

## ARTICLES

**Two interacting electrons in a quasiperiodic chain**

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We study numerically the effect of on-site Hubbard interaction  $U$  between two electrons in the quasiperiodic Harper's equation. In the periodic chain limit, by mapping the problem to that of one electron in two dimensions with a diagonal line of impurities of strength  $U$  we demonstrate a band of resonance two-particle pairing states starting from  $E=U$ . In the ballistic (metallic) regime we show explicitly interaction-assisted extended pairing states and multifractal pairing states in the diffusive (critical) regime. We also obtain localized pairing states in the gaps and the created subband due to  $U$ , whose number increases when going to the localized regime, which are responsible for reducing the velocity and the diffusion coefficient in the qualitatively similar to the noninteracting case ballistic and diffusive two-particle dynamics. In the localized regime we find propagation enhancement for small  $U$  and stronger localization for larger  $U$ , as in disordered systems. [S0163-1829(97)07940-X]

**I. INTRODUCTION**

Anderson localization<sup>1</sup> can be also studied in quasiperiodic systems via the Harper's equation, which also describes electrons in a square lattice with an added strong magnetic field,<sup>2-4</sup> superconducting networks,<sup>5</sup> etc. This model presents a very useful alternative to the study of one-dimensional (1D) disordered systems, since, apart from localization it can also display metallic behavior associated with ballistic motion and critical behavior (mobility edge) with ordinary diffusion,<sup>6,7</sup> somehow mimicking more realistic three-dimensional (3D) disordered systems. In this paper we report results that relate to the problem of what happens to the electronic eigenstates and the corresponding quantum dynamics of two electrons moving in a quasiperiodic potential in which the interaction between them is taken into account.

The study of two Hubbard interacting particles (THIP) localized by a random potential has been pioneered by Shepelyansky.<sup>8</sup> This author and others<sup>9-14</sup> produced very interesting analytical and numerical work within the Anderson-Hubbard model, which showed weakening of Anderson localization, known always to be caused by disorder in 1D, due to the effect of the two-particle interaction. The enhanced propagation effect of the interacting electron pair on scales  $\xi$  larger than the single-particle localization length  $\xi_1$  due to the interaction was also displayed in disordered mesoscopic rings threaded by magnetic flux, by showing a pairing effect via  $h/2e$ -periodic, instead of  $h/e$ -periodic, eigenstates.<sup>11</sup> However, a previous diagonalization study for 1D disordered system<sup>15</sup> revealed that few states in the main band show a weak propagation enhancement, while states with two locally paired electrons are usually even more localized in the presence of the interaction. Moreover, it was pointed out that for large positive  $U$  stronger localization occurs when compared to the noninteracting case. In a recent work,<sup>16</sup> it is demonstrated by a transfer matrix study that no propagation enhancement is possible for THIP in an infinite disordered chain at  $E=0$  (see, however, Ref. 17).

These rather conflicting results can be partially understood by the fact that most works, apart from the direct exact diagonalization or dynamical approaches, rely on a mapping of the THIP problem to a superimposed banded random matrix ensemble (SBRME). It was suggested that if the interaction is expressed in the noninteracting localized basis a random band matrix with additional disorder in the matrix diagonal appears (SBRME) and the enhancement of the pair localization length  $\xi \propto \xi_1^2$ , where  $\xi_1$  is the one-particle localization length, is easily obtained.<sup>8</sup> However, the reduction to a SBRME relies on a questionable assumption about chaoticity of the noninteracting localized states within  $\xi_1$ , so that the relevant matrix model could be different.<sup>18</sup> Moreover, since in the one-particle localized basis the interaction is relevant only when the two particles are localized around positions close to each other, the obtained localization weakening that occurs for mesoscopic systems vanishes for an infinite chain.<sup>16</sup> It must be also pointed out that since in most of the previous works only the localized case with finite  $\xi_1$  is considered it could be reasonable to expect more dramatic pairing effects for extended noninteracting eigenstates that are always overlapping.

The model considered in this paper allows us to study the fate of extended and critical one-electron states in the presence of Hubbard interaction. We find a kind of pairing effect for certain two-particle states in the metallic and the critical regimes with the simultaneous appearance of localized pairing states in the gaps and the created subband due to the interaction.<sup>19</sup> These localized states reduce the corresponding THIP dynamics although it remains similar in nature to the noninteracting case in all three regimes. However, we obtain a weak enhancement of propagation in the localized regime when the interaction is switched on and even stronger localization for larger  $U$ .

In Secs. II and III, we introduce the Harper-Hubbard model and consider by diagonalization methods two interacting electrons moving in a tight-binding quasiperiodic potential of strength  $\lambda$ , for various values of the local electron-

electron Hubbard interaction  $U$ . In the absence of the interaction  $U$  it is known<sup>4</sup> that there are extended states for  $\lambda < 2$ , a mobility edge for  $\lambda = \lambda_c = 2$  and a finite one-electron localization length  $\xi_1 = 1/\ln(\lambda/2)$  independent of energy for  $\lambda > 2$ . In Sec. IV we present our results from the numerical diagonalization of the corresponding two interacting electrons Harper-Hubbard equation, by showing explicitly extended pairing states in the metallic case  $\lambda < 2$  or multifractal pairing states at the mobility edge  $\lambda = 2$ . We do not find extended or multifractal pairing states for the insulator but a weak propagation enhancement with the simultaneous appearance of localized pairing states.<sup>15</sup> In Sec. V we address the question of the electron localization dynamics in the presence of  $U$ . The time evolution of a quantum wave packet in the presence of interactions shows ballistic motion for  $\lambda < 2$ , diffusion for  $\lambda = 2$  and ceases to expand for  $\lambda > 2$  as for the noninteracting metallic, critical, and localized regimes, respectively.<sup>6,12</sup> In the presence of the interaction a decreasing  $U$ -dependent electron velocity and diffusion coefficient, due to the appearance of localized states, is obtained for the metallic and the critical regimes, respectively. In the localized regime for high  $U$  stronger localization occurs, in agreement with previous results on the Anderson-Hubbard model.<sup>15</sup> Finally, in Sec. VI we discuss our results and present the conclusions which arise from the present study.

## II. THE HARPER-HUBBARD MODEL

The Harper-Hubbard tight-binding equation for two interacting particles is<sup>20,21</sup>

$$\begin{aligned}
 H = & \sum_{n=1}^N \sum_{\sigma} (c_{n+1,\sigma}^{\dagger} c_{n,\sigma} + c_{n,\sigma}^{\dagger} c_{n+1,\sigma}) \\
 & + \sum_{n=1}^N \sum_{\sigma} \lambda \cos(2\pi\phi n) c_{n,\sigma}^{\dagger} c_{n,\sigma} \\
 & + \sum_{n=1}^N U c_{n,\uparrow}^{\dagger} c_{n,\uparrow} c_{n,\downarrow}^{\dagger} c_{n,\downarrow}, \quad (1)
 \end{aligned}$$

where  $c_{n,\sigma}^{\dagger}$  and  $c_{n,\sigma}$  are the creation and destruction operators for the electron at site  $n$  with spin  $\sigma$ ,  $\lambda \cos(2\pi\phi n)$  is the potential at site  $n$ , with  $\phi$  an irrational number usually chosen as the golden mean  $\phi = (\sqrt{5}-1)/2$  and  $U$  is the strength of the local Hubbard interaction between the two electrons. The Hilbert space can be conveniently divided into one singlet subspace with total spin  $S=0$  and three triplet subspaces with total spin  $S=1$ ,  $S_z=1,0,-1$ , respectively. The three triplet subspaces are energy degenerate and since they permit no double occupation the triplet states are not affected by the Hubbard interaction. In a chain of  $N$  sites the singlet subspace is spanned in the basis of  $N(N+1)/2$  spatially symmetric wave functions

$$\begin{aligned}
 & |\psi(n_1, n_2)\rangle_s \\
 = & \begin{cases} \frac{1}{\sqrt{2}} (c_{n_1,\uparrow}^{\dagger} c_{n_2,\downarrow}^{\dagger} + c_{n_2,\uparrow}^{\dagger} c_{n_1,\downarrow}^{\dagger}) |0\rangle & \text{for } n_1 = n_2, \\ (c_{n_1,\uparrow}^{\dagger} c_{n_2,\uparrow}^{\dagger}) |0\rangle & \text{for } n_1 \neq n_2, \end{cases} \quad (2)
 \end{aligned}$$

which are antisymmetric with respect to the exchange of the spins and permit double occupancy.

## III. METHOD OF CALCULATION

We carried out exact diagonalization of  $H$  in the singlet subspace where the Hubbard interaction is relevant and found out all the eigenvalues and eigenvectors for finite  $N$  sites with various  $\lambda$ 's and  $U$ 's. In order to measure the degree of localization for the interacting electrons we calculate the one-particle spatial extent  $\xi^{(j)}$  in the  $j$ th two-electron wave function via<sup>15</sup>

$$\xi^{(j)} = \sum_{n_1=1}^N \sum_{n_2=1}^{n_1} |a_{n_1, n_2}^{(j)}|^2 \sqrt{(n_1 - \bar{x}_1)^2 + (n_2 - \bar{x}_2)^2}, \quad (3)$$

with mean positions

$$\bar{x}_{1,2} = \sum_{n_1=1}^N \sum_{n_2=1}^{n_1} |a_{n_1, n_2}^{(j)}|^2 n_{1,2} \quad (4)$$

of the electrons 1 and 2, where  $a_{n_1, n_2}^{(j)}$  is the normalized coefficient of the wave function in the basis of Eq. (2). It must be mentioned that in the way  $\xi$  is defined it can estimate the spatial extend of each electron averaged over the second electron and is related to a quantity known as the participation ratio.<sup>15</sup> Moreover,  $\xi$  should correspond to the true localization length if the wave functions decay exponentially. Another important quantity used in this study is the mean value of the distance between the two electrons in the chain, which can be calculated for each two-particle wave function via

$$d^{(j)} = \sum_{n_1=1}^N \sum_{n_2=1}^{n_1} |a_{n_1, n_2}^{(j)}|^2 |n_1 - n_2|. \quad (5)$$

The distance  $d$  measures the correlation between the two electrons so that a small  $d$  defines a pairing two-electron eigenstate, which can be either delocalized in the metallic regime, multifractal in the critical regime, or localized mostly in the insulating regime  $\lambda > 2$ .

## IV. TWO-PARTICLE PAIRING STATES

We diagonalize the Hamiltonian matrix for Fibonacci number chain lengths  $N$ , e.g.,  $N=89$  if the rational approximant of  $\phi = (\sqrt{5}-1)/2$  is  $\frac{55}{89}$ , so that the potential is periodic with period  $N$ . In Fig. 1(a) we plot  $\xi$  and  $d$  versus the corresponding eigenvalue  $E$  for the 1D pure  $\lambda=0$  case with interaction  $U=1$ . The striking characteristic is a band of  $N$  states, out of the total of  $2N^2$  two-particle states, which have extremely small distance  $d$  starting from the energy  $E=U$  where  $d$  is precisely zero [see Fig. 1(a)]. These pairing states have one sharp peak at the diagonal line of the plane where  $n_1=n_2$ , which implies that the particles always stay very close to each other. In Figs. 1(b)–1(e) we plot some such characteristic wave function amplitudes in the plane of the two-electron coordinates  $n_1$  and  $n_2$  where the nonzero amplitudes appear in or very close to the diagonal line.

Extended pairing states due to the interaction but having a finite width  $d$  are also seen in Fig. 2 for the ballistic case  $\lambda=1$  for  $U=1$ . These states are identified from Fig. 2(a) by plotting in Figs. 2(b) and 2(c) only states that have small  $d$ . The extended pairing states in the metallic regime ( $\lambda < 2$ ) have their number progressively reduced when in-

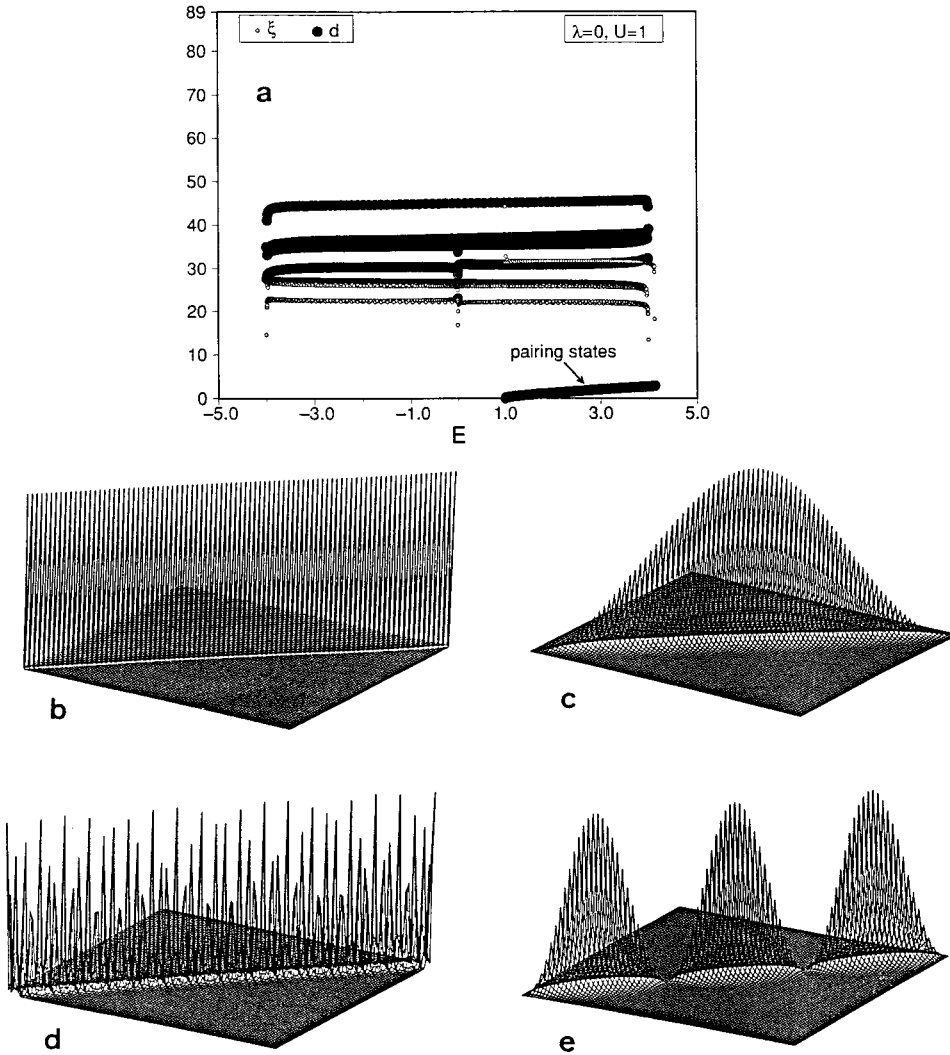


FIG. 1. (a) The electron spatial extend  $\xi$  (open circles) and the mean distance  $d$  (black dots) between two electrons as a function of the two-electron wave function energy  $E$  for the periodic Hubbard chain of  $\lambda=0$  with interaction strength  $U=1$ . (b), (c), (d), (e) Amplitude distributions for extended pairing states with  $E=U$ ,  $E=4.1225$ ,  $E=2.5119$ , and  $E=4.1173$ , respectively, as a function of the two-electron coordinates  $n_1$  and  $n_2$  and the same parameters as in (a).

creasing  $\lambda$  towards  $\lambda=2$ . Figure 3(a) accounts for the critical case  $\lambda=2$  where still a few pairing states are seen, such as in Fig. 3(b), with a displayed kind of multifractality along the diagonal.<sup>7</sup> However, apart from extended or multifractal pairing states we also obtain another kind of localized pairing states, which occur in pairs of almost identical energies and similar amplitude distributions. In Fig. 3(c) one such state is shown where a double peaked structure is displayed along the diagonal having small  $d$  and misleadingly large  $\xi$  due to our definition of  $\xi$ , since such pairing states are strongly localized in two spatial positions along the diagonal. The localized pairing states correspond to a physical picture of localization due to Mott,<sup>22</sup> and they are more frequently encountered in the insulating  $\lambda>2$  regime. They involve tunneling transitions between two-particle localized states spaced at a distance proportional to  $\xi_1$  apart, having energies that differ by very small amounts. In Fig. 4(a) we demonstrate  $\xi$  and  $d$  in the critical regime  $\lambda=2$  with a higher value of the interaction strength  $U=5$ . In Figs. 4(b) and 4(c) we show two multifractal pairing states. In the plot of Fig. 5 we show  $\xi$  and  $d$  for the insulating regime  $\lambda=3$  with localized pairing states having two separate maxima [Figs. 5(b) and 5(c)] and no extended or multifractal pairing states survive in this case.

We find that localized two-particle states due to the inter-

action also appear in the metallic and the critical regimes. These pairing states have small  $d$  and are located either in the gaps or in the subband created by the interaction  $U$ . They are identified from Figs. 2(a), 3(a), 4(a), and 5(a) and for the critical  $\lambda=2$  case also in Figs. 6(a)–6(c) from the integrated density of states, which is known to be multifractal “devil’s staircase” for noninteracting electrons. For the THIP four major gaps (plateaus) are seen to coexist with smaller gaps on all scales. In the created subband for large positive energy the localized pairing states due to the effect of the interaction  $U$  are clearly seen. It must be emphasised that localized pairing states are found for  $\lambda<2$  only in the presence of finite interaction ( $U>0$ ). Moreover, we mention that the results described in this section did not change qualitatively by varying the system size.

## V. TWO-PARTICLE DYNAMICS

The study of the wave packet dynamics provides global information for the changes due to the interaction of all the relevant wave functions. If we put two electrons at the same initial site, e.g., the chain center 0 at  $t=0$ , the mean-square displacement  $\langle[\Delta x(t)]^2\rangle$  for each electron at subsequent times  $t$  can be calculated from all the singlet eigensolutions of Eq. (1) from the variance

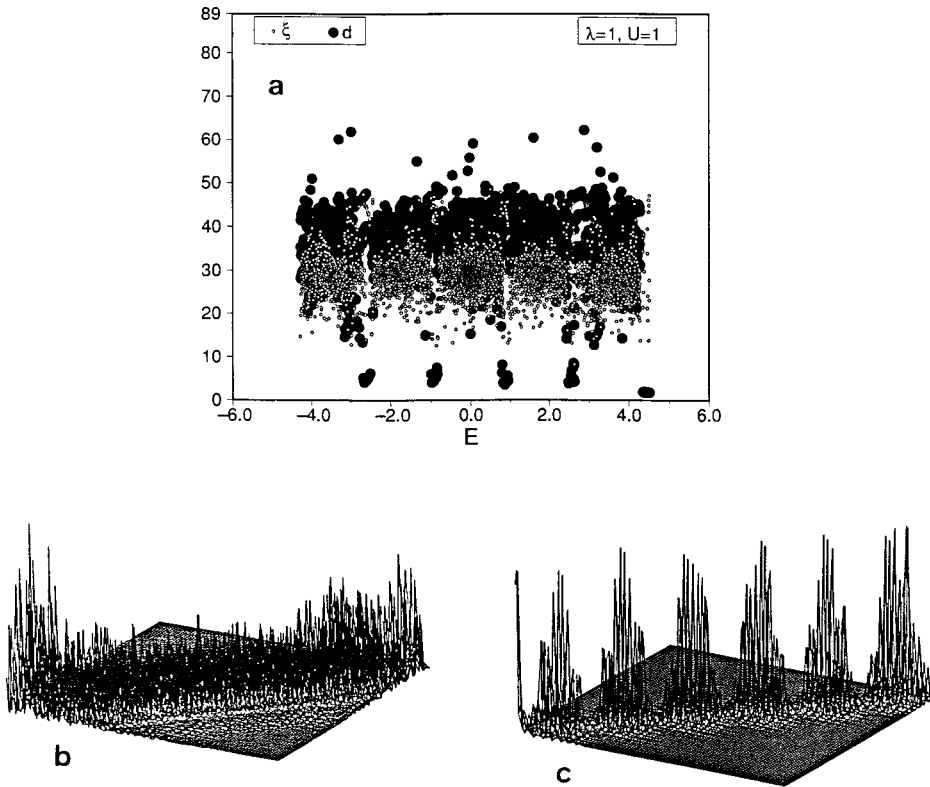


FIG. 2. (a) The  $\xi$  and  $d$  versus the energy  $E$  of the two-electron wave functions in the *ballistic* case  $\lambda=1$  with the interaction strength  $U=1$ . Amplitude distributions (b) for the extended pairing state  $E=-0.0013$  and (c) for  $E=-2.5707$ .

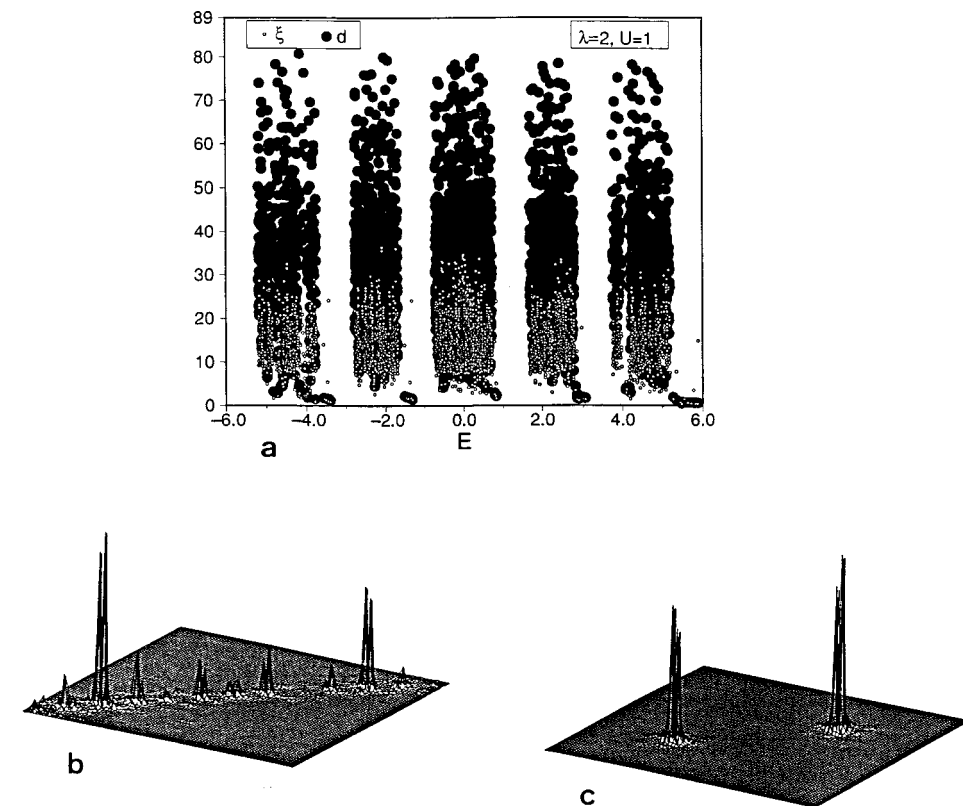


FIG. 3. (a) The  $\xi$  and  $d$  versus the energy  $E$  of the two-electron wave function for the *diffusive* case with  $\lambda=\lambda_c=2$  and the interaction strength  $U=1$ . Amplitude distributions (b) for the pairing state  $E=-0.5231$  which has a multifractal character and (c) for  $E=0.8274$  which is localized in the Mott sense.

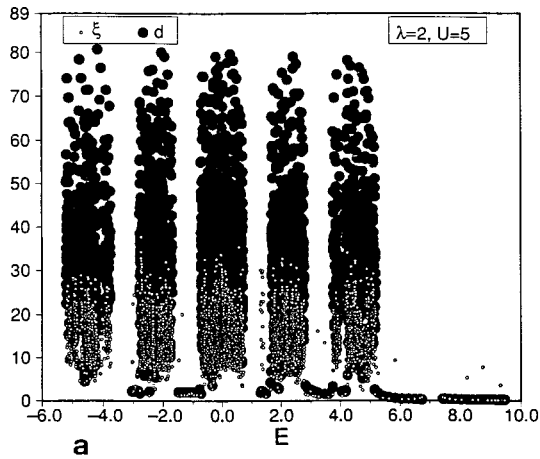


FIG. 4. (a) The  $\xi$  and  $d$  versus the energy  $E$  of the two-electron wave function for the critical *diffusive* case  $\lambda=2$  with  $U=5$ . The states (b)  $E=1.3631$  and (c)  $E=1.3752$  display a multifractal character.

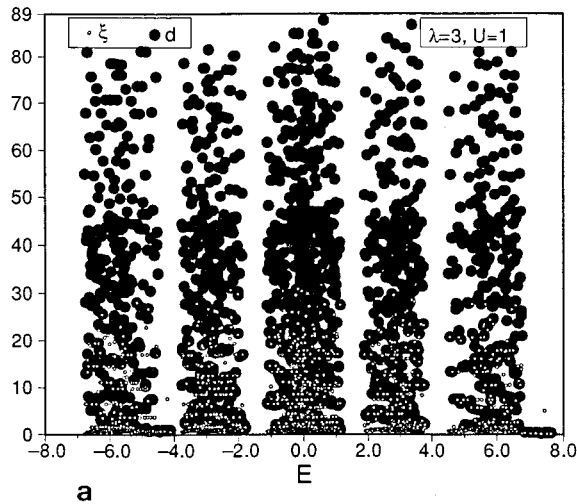
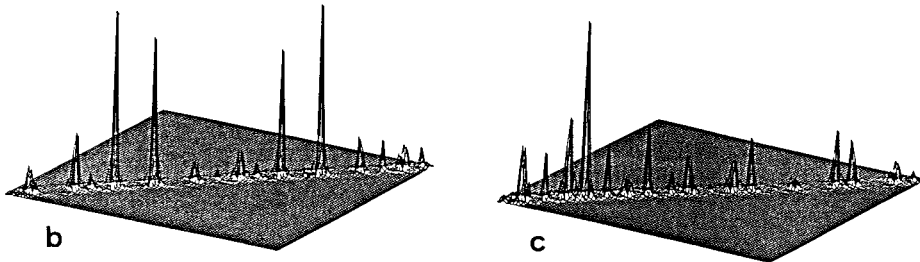
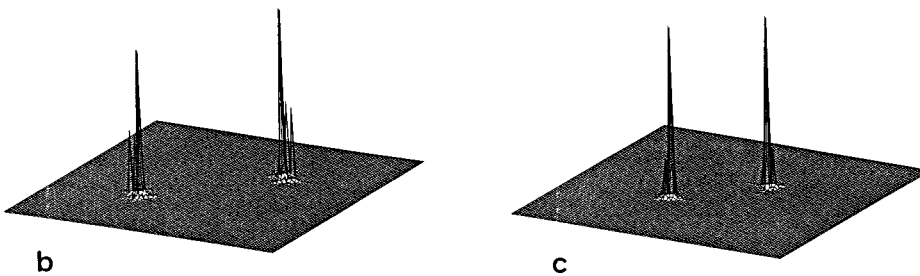


FIG. 5. (a) The  $\xi$  and  $d$  versus the energy  $E$  of the two-electron wave function for the insulating *localized* case  $\lambda=3$  with  $U=1$ . The (b)  $E=-0.0646$  and (c)  $E=0.9083$  correspond to localized pairing states in the Mott sense.



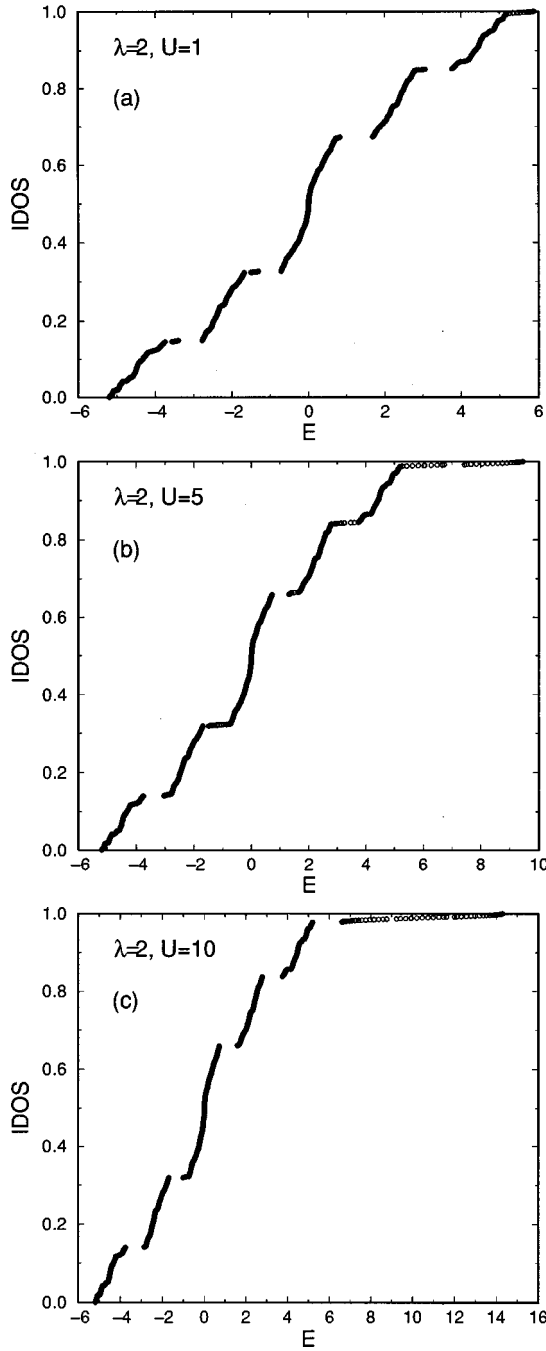


FIG. 6. (a), (b), (c) The integrated density of states for the critical case  $\lambda=2$  with various values of the interaction strength  $U$ . The main gaps correspond to the empty plateaus.

$$\begin{aligned}
 \langle \Delta x^2(t) \rangle &= \frac{1}{2} \langle n_1^2 + n_2^2 \rangle \\
 &= \sum_{n_1=1}^N \sum_{n_2=1}^{n_1} \left| \sum_j e^{-iE_j t} a_{0,0}^{(j)*} a_{n_1, n_2}^{(j)} \right|^2 (n_1^2 + n_2^2) / 2,
 \end{aligned} \tag{6}$$

where  $\langle \dots \rangle$  denotes quantum average and the factor of 2 in the denominator transforms  $\langle \Delta x^2(t) \rangle$  to correspond to one electron, in order to agree with previous one-electron dynamics for  $U=0$ . For the adopted initial condition, in which the two electrons are at the same site, only the singlet states with additional on-site energy due to  $U$  are allowed. Alterna-

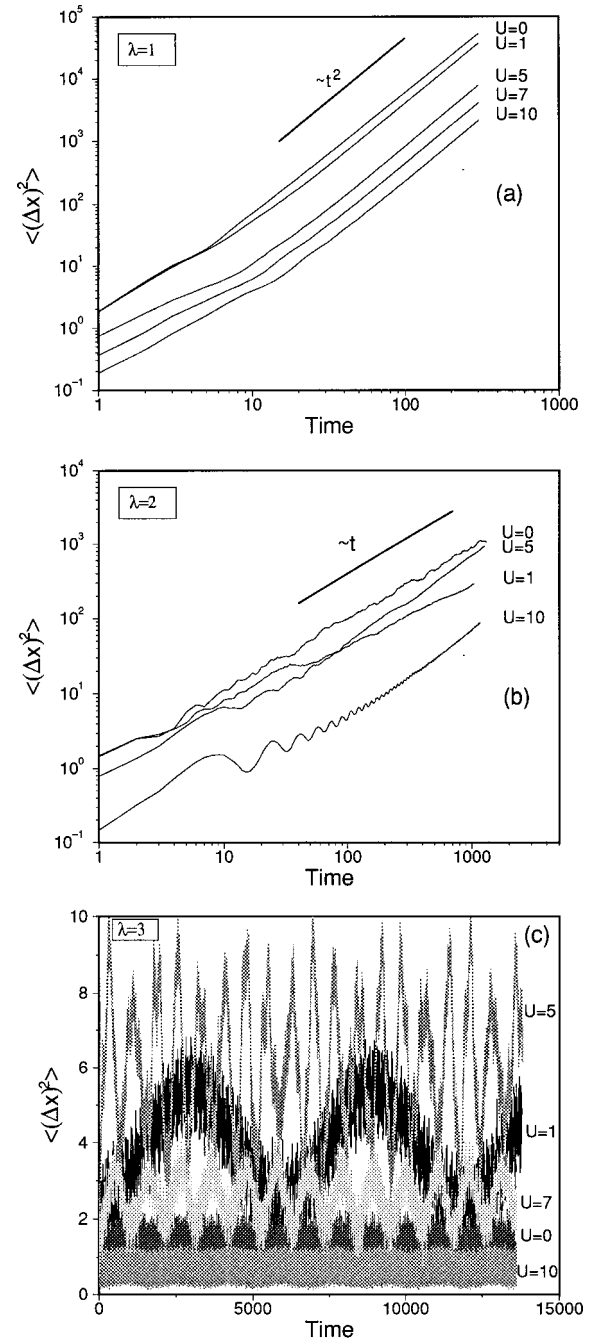


FIG. 7. The mean-square displacement  $\langle [\Delta x(t)]^2 \rangle$  of a wave packet for the approximant  $\phi=10946/17711$  with the two electrons initially located at the chain center of long length  $N=17711$ , which ensures that the wave does not reach the ends of the chain. The values of the interaction strength  $U$  are denoted in the figures: (a) log-log plot for the ballistic case  $\lambda=1$ , (b) log-log plot for the diffusive case  $\lambda=\lambda_c=2$  and (c) ordinary plot for the localized case  $\lambda=3$ .

tively, we have integrated the corresponding two-dimensional equations of motion using a Runge-Kutta algorithm, in order to obtain results for much longer chains of  $N=17711$ . Figure 7(a) shows the obtained  $\langle [\Delta x(t)]^2 \rangle$  for  $\lambda=1$  where is seen that the ballistic motion  $\langle [\Delta x(t)]^2 \rangle \propto t^2$ , remains valid also for finite  $U$  but with a reduced velocity. In the critical case  $\lambda=2$  diffusion with  $\langle [\Delta x(t)]^2 \rangle \propto t$  is obtained in Fig. 7(b) reducing in magnitude by increasing  $U$ , although a tendency for more enhanced propagation

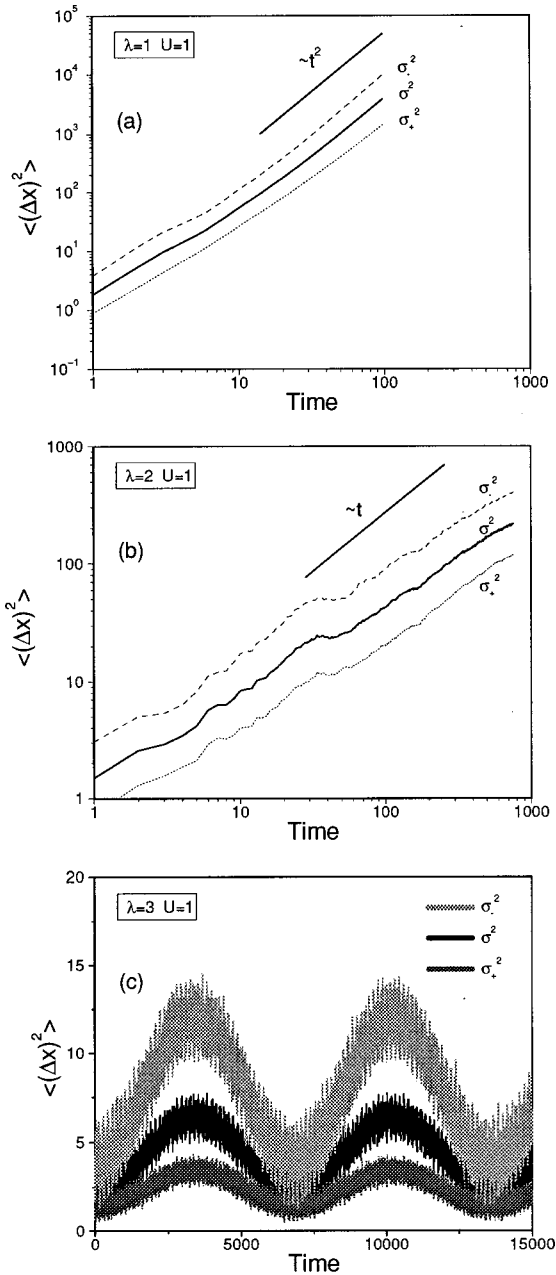


FIG. 8. A comparison between the mean-square displacements  $\sigma^2 = \langle[\Delta x(t)]^2\rangle$ , the pair mean-square displacement  $\sigma_+^2$  and the pair size  $\sigma_-^2$  with the rest of parameters as in Fig. 7. The values of the interaction strength  $U=1$ : (a) log-log plot for the *ballistic* case  $\lambda=1$ , (b) log-log plot for the *diffusive* case  $\lambda=\lambda_c=2$  and (c) ordinary plot for the *localized* case  $\lambda=3$ .

is seen when  $U=5$ . For the insulator in Fig. 7(c)  $\langle[\Delta x(t)]^2\rangle$  shows many oscillations and asymptotically reaches larger values for finite  $U=1$  or  $5$  when compared to  $U=0$ , which indicates the familiar weakening of localization due to the interaction.<sup>9–14</sup> However, for very large  $U=7$  or  $10$  the relevant wave functions for the dynamical process lie mostly in the subband created above the main band, which corresponds to localized pairing states having much shorter localization lengths, and as a result the mean-square displacement becomes very short [Fig. 7(c)] indicating a localizing effect of the interaction.<sup>15</sup> Therefore, a decrease of the degree of localization due to the interaction is demonstrated in the local-

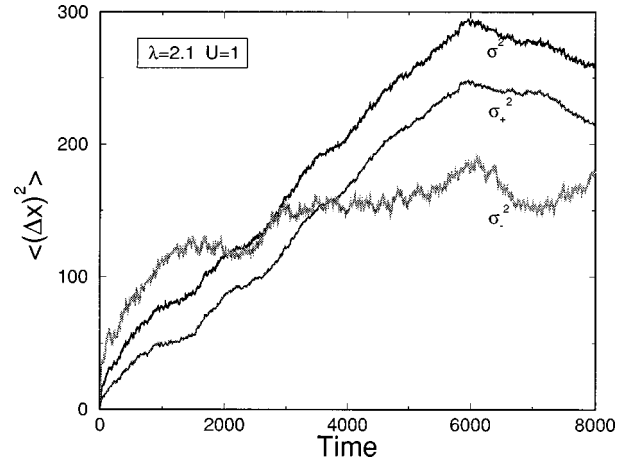


FIG. 9. The pair mean-square displacement  $\sigma_+^2$  and the pair size  $\sigma_-^2$  for the weakly localized case  $\lambda=2.1$  with interaction strength  $U=1$ . It is seen that for large times  $\sigma_+^2$  becomes greater than  $\sigma_-^2$  denoting coherent pair propagation in this regime.

ized regime for not too large  $U$ , in agreement with the original reported tendency.

It must be mentioned that our definition of  $\sigma^2 = \frac{1}{2}\langle n_1^2 + n_2^2 \rangle$  of Eq. (6) focuses on the properties of one interacting electron and is different from both  $\sigma_+^2 = \frac{1}{4}\langle (n_1 + n_2)^2 \rangle$  and  $\sigma_-^2 = \langle (n_1 - n_2)^2 \rangle$  introduced in Refs. 8 and 18 to examine coherent propagation of two electrons. Our results displayed in Fig. 8 for the metallic, critical, and localized case show a similar behavior of the electron ( $\sigma^2$ ) and pair ( $\sigma_+^2$ ) propagation as well as for the squared pair size ( $\sigma_-^2$ ). From these results, since the obtained propagation behavior in the diagonal and its vertical of the effective two-dimensional lattice are similar, no coherent pair propagation can be concluded. In order to test our conclusion for the insulating regime we also consider the weakly localized case with  $\lambda=2.1$ . The obtained dynamics shown in Fig. 9 eventually gives  $\sigma_+^2 > \sigma_-^2$  for larger times, as for disordered systems,<sup>8</sup> which can be interpreted as denoting coherent pair propagation enhancement.

## VI. DISCUSSION AND CONCLUSIONS

It can be shown<sup>8,10</sup> that the interacting electron problem in the periodic  $\lambda=0$  case can be mapped onto an equation for a single electron moving in an effective two-dimensional lattice with a line of impurities of energy  $U$  along the diagonal. The impurities naturally lead to  $N$  resonance states at energies starting from  $E=U$  as seen in Fig. 1(a), having amplitude only on the impurity sites along the lattice diagonal. In this way extended pairing states naturally appear, for example, precisely at  $E=U$  a two-particle pairing state can be found exactly [Fig. 1(b)] having a constant amplitude on the diagonal and zero elsewhere. It is very well known that such resonance extended states can also appear at certain energies in noninteracting 1D chains with distributed large segments of identical impurities.<sup>23</sup>

We show that quasiperiodicity in addition to the interaction also permits such an exact mapping of THIP to a single-electron equation moving in a two-dimensional lattice with a symmetric potential  $\lambda \cos(2\pi\phi n_1) + \lambda \cos(2\pi\phi n_2)$  at the co-

ordinate  $n_1, n_2$ , which denote the positions of the two electrons, in addition to the line of impurities  $U\delta_{n_1, n_2}$  along the diagonal. In analogy with the one-dimensional large impurity case where additional small perturbations are known to allow the survival of a weak resonant effect at certain energies, remnant of the extended states in the absence of such perturbation,<sup>23</sup> we similarly obtain a kind of pairing states having finite but small distance between the two electrons. In this paper we demonstrate by exact diagonalization of the THIP Hamiltonian in a finite quasiperiodic Harper's chain such two-particle extended or multifractal pairing states due to the interaction for the metal and at the critical point. In these regimes we also find localized pairing states due to the interaction in the gaps or the created subband, also according to the Mott resonance theory of localization. In the localized regime  $\lambda > 2$  we find mostly localized pairing states with short localization lengths.

In disordered systems previous attempts to consider the electron-electron interactions are based on perturbation theories<sup>24,25</sup> or more rigorous solutions for special cases.<sup>26,27</sup> In this paper by a numerical diagonalization study the interaction between two electrons a kind of pairing effect for certain delocalized states is demonstrated, which occurs via

extended or multifractal states. Localized pairing states are also found due to the interaction in all regimes.<sup>19</sup> Our results are confirmed for both repulsive and attractive on-site Hubbard interactions and it is probably worth noting that in the case of an attractive interaction ( $U$  negative) the subband created by the interaction lies below the band bottom of the noninteracting case so that the ground state is always a localized pairing state for the metal and the insulator. The localized pairing states might also affect physical quantities since they can decrease the velocity and the diffusion coefficient in the metallic and the critical regimes. Moreover, in the corresponding dynamics we demonstrate a tendency for weakening of localization in the insulating  $\lambda > 2$  regime for small  $U$  but even stronger localization for higher  $U$ .

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