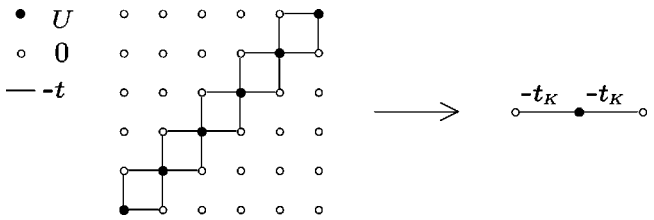

FIG. 1. Representation of the two-body problem as a graph standing in the $\mathbf{Z}^2$ lattice and its reduction after projection along (1,1). $t_K = t(1+e^{-iKb})$.

moving in the graph displayed in Fig. 1 where each site (i,j) of the $\mathbf{Z}^2$ lattice (with appropriate boundary conditions) corresponds to the ket $|i,j\rangle$. Using the invariance of the system under a translation of the center of mass [direction (1,1) in $\mathbf{Z}^2$], diagonalizing H can be simply achieved by introducing the following Bloch waves:

$$|\varphi_0(K)\rangle = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} e^{iKnb} |n,n\rangle, \tag{3}$$

$$|\varphi_\pm(K)\rangle = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} e^{iKnb} |n,n\pm 1\rangle, \tag{4}$$

where $b = a\sqrt{2}$ and where $K = 2\pi j/Nb (j \in [0,N-1])$ is the total momentum of the two particles. Indeed, one has

$$\langle \varphi_0(K)|H|\varphi_\pm(K')\rangle = -t(1+e^{-iKb})\,\delta_{K,K'}, \tag{5}$$

$$\langle \varphi_0(K)|H|\varphi_0(K')\rangle = U\,\delta_{K,K'}, \tag{6}$$

where $\delta_{K,K'}$ is the usual Kronecker symbol, so that the eigenvalues of H are given by $\varepsilon = 0$ for the triplet states (non sensitive to U) and for all the trivial configurations corresponding to isolated particles, and by

$$\varepsilon_\pm(K) = \frac{1}{2}\left[U \pm \sqrt{U^2 + 32t^2\cos^2(Kb/2)}\right], \tag{7}$$

for the singlet states. Note that this result has already been obtained by Hirsch in a different context.[34,35] The most surprising fact is the emergence of a dispersive band $\varepsilon_-(K) < 0$ associated to two-body bound states for any U. In particular, the ground state is obtained for $\varepsilon_-(K=0)$. This can be understood invoking the competition between the kinetic term that lowers the energy and that is enhanced when particles are close together, and the interaction term that favors the opposite situation. An interesting issue is to know whether this feature still holds for more than two particles. To tackle this task, we shall now analyze the three-body problem that is, fortunately, still tractable analytically.

III. THE THREE-BODY PROBLEM

As previously, we consider the three-body problem in the one-dimensional chain as a single-body problem in a graph standing in the $\mathbf{Z}^3$ lattice. Using, once again, the invariance of the system under a translation of the center of mass [direction (1,1,1) in $\mathbf{Z}^3$], it is convenient to build the following Bloch waves

$$|\varphi_{i,j,k}(K)\rangle = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} e^{iKnc} |i+n,j+n,k+n\rangle, \tag{8}$$

where $c = a\sqrt{3}$ and where $K = 2\pi j/Nc (j \in [0,N-1])$ is the total momentum of the three fermions. Remark that $|\varphi_{i,j,k}\rangle \propto |\varphi_{i',j',k'}\rangle$ if $(i,j,k) \equiv (i',j',k')$ mod (1,1,1) so that one must only consider nonequivalent Bloch function. Here, we have chosen to affect the phase 1 to the ket $|i,j,k\rangle$ such that $(i^2+j^2+k^2)$ is minimum. After projection along (1,1,1) the graph is the so-called *sextopus* displayed in Fig. 2.

Note that in this latter graph, we have not put the site corresponding to $|\varphi_{0,0,0}(K)\rangle$ since it is forbidden for spin 1/2 fermions but that would be allowed for bosons. It is readily seen with this representation that there are two types of regions: (i) the ''bulk'' where the three particles are close together and where there could possibly exist three-body bound states and (ii) the ''legs'' corresponding to a situation where one particle is motionless and the two others propagate together. One also observes that K plays the role of a ''pseudomagnetic field'' for the system so that the ground states will be obtained for $K = 0$ (zero field condition). For an arbitrary value of $K \neq 0$ mod π/c, the *sextopus* has the dihedral symmetry D_3 and can be easily diagonalized for any N. Note that when the three electrons have the same polarization, the system is frozen since the particles cannot move. It implies that the energy of the quadruplet $S = 3/2$ is simply 0. The only interesting situation thus arises in the sector $S = 1/2$ whose spectrum is shown in Fig. 3 as a function of K for a given U.

One clearly observes two distinct components. First, for a fixed K, there are two dispersive bands that correponds to scattering states (one two-body bound state + one motionless particle) propagating ballistically in the ''legs.'' Their precise form is given by Eq. (7). Second, one observes much more interesting states out of those bands. As we shall see thereafter, these states are actually three-body bound states and the most remarkable fact is that the ground state is always given by such a state for any U. To analyze more precisely this surprising phenomenon, we focus on the case $K = 0$ for which the ground state is obtained. In this case, the symmetry of the *sextopus* is D_6 and it is possible to look for bound states in each representation schematized in Fig. 4. Each site represented in Fig. 4 symbolizes a state vector with fixed angular momentum. Note that the representations indexed by $l = 0,3$ corresponds to a fully space symmetric wavefunction that can, in no case, be an eigenstate for three spin 1/2 fermions.

We thus look for a bound eigenstate $|\Psi\rangle = \Sigma_n \psi_n |n\rangle$ where $|n\rangle$ is the ket corresponding to the nth site of the half-chains labeled by $l \in [1,2]$ (or equivalently $l \in [4,5]$). For all $n \geqslant 3$, we set $\psi_n = C_\lambda e^{-\lambda(n-3)b}$ for n odd and $\psi_n = D_\lambda e^{-\lambda(n-3)b}$ for n even, and we seek for complex λ such that $\mathrm{Re}(\lambda b) \geqslant 0$ and $\mathrm{Im}(\lambda b) \equiv 0$ mod π, this latter condition ensuring to have a real eigenenergy. Such a state is an eigenstate if the secular equations are satisfied:

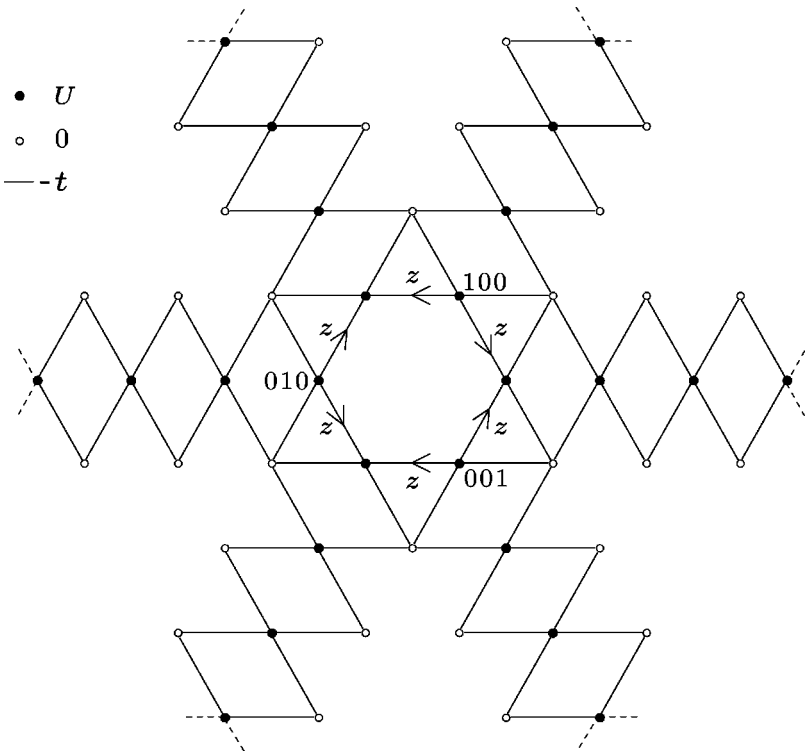

FIG. 2. Representation of the three-body problem graph after projection perpendicularly to the direction (1,1,1) in the $\mathbf{Z}^3$ lattice. The sites denoted ijk correspond to the ket $|\varphi_{i,j,k}(K)\rangle$ and $z=-2te^{-iKc}$.

$$[\varepsilon_{\pm}^{B}(\lambda)-U_l]\psi_1=-2t_l\psi_2,$$

$$\varepsilon_{\pm}^{B}(\lambda)\psi_2=-2t_l(\psi_1+\psi_3), \tag{9}$$

$$[\varepsilon_{\pm}^{B}(\lambda)-U]\psi_3=-2t_l\psi_2-\sqrt{2}t\psi_4,$$

where $U_l=U-4t\cos(2\pi l/6)$ and $t_l=t\cos(\pi l/6)$ and

$$\varepsilon_{\pm}^{B}(\lambda)=\frac{1}{2}[U\pm\sqrt{U^2+32t^2\cosh^2(\lambda b/2)}]. \tag{10}$$

We emphasize that the periodic boundary condition adds restrictions on λ but since the amplitude decreases exponentially, they are not relevant provided N is larger than the localization length $1/\lambda$. A simple inspection of the secular system (9) allows one to show that it always has, at least, one solution λ_0 (for any $U>0$) associated to $\varepsilon_{-}^{B}(\lambda_0)$ which is, thereby, the ground state of the system. We have plotted in Fig. 5 the dependence of the two-body and three-body ground states energy as a function of U for spin 1/2 fermions.

When U goes to infinity, both energies converges toward zero but, as noticed previously, the three-body ground state has always a lower energy than the two-body one. In addition, the localization length $1/\lambda_0$ tends to infinity which sounds quite natural for strong repulsion.

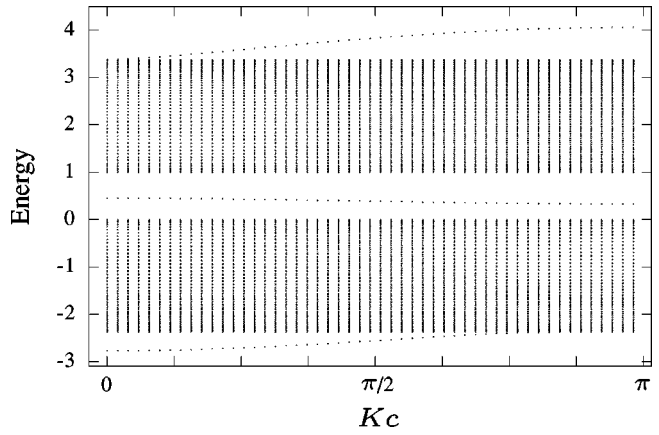

FIG. 3. Spectrum of the three-body problem as a function of Kc for $U=1$ and $N=100$ ($t=1$).

IV. THE FINITE DENSITY CASE

A natural question then arises: are there still many-body bound states at higher densities? Indeed, if we now consider four electrons, we can figure out more complex scattering processes where two two-body bound states collide with each other, or where a bound pair oscillates between two isolated particles. In these cases, one may expect the emergence of four-body bound states. Unfortunately, this problem is too complicated to be completely analyzed by elementary methods. We have searched for the possibility of binding together two two-body ground states by means of a variational method. In this approach, the four-particle state space has been decomposed in two sectors. The first one corresponds to two isolated two-particle states whose centers of mass are separated by at least 2.5 lattice spacings. In this region, we assumed an exponential decay of the wave func-

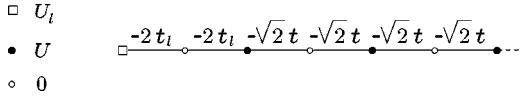

FIG. 4. Nontrivial graph of each irreducible representation of D_6 indexed by $l\in[0,5]$. U_l and t_l are defined in the text.

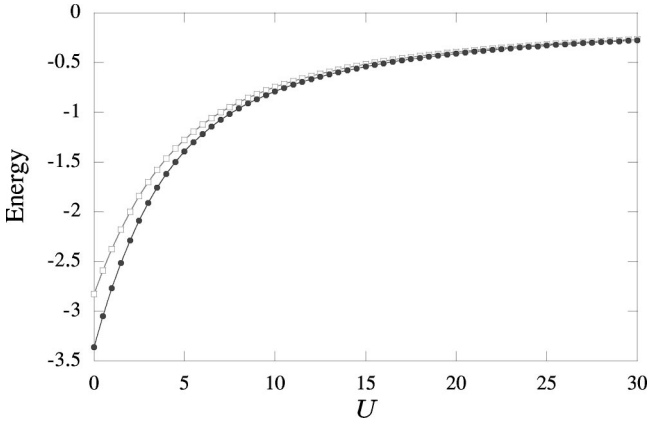

FIG. 5. Variation of the ground state energy of the two-body (□) and three-body (●) problems as a function of the interaction U ($t=1$).

tion with the relative separation of the two center of mass positions. The second region corresponds to real space configurations where each of the four particles is close to any other. In the simplest version, this defines, after taking global translation invariance into account, a finite set of 18 configurations. It is important to note that two two-body bound states collision may generate real space configurations where a bound pair escapes to infinity leaving two unpaired electrons which may remain at an arbitrary large final distance from each other. This is illustrated on the sequence shown in Fig. 6.

However, the typical decay length for the escape of a single pair is likely to be significantly shorter than the one for two bound pairs. Thus, we have not kept these asymptotic states with a single pair in our variational approach. This search for four-particle bound states has always failed so far. Of course, this lack of evidence does not constitute a proof of the absence of such bound states in the spectrum, but we believe that four-particle binding is unlikely in this model. The main reason for that is the Pauli principle which severely restricts the possibility of particle hopping in a close packing configuration. Therefore, we suggest that the finite but small density system will form a Luttinger liquid of bound pairs. The absence of four-particle binding may mean that residual interactions between these bound pairs are repulsive, allowing a well-defined thermodynamic limit. This picture of a fluid of bound pairs is in fact reminiscent of the attractive Hubbard model.[33] Indeed, a detailed analysis of the Bethe ansatz spectrum[36] shows that this model is precisely described in its low-energy limit in terms of a Luttinger liquid of spinless two-particle bound states. By analogy, we thus also expect a gap in the spin excitation spectrum of our model. Actually, the ground state and the thermodynamical properties of both models should be quite similar. However, dynamical quantities might produce some meaningful differences. For instance, it would be very interesting to investigate in more details the behavior of the single electron Green's function. In our simple-minded picture, adding an electron to a state with an even number of particles indeed leaves an unpaired spin. By contrast to the usual spin charge separated liquid and to the attractive Hubbard model in particular, our model opens the possibility of sustaining three-body bound states between this extra electron and a pair taken from the Luttinger liquid ground state. This interesting question clearly deserves further studies. Instead of adressing this issue here, we shall turn to a very simple description of the finite density system. For large particle densities, the two-particle bound states have to overlap in real space, and it is no longer clear that they provide a good basis to understand the ground state properties. In the following, we shall assume that the quantum state of the finite density system is not too far from a Slater determinant of plane waves. Let us now write the Hamiltonian (1) in momentum space:

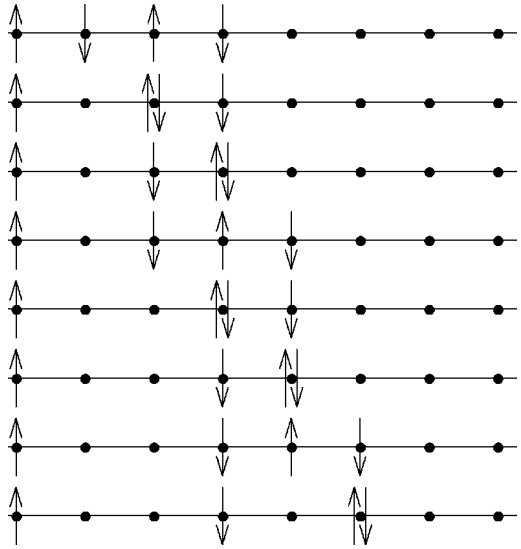

FIG. 6. A possible way to obtain an isolated pair and two frozen electrons from a four-body compact configuration.

$$H=\frac{1}{N}\sum_{k,k',p,p',\sigma}\delta_{p+p',k+k'} \times f(p,p';k',k)c^{\dagger}_{p,\sigma}c^{\dagger}_{p',-\sigma}c_{k',-\sigma}c_{k,\sigma}, \qquad (11)$$

where $c_{p,\sigma}=(1/\sqrt{N})\Sigma_n e^{inpa}c_{n,\sigma}$ and p is the momentum of the state. We keep the same notation c for operators either in real or in momentum space since no confusion is possible here. The interaction function is given by

$$f(p,p';k',k)=\frac{U}{2}-t[\cos(pa)+\cos(p'a)+\cos(k'a) +\cos(ka)]. \qquad (12)$$

The expectation value of H taken on any free particle state written using the plane wave single particle basis is given by

$$\langle H\rangle=\frac{2}{L}\sum_{k,k'} f(k,k';k',k)n_{k,\uparrow}n_{k',\downarrow}. \qquad (13)$$

To determine the most stable Slater determinant of plane

waves, we consider a single particle-hole excitation away from a reference state whose occupation numbers in momentum space are denoted by $n^{(0)}_{k,\sigma}$. For instance, we consider $n_{k,\uparrow}=n^{(0)}_{k,\uparrow}+\delta_{k,p}-\delta_{k,q}$ and $n_{k,\downarrow}=n^{(0)}_{k,\downarrow}$. The average energy change induced by this particle-hole excitation is

$$\langle \delta H\rangle_{p,q}=\frac{2}{L}\sum_{k'}\left[f(p,k';k',p)-f(q,k';k',q)\right]n^{(0)}_{k,\downarrow} \tag{14}$$

$$=-4t\frac{N_\downarrow}{N}[\cos(pa)-\cos(qa)], \tag{15}$$

where N_σ is the total number of spin σ electrons. This shows that the average energy is minimal provided the occupied state (momenta) fills the usual Fermi intervals $[-k_{F,\sigma},k_{F,\sigma}]$ for $\sigma=\uparrow,\downarrow$. From these considerations, and from the expression (11), it is very natural to separate the diagonal and off-diagonal part of H. We thus have

$$H_{\text{diag}}=\frac{U}{N}N_\uparrow N_\downarrow-2\sum_{k,\sigma}t_{\text{eff},\sigma}\cos(ka)c^\dagger_{k,\sigma}c_{k,\sigma}, \tag{16}$$

with $t_{\text{eff},\sigma}=2tN_{-\sigma}/N$. Up to a global shift, H_{diag} exhibits the same structure as a pure hopping Hamiltonian for free particles, but its hopping term depends on the particle density as it is induced by a two-particle interaction process. Along the same line, one has

$$H_{\text{off-diag}}=\frac{1}{N}\sum_{k,k',p,p',\sigma}\delta_{k+k',p+p'}(1-\delta_{k,p})\times f(p,p',k',p)c^\dagger_{p,\sigma}c^\dagger_{p',-\sigma}c_{k',-\sigma}c_{k,\sigma}. \tag{17}$$

Let us assume that the ground state is not too remote from the usual noninteracting Fermi sea. In this case, the four wave vectors involved in Eq. (17) are close to Fermi points so that $H_{\text{off-diag}}$ is well approximated by

$$H_{\text{off-diag}}\simeq\frac{1}{N}\sum_{k,k',p,p',\sigma}\delta_{k+k',p+p'}(1-\delta_{k,p})\times\frac{U_{\text{eff}}}{2}c^\dagger_{p,\sigma}c^\dagger_{p',-\sigma}c_{k',-\sigma}c_{k,\sigma}, \tag{18}$$

with $U_{\text{eff}}=U-8t\cos(k_Fa)$. This result is similar to the one obtained by Airoldi and Parola in a more general model.[20] Expression (18) is expected to be valid when $|U_{\text{eff}}|$ is smaller than the effective bandwidth which is of the order $t(N_\uparrow+N_\downarrow)/N$. When this condition is satisfied, we see that the model becomes equivalent to a one-dimensional Hubbard model with an effective interaction parameter U_{eff}. Note that the terms we have neglected going from Eqs. (17),(18) involve the momentum dependence of the bare interaction vertex on the external legs so they are irrelevant in the usual renormalization group analysis of weakly interacting fermions in one dimension.[37] The most interesting consequence of Eq. (18) is obtained for a less than half-filled system ($|k_Fa|<\pi/2$) so that $\cos(k_Fa)>0$. In this case, the model exhibits a qualitative change from an effective attraction to an effective repulsion as the bare on-site repulsion U crosses the value $8t\cos(k_Fa)$. From the previous argument, we expect a one-dimensional Fermi liquid for $U=8t\cos(k_Fa)$ as the off-diagonal interaction is then purely composed of irrelevant terms. As the density increases, the size of the attractive regions is reduced since the critical value of U decreases. Note that for dilute systems, this effective Hubbard model is supposed to be valid only for a narrow interval of values of U around $8t\cos(k_Fa)$ since the effective single electron bandwidth is small. In the dilute and attractive regime, it is therefore more accurate to work within the picture of a Bose gas of bound pairs.

V. CONCLUSIONS

To conclude, we have shown that a simple one-dimensional model in which the particle hopping is completely assisted by the presence of another particle in its neighborhood generates some interesting conducting states at finite density. For the less than half-filled system, in the presence of an on-site repulsion U, we have established the existence of two regimes for the effective interaction depending on the strength of U. In the attractive regime, the elementary building blocks of the system are likely to be the two-particle bound states discussed in Sec. II. Indeed, these states appear for any value of U and they are characterized by a very tight binding in real space. In this regime, our model is strongly reminiscent of the one-dimensional attractive Hubbard model. An interesting difference remains the existence of three-particle bound states detailed in Sec. III that are absent in the attractive Hubbard model.[33] In the present work, the existence of these bound states have only been established in the zero density limit. It would be interesting to know whether they could survive in the presence of a finite particle density, since they could eventually show up in the single electron spectral function.

Finally, we would like to make a few comments regarding the original motivation of this study, namely, the investigation of interaction effects in tight-binding models for which all single-particle eigenstates are localized in Aharonov-Bohm cages. A quasi-one-dimensional example illustrating this phenomenon has been analyzed in details in Ref. 31 for the two-body problem. Though the results obtained here have strong similarities with this latter model, they have also important qualitative differences. A common point is the possibility to form extended states for the two-particle problem which are tightly bound in real space independently of the local bare repulsion strength. However, the main difference lies in the fact that for Aharonov-Bohm cage models, these extended two-particle eigenstates are, at best, degenerate with the localized ground states and they are in most cases excited states.[30] In the finite density case, it is by no means obvious that these strongly localized systems become con-

ducting by contrast to the one studied here. Nevertheless, we believe that if such conducting states appear in the presence of Aharonov-Bohm cages, two-particle bound states will play a major role. In this context, such models with strongly correlated (or purely assisted) hopping may provide a simple and efficient way to describe possible conducting states induced by interactions in otherwise localized systems.

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