Interaction induced delocalisation for two particles in a periodic potential

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We consider two interacting particles evolving in a one-dimensional periodic structure embedded in a magnetic field. We show that the strong localization induced by the magnetic field for particular values of the flux per unit cell is destroyed as soon as the particles interact. We study the spectral and the dynamical aspects of this transition.

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As shown by Anderson in 1958\(^[1]\), a quantum particle in a disordered potential may be trapped in spatially localized eigenstates. A natural question which arises is whether such a dramatic effect operates in a many-body interacting system. This issue has been strongly revived by a series of experiments on Si MOSFETs\(^[2]\) which seem to indicate a metal-insulator transition in two dimensions. Since then, a lot of experimental and theoretical activity has been dedicated to this highly controversial topic\(^[3]\). Given the complexity of the full many-body systems, various groups have studied the already non trivial two-particle problem\(^[4]\). In particular, D. L. Shepelyansky has shown convincingly that some two-particle eigenstates exhibit much larger localization length than single particle ones. Note however that in other situations such as in quasiperiodic systems, interactions may generate strongly localized two-particle eigenstates\(^[5]\). In addition, it seems that for repulsive interactions these interesting effects do not appear in the vicinity of the two-particle ground state, and this leaves open questions for the many electron case.

Recently, it has been shown that an extreme localization mechanism induced by the magnetic field can lead to a complete confinement of the particle motion inside Aharonov-Bohm cages\(^[6]\). Contrary to the Anderson localization, this phenomenon occurs in pure two-dimensional systems, \textit{i.e.} without disorder, and is due to a subtle interplay between the structure geometry and the magnetic field. Two series of experiments have confirmed the existence of these Aharonov-Bohm cages. In the first one\(^[7]\), superconducting wire networks with the adapted structure exhibit a striking reduction of the critical current for the predicted values of the magnetic field. The second experiments\(^[8]\) measure the magneto-resistance oscillations in two-dimensional mesoscopic structures with a small number of conduction channels and large electronic mean free path. A clearcut dip at half a flux quantum per loop is observed and confirms the presence of this peculiar localization process.

It is therefore very natural to ask whether these cages survive for interacting particles. In this letter, we present an exactly solvable model for two interacting particles under a magnetic field. To simplify, we deal with a quasi-one-dimensional model which exhibits Aharonov-Bohm cages. We show that for half a flux quantum per loop, dispersive two-particle bound states appear even for repulsive local interaction. In this system, the two-particle ground state is non dispersive but the first dispersive band is rather close in energy. Slightly away from these remarkable fluxes, these bound states survive until they merge in a two-particle continuum. Finally, we are led to speculate that a finite repulsive local interaction is able to turn the fully localized non interacting system into a strongly correlated metal provided the electron density is large enough.

We consider a one-dimensional chain of square loops with periodic boundary conditions displayed in Fig.\(^[9]\) embedded in a uniform perpendicular magnetic field \(\mathbf{B}\), which is a bipartite periodic structure with three sites per unit cell. As we shall see, the various characteristics of this system are similar to those discussed in Ref.\(^[1]\) for two-dimensional tilings. Hereafter, we fix the total polarization to zero which is equivalent to consider two particles with opposite spin (\(\uparrow\) and \(\downarrow\)).

Let us consider the standard Hubbard Hamiltonian:

\[
H = \sum_{(i,j),\sigma = \uparrow,\downarrow} t_{ij} c_{i,\sigma}^{\dagger} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow},
\]

where \(c_{i,\sigma}^{\dagger}\) (resp. \(c_{i,\sigma}\)) denotes the creation (resp. annihilation) operator of a fermion with spin \(\sigma\), \(n_{i,\sigma} = c_{i,\sigma}^{\dagger} c_{i,\sigma}\) the density of spin \(\sigma\) fermion on site \(i\), and \(\langle \ldots \rangle\) stands for nearest neighbor pairs. Note that, since the particle considered here are fermions, the interaction term \(U\) is only efficient in the singlet sector where the orbital part
of the wave function is symmetric. When \( B = 0 \), the hopping term \( t_{ij} = 1 \) if \( i \) and \( j \) are nearest neighbors and 0 otherwise. In the presence of a magnetic field \( \mathbf{B} \), \( t_{ij} \) is multiplied by a phase factor \( e^{i\gamma_{ij}} \) involving the vector potential \( \mathbf{A} \):

\[
\gamma_{ij} = \frac{2\pi}{\phi_0} \int_{j}^{i} \mathbf{A} \cdot d\mathbf{L},
\]

where \( \phi_0 = \frac{hc}{e} \) is the flux quantum. For convenience, we choose a gauge in which only one hopping term per unit cell is modified (see in Fig. 1). The whole spectrum only depends on the reduced flux \( f = \phi/\phi_0 \) where \( \phi = Ba^2/2 \) is the magnetic flux through an elementary square (\( a \) is the unit cell vector length).

![FIG. 1. Square chain under a uniform magnetic field. The magnetic flux per unit cell is denoted by \( \phi \) and \( \gamma = 2\pi \phi/\phi_0 \).](image)

Let us first analyze the one-particle problem. In this case, the translation invariance of the system along the chain direction allows one to straightforwardly compute the one-particle spectrum that consists of three bands:

\[
\epsilon_{\alpha}(k) = 2\alpha \sqrt{1 + \cos(2\gamma) \cos(ka)}, \quad k \in [0, 2\pi/a],
\]

where \( \alpha = 0, \pm 1 \) is the band index and \( \gamma = 2\pi f \). The weight of each band in the normalized density of states equals \( 1/3 \). The existence of a non dispersive band at \( \varepsilon = 0 \) is simply due to the bipartite character of the structure, its degeneracy being equal to the difference between the number of sites of each family. The most striking feature is that for \( f = 1/2 \) (half a flux quantum per unit square), the spectrum is made up of three non dispersive bands. As discussed in Ref. [8], this property leads to a complete lock-in of any wave packet spreading inside the so-called Aharonov-Bohm cages. One thus has a transition induced by the magnetic field.

For \( U = 0 \), the two-particle spectrum is the addition of the one-particle spectra so that the eigenenergies are labelled by four quantum numbers:

\[
\epsilon_{\alpha_\sigma, \alpha_\bar{\sigma}}(k_1, k_2) = \epsilon_{\alpha_\sigma}(k_1) + \epsilon_{\alpha_\bar{\sigma}}(k_2),
\]

where \( \alpha_\sigma = 0, \pm 1 \) (resp. \( k_\sigma \)) is the band index (resp. the wave vector) of the spin \( \sigma \) particle. Thus, for \( f = 1/2 \), the spectrum consists of five non dispersive bands corresponding to \( \epsilon = 0, \pm 2, \pm 4 \) and the space evolution of any two-particle wave function is confined in an Aharonov-Bohm cage that is merely the superposition of each one-particle cage.

![FIG. 2. Eigenstates of the one-particle problem for \( f = 1/2 \) (non normalized cage solutions).](image)

We now address the interacting case where \( U \neq 0 \). The main question is whether or not the latter system remains frozen when the particles are interacting. In other words, can a (local) interaction term destroy the cages and authorize any propagation? In general, a two-particle problem with on-site interaction in a \( D \)-dimensional structure can be viewed as a single particle one in a \( 2D \)-dimensional structure with a local potential in the hyperplane corresponding to a double occupancy of a site. Taking advantage of the translation invariance, this problem can then be mapped onto a (continuous) family of \( D \)-dimensional problems with a finite number of impurity sites which are often easier to solve. [4] The same approach could in principle be used here but given the very special nature of the non interacting system for \( f = 1/2 \), it is most easily carried out by using the minimally extended one-particle eigenstates displayed in Fig. 2.

These states have non vanishing amplitude only on a finite number of sites and thus reflect the absence of propagation at \( f = 1/2 \). We denote them by \( |i, \varepsilon_\alpha\rangle \), where \( i \) is the cell number centered on each 4-fold coordinated site and \( \varepsilon_\alpha = 0, \pm 2 \).

The two-particle state space is then given by the tensor product of the one-particle state:

\[
|i, \alpha; i', \alpha'\rangle = |i, \varepsilon_\alpha\rangle_\uparrow \otimes |i', \varepsilon_{\alpha'}\rangle_\downarrow,
\]

for all \( i, i', \alpha, \alpha' \). It is worth stressing that since the \( |i, \varepsilon_\alpha\rangle \) are confined eigenstates of the one-particle hamiltonian, most of these two-particle eigenstates are not affected by \( U \). This local interaction term only acts on states for which the two particles have a non vanishing probability to be on the same site, i.e. such that \( |i - i'| \leq 1 \). As a result, the number of states which are sensitive to \( U \) scales linearly with the total number of cells \( N \) whereas in the generic case \( (f \neq 1/2) \), it is proportional to \( N^2 \). To proceed further, let us remark that the states sensitive to \( U \) are space-symmetric:

\[
|i, \alpha; i', \alpha'\rangle_S = \frac{1}{\sqrt{2}} (|i, \alpha; i', \alpha'\rangle + |i', \alpha'; i, \alpha\rangle),
\]
if \( i \neq i' \) or \( \alpha \neq \alpha' \), and \( |i, \alpha; i, \alpha\rangle = |i, \alpha; i, \alpha\rangle \). Moreover, since the problem is invariant under a translation of the center of mass, it is convenient to build Bloch waves:

\[
|\varphi_0(\alpha, \alpha', K)\rangle = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} e^{iKna} |n, \alpha; n, \alpha'\rangle
\]

\[
|\varphi_1(\alpha, \alpha', K)\rangle = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} e^{iKna} |n, \alpha; n + 1, \alpha'\rangle,
\]

where \( K = 2\pi j/Na (j = 0, N - 1) \) is a wave vector lying in the first Brillouin zone. In the following, we shall always consider the limit where \( N \) tends to infinity. One then has to calculate the matrix element of the Hamiltonian in each irreducible representation labelled by \( K \), and restrict this analysis to the \((15 \times 15)\) subspace generated by \(|\varphi_0\rangle\) and \(|\varphi_1\rangle\). For any \((\alpha, \alpha', \beta, \beta', K_l, K_m)\) one has:

\[
\langle \varphi_0(\alpha, \alpha', K_l)|H|\varphi_1(\beta, \beta', K_m)\rangle = 0
\]

\[
\langle \varphi_1(\alpha, \alpha', K_l)|H|\varphi_1(\beta, \beta', K_m)\rangle = \lambda_{\alpha, \alpha', \beta, \beta'} \delta_{l,m},
\]

where \( \lambda_{\alpha, \alpha', \beta, \beta'} \) is a \( K_{l,m}\)-independent scalar and where \( \delta_{l,m} \) is the usual Kronecker symbol. This implies that the eigenvalues of the \((9 \times 9)\) subspace generated by \(|\varphi_0\rangle\) are non dispersive. These eigenvalues are given by the five \( U\)-dependent roots of the characteristic polynomial:

\[
P(\epsilon, U) = \epsilon^5 - U \epsilon^4 - 20 \epsilon^3 + 16U \epsilon^2 + 64\epsilon - 24U,
\]

and four \( U\)-independent values \( \pm 2, 0 \) (two-fold degenerated) resulting of additional symmetry between \( \alpha \) and \( \alpha' \). The non dispersive part of the spectrum is shown in Fig. 3 for \( U \geq 0 \).

\[\text{FIG. 3. Non dispersive part of the two-particle spectrum at } f = 1/2 \text{ versus the interaction.}\]

We emphasize that since the spectrum of the Hubbard Hamiltonian (in a bipartite structure) is odd under the transformation \( U \rightarrow -U \), we can restrict our analysis to the repulsive case. In the large \( U \) limit, the five roots of \( P \) tend toward \( \pm \sqrt{8 \pm 2\sqrt{10}}, U \); this latter value simply corresponding to a situation where the two particles are localized on the same site (anti-bonding state).

A much more interesting component of the spectrum is provided in the \((6 \times 6)\) subspace generated by \(|\varphi_0\rangle\). In this subspace, the eigenvalues are given by the roots of the following characteristic polynomial:

\[
Q(\epsilon, U, K) = \epsilon^6 - 2U \epsilon^5 + (U^2 - 20) \epsilon^4 + 28U \epsilon^3 + 8 (8 - U^2) \epsilon^2 - 4U(14 - 3 \cos(Ka)) \epsilon + 4U^2(2 + \cos(Ka)).
\]

Contrary to the previous case, these eigenvalues obviously depend on \( K \), and the associated non degenerated eigenstates are extended (Bloch-like). This dispersive component of the spectrum is displayed in Fig. 4.

\[\text{FIG. 4. Dispersive part of the two-particle spectrum at } f = 1/2 \text{ versus the interaction.}\]

In the large \( U \) limit, the asymptotic eigenvalues are given by \( U \) (twice degenerated) and \( \pm \sqrt{4 \pm 2 \sqrt{2 - \cos(Ka)}} \), and there still remains a \( K\)-dependent component in the spectrum.

The physical consequences of this dispersion are important. Indeed, let us consider a generic two-particle initial state having a non zero overlap with one of the \(|\varphi_0\rangle\). The emergence of dispersive states for \( U \neq 0 \) indicates that it is now possible for this wave packet to spread over the whole system whereas it was completely trapped inside the Aharonov-Bohm cage in the non interacting case. Moreover, since the dispersive eigenstates are extended, the propagation is ballistic.

For other values of the reduced flux, the full solution of the two-particle problem cannot be cast in a simple analytic form, although it is possible to reduce it into a scattering problem for one particle moving on a chain in the presence of three static impurities. Nevertheless, let us analyze the neighborhood of the half-flux parametrized
by \( \delta f = |f - 1/2| \). For \( f \neq 1/2 \), all the single-particle eigenstates become extended, except those corresponding to the flat band at \( \varepsilon = 0 \). The non dispersive two-particle states which are insensitive to \( U \) at \( f = 1/2 \) evolve into several two-particle continua, whose band width scales as \( \delta f \) for small \( \delta f \). The non dispersive states which are sensitive to \( U \) become dispersive with a band width scaling as \( (\delta f)^2/U \) (see inset in Fig. 5). The corresponding wave functions still exhibit a binding of the two particles. Finally, as displayed in Fig. 5, the dispersive states at \( f = 1/2 \) remain dispersive. All these dispersive bound states evolve smoothly as a function of \( \delta f \) until their energies merge in the two-particle continuum, which occurs for \( \delta f \sim U \) at small \( U \). As \( \delta f \) further increases, the total number of bound states gradually decreases.

![Fig. 5. Low-energy spectrum for \( U = 0.01 \) as a function of the reduced flux.](image)

Since, in this study, the effect of the interaction term between the two particles is clearly to induce a delocalization process, one can expect that for finite density of particles, a subtle correlated conducting state will emerge. Note however that in this system, the energy of two particles is minimal when they do not interact, either because they are far apart or because their orbital wave function is antisymmetric. We therefore conjecture that the many body ground state will remain localized up to a filling factor equal to \( 1/3 \). At this point, the lowest flat band is completely filled with a fully polarized electron sea. The next electron will have an opposite spin and is thus likely to delocalize along the chain. This problem obviously deserves further investigations. Let us also remark that, here, we consider a quasi-one-dimensional model to simplify the calculations, but a similar physics is expected for other tight-binding models which exhibit single-particle confinement inside Aharonov-Bohm cages. Nevertheless, in more general systems, we do not expect to see non dispersive states sensitive to \( U \). In this context, an interesting open question is whether it is possible to find situations where the ground state of the two-particle spectrum is dispersive, even for repulsive interaction.

How could this interaction induced delocalization be observed experimentally? The two-particle system might be accessible in a Josephson junction or a quantum dot array in the Coulomb blockade regime. Such experimental situations shall be described by a model with on-site disorder, but, very likely, some two-particle states would still exhibit a much larger localization length than single particle ones. Ongoing experiments on ballistic semi-conducting networks with special two-dimensional geometry may also manifest some interaction effects on this Aharonov-Bohm localization. In these structures, the interaction strength can be varied by changing the electronic density or by polarizing the system with a tilted magnetic field. Clearly, a better understanding of the many electron case needs to be achieved.

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[1] P. W. Anderson, Phys. Rev. 109, 1492 (1958).
[2] S. V. Kravchenko et al., Phys. Rev. Lett. 77, 4938 (1996).
[3] See for instance a recent survey by B. L. Altshuler, D. S. Maslov and V. M. Pudalov, cond-mat/003032.
[4] D. L. Shepelyansky, Phys. Rev. Lett. 73, 2607 (1994).
[5] Y. Imry, Europhys. Lett. 30, 405 (1995).
[6] D. Weinmann, A. Müller-Groeling, J. L. Pichard and K. Frahm, Phys. Rev. Lett. 75, 1598 (1995).
[7] A. Barelly, J. Bellissard, P. Jacquod and D. L. Shepelyansky, Phys. Rev. Lett. 77, 4752 (1996).
[8] J. Vidal, R. Mosseri and B. Douçot, Phys. Rev. Lett. 81, 5888 (1998).
[9] C. C. Abilio et al., Phys. Rev. Lett. 83, 5102 (1999).
[10] C. Naud, G. Faini, D. Mailly and B. Etienne, cond-mat/0006400.
[11] R. E. Peierls, Z. Phys. 80, 763 (1933).
[12] M. Caffarel and R. Mosseri, Phys. Rev. B 57, 12651 (1998).
[13] We have also added the \( U \)-independent eigenvalues \( \varepsilon = \pm 4 \) provided by the space-antisymmetric states.
[14] B. Sutherland, in *Exactly solvable problems in condensed matter and relativistic field theory*, Proceedings, Panchgani, India, edited by B. S. Shastry, S. S. Jha, and V. Singh (Springer-Verlag, Berlin Heidelberg New-York Tokyo, 1985), p. 9 ; R. Mosseri, J. Phys. A 33, L319 (2000).
[15] The dimension of this subspace is different from the one generated by the \( |\varphi_1\rangle \) since, for any \( (\alpha, \alpha', K) \) one has : \( |\varphi_0(\alpha, \alpha', K)\rangle = |\varphi_0(\alpha', \alpha, K)\rangle \).
[16] Such a situation occurs as soon as the two one-particle wave functions overlap each other. For example, one can considers a initial configuration where the two particles are localized on the same site.