Double Butterfly Spectrum for Two Interacting Particles in the Harper Model

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We study the effect of interparticle interaction U on the spectrum of the Harper model and show that it leads to a pure-point component arising from the multifractal spectrum of the noninteracting problem. Our numerical studies allow us to understand the global structure of the spectrum. An analytical approach developed permits us to understand the origin of localized states in the limit of strong interaction U and fine spectral structure for small U. [S0031-9007(96)01788-7]

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Recently a great deal of attention has been devoted to the investigation of incommensurate systems exhibiting singular continuous spectrum with many interesting multifractal properties (see, e.g., [1–3]). Among the physical models, one of the most popular is the Harper model of electrons on a two-dimensional square lattice in the presence of a perpendicular magnetic field [4,5]. This system can be reduced to the study of a rather simple model of particle dynamics on a one-dimensional quasiperiodic lattice. The energy spectrum exhibits multifractal properties and the band spectrum for rational values of magnetic flux looks like a butterfly. In spite of the academic character of such a model, experiments have been performed during the last ten years exhibiting this multifractal butterfly structure. One of the first among them was performed in 1985 using superconducting networks [6] and more recently experiments with superlattices also allowed us to observe the first hierarchical steps of multifractal butterfly structure [7].

An in-depth understanding of such an intricate spectral structure attracted the interest of mathematicians and physicists who developed new approaches for its investigation such as noncommutative geometry [8], pseudodifferential operators [9], functional analysis [10], renormalization group approach [11,12], and thermodynamical formalism [13]. All these tools allowed us to study the problem on rigorous mathematical ground and to understand the properties of eigenstates. For example using the duality between momentum and spatial coordinate [14], it is possible to prove rigorously the existence of localized or delocalized states [15,16]. It was also found that quantum systems which are chaotic in the classical limit may have quite unusual properties in the presence of underlying quasiperiodic structure [1,13,17].

All the works mentioned above were done for one particle dynamics. However, even from the physics of the original Harper model, it is clear that the interaction between electrons on the square lattice in the presence of magnetic flux plays an important role. Therefore it is natural to address the question of the influence of interaction on multifractal spectrum. The most simple example of such a case is an interaction between two particles. Recently it was found that in the case of random potential even such a simple model has a number of unexpected properties [18]. For example, repulsive/attractive short range interaction leads to the appearance of effective pair states in which two particles propagate together on a distance much larger than the one-particle localization length without interaction. Surprisingly the first numerical studies of interaction effect in a quasiperiodic potential showed an opposite tendency [19]. Namely, repulsive/attractive interaction leads to the appearance of localized states while in the absence of interaction multifractal spectrum generated quasidiffusive spreading of wave packets on the lattice. However, the numerical approach used in [19] allowed us to study only the wave packet evolution while the structure of the spectrum itself was not directly accessible. Therefore, to understand the spectral structure and the nature of eigenstates, we performed numerical simulations by direct diagonalization based upon the Lanczos algorithm.

As a basic model for our investigations we consider the model of two interacting particles (TIP) in the Harper problem described by the following eigenvalues equation:

$$[2\lambda\cos(\gamma n_1+\beta_1)+2\lambda\cos(\gamma n_2+\beta_2)+U\delta_{n_1,n_2}]\varphi_{n_1,n_2}+\varphi_{n_1+1,n_2}+\varphi_{n_1-1,n_2}+\varphi_{n_1,n_2+1}+\varphi_{n_1,n_2-1}=E\varphi_{n_1,n_2}\,. \quad (1)$$

Without interaction, each particle moves in quasiperiodic Harper potential and $\gamma/2\pi=\phi/\phi_0=\alpha$ is the ratio between the magnetic flux within one unit cell of the square lattice and the flux quantum $\phi_0=h/e$. The parameter α plays the role of an effective Planck's constant and $\beta_{1,2}$ are related to the quasimomentum components in the noninteracting problem. The parameter λ characterizes the strength of the quasiperiodic potential and for the case of electrons on a square lattice $\lambda=1$ [5]. Strong analytical and numerical evidence has been given that the spectrum is pure point and the states are localized when $\lambda>1$ while for $\lambda<1$ the spectrum is continuous with extended eigenstates [1,10,14,20]. The strength of the short range on-site interaction is characterized by U. We concentrate our investigations on the case $\lambda=1$, $\beta_{1,2}=\beta$ when for $U=0$ the spectrum is multifractal for irrational values of $\gamma/2\pi$. We consider only the symmetric TIP states.

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In the absence of interaction, the corresponding two particle spectrum results from the superposition of two one-particle spectra of the Harper model and is shown in Fig. 1(a).

When increasing the strength of the interaction U, the spectrum is split into two butterflies which are slightly shifted one in respect to the other. However, one of them remains almost at the same place corresponding to the noninteracting case of Fig. 1(a). The shifted butterfly moves to the right since the repulsive interaction $U > 0$ gives a global increase of energy. A typical case $U = 1$ of the double butterfly spectrum is presented in Fig. 1(b).

The main features which can be immediately observed in Fig. 1(b) are the smoothness of the edge of the shifted butterfly, the less dense character of its spectrum, and the filling of some internal energy gaps (see, for example, near $\alpha = 0.6$ and $E = -1.5$). However, the gaps in the spectrum still exist on all scales.

The shift of one butterfly and the almost unchanged form for the other at moderate values of interaction U can be understood in the following simple way. For that we choose small values of flux $\alpha \ll 1$ and use the perturbation theory in U on the basis of harmonic oscillator functions to get analytical expressions for the Landau sublevels at the spectrum edge. Without interaction, the band edge is given by $E_{\pm}(\alpha) = \pm 8 \mp 4\pi\alpha(m_1 + m_2 + 1) \pm \pi^2\alpha^2[2 + (2m_1 + 1)^2 + (2m_2 + 1)^2]/4 + \mathrm{O}(\alpha^3)$, which is a superposition of two Hofstadter butterflies in the semiclassical regime [21]. The integers m_1, m_2 are the Landau quantum numbers for oscillator states near the bottoms of potential minima. If two particles are located in different minima, the interaction between them is negligibly small and the energy levels are not shifted by U. These energy states correspond to a nonshifted butterfly with dense spectrum since there are many states when TIP are separated from each other. If TIP are located in the same potential minimum, the interaction gives an energy shift which in the first order of perturbation theory is $\Delta E_{\pm} = U\sqrt{\alpha}$ for $m_{1,2} = 0$ and $m_{1,2} = (0; 1)$ being in good agreement with numerical data for $U < 1$ as can be seen in Fig. 2(a). This shows that the shifted butterfly corresponds to the case when the

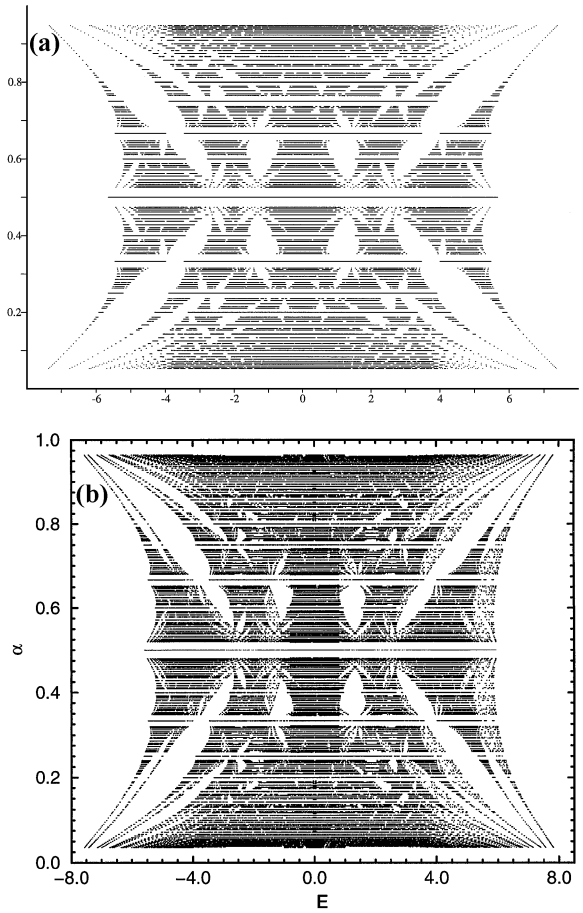

FIG. 1. Spectrum of the two particle Harper problem [(a) up], with $U = 0$ obtained for rational values of $\gamma/2\pi = \alpha = p/q$ with $q \leq 19$; [(b) down] with $U = 1$ and $q \leq 23$.

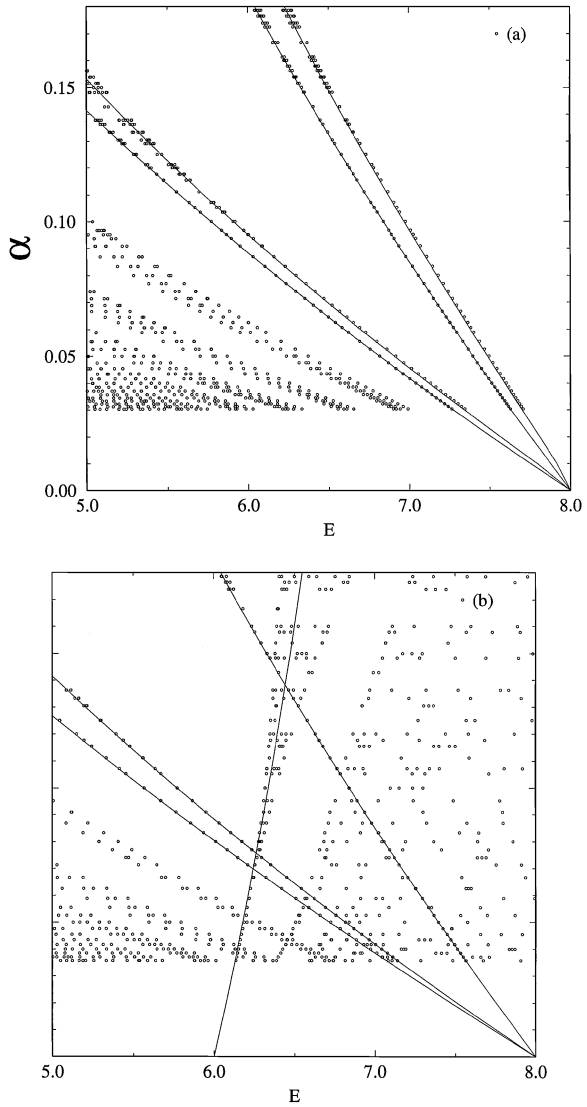

FIG. 2. Energy band edges (a) $U = 0.4$, dots are numerical data, and solid curves are perturbation theory results (see text); (b) $U = 10$, dots are data from Fig. 4, and solid curves are given by theory described in the text.

two particles are located near each other. The density of such states is smaller than in the case when particles are far from each other and that is why the shifted butterfly is less dense.

Direct analysis of eigenstates for irrational flux values (which are approximated by a continuous fraction expansion) also shows that the states in the shifted part correspond to the situation where two particles stay near each other. However, contrary to the TIP in a random potential, the particles here cannot propagate together and stay exponentially localized near the origin as can be seen with the typical 3D plot of Fig. 3.

We also investigated the structure of eigenstates in the more dense part of the spectrum (nonshifted butterfly). In that case the eigenstates are delocalized and quite similar to those corresponding to the noninteracting case. Here the two particles mainly spread quasidiffusively along the quasiperiodic lattice and interaction is not important for them in agreement with [19]. The properties of eigenstates can also be analyzed with the help of the inverse participation ratio (IPR) $\xi = (\sum_{n_{1,2}} W_{n_1,n_2}^2)^{-1}$ (Fig. 4). The localized states with small ξ correspond to the part of the shifted butterfly with the less dense spectrum while the unshifted butterfly is associated to large ξ with delocalized states. It is interesting to determine the IPR ξ_0 in the noninteracting eigenstates basis. Such an approach has been quite useful for TIP in a random potential [22] but the situation for TIP in the Harper model is quite different. Namely, the delocalized states have a very small value of ξ_0 while the localized ones are delocalized in the noninteracting eigenstates basis and have very large ξ_0 (see Fig. 3).

With a further increase of U the shifted butterfly goes on moving to the right and becomes more and more deformed. Starting from the interaction strength $U \geq 10$, this butterfly is transformed into a spectral band with a width two times smaller than the original spectrum at $U = 0$. The center of this band is located at energy $E \approx U$. A typical example of a global spectrum is shown in Fig. 5.

The physical reason for the appearance of such a separated spectral band can be understood in the following way. For strong U, there are states for which TIP are localized on the same site so that $n_{1,2} = n$. According to (1) the energy of the states is $E_n = 4\lambda \cos(\gamma n + \beta) + U$. The transition between these states can be obtained with first order perturbation theory in $1/U$ which gives the effective eigenvalue equation

$$[4\lambda \cos(\gamma n + \beta) + U]\phi_n + V_{\text{eff}}(\phi_{n+1} + \phi_{n-1}) = E\phi_n . \quad (2)$$

Here V_{eff} is the hopping between such states due to virtual transitions via states with $n_1 \neq n_2$. For $U \gg 1$, the energy difference between diagonal and off-diagonal states is very large and therefore $V_{\text{eff}} \sim 1/U$. The equation for diagonal eigenstates has the form of the Harper equation with $\lambda_{\text{eff}} = 2\lambda/V_{\text{eff}} \gg 1$. Because of this, these states are exponentially localized so that particles stay near the origin. In some sense, the interaction renormalizes the constant $\lambda \rightarrow \lambda_{\text{eff}}$ in the Harper equation for a pair of particles. For strong U, the renormalized λ_{eff} is much larger than 1 that, according to the Aubry duality [14], leads to a localization of TIP pairs in the quasiperiodic potential. Our conjecture is that in a sense λ_{eff} remains larger than 1 even for moderate values of $U \sim 1$. In a sense interaction breaks Aubry duality leading to the appearence of a localized TIP phase. However more rigorous analytical confirmations of this conjecture are desirable especially keeping in mind that in a random potential the interaction with $U \sim 1$ leads to delocalization of TIP pair states. The expressions for the TIP energy edges of a shifted spectral band can be found using semiclassical analysis at small flux values [8,23]. For Fig. 2(b), they give $E = 6.0 + 0.59 \times 2\pi\alpha + \mathrm{O}(\alpha^2)$ [24] in agreement with numerical data.

For the part of the spectrum represented by the unshifted butterfly at $U \gg 1$, the eigenstates become more and more similar to asymmetric TIP configuration, i.e., $\phi_{n_1,n_2} = \mathrm{sgn}(n_1 - n_2)(\chi_{n_1}^{(1)}\chi_{n_2}^{(2)} - \chi_{n_2}^{(1)}\chi_{n_1}^{(2)})/\sqrt{2}$,

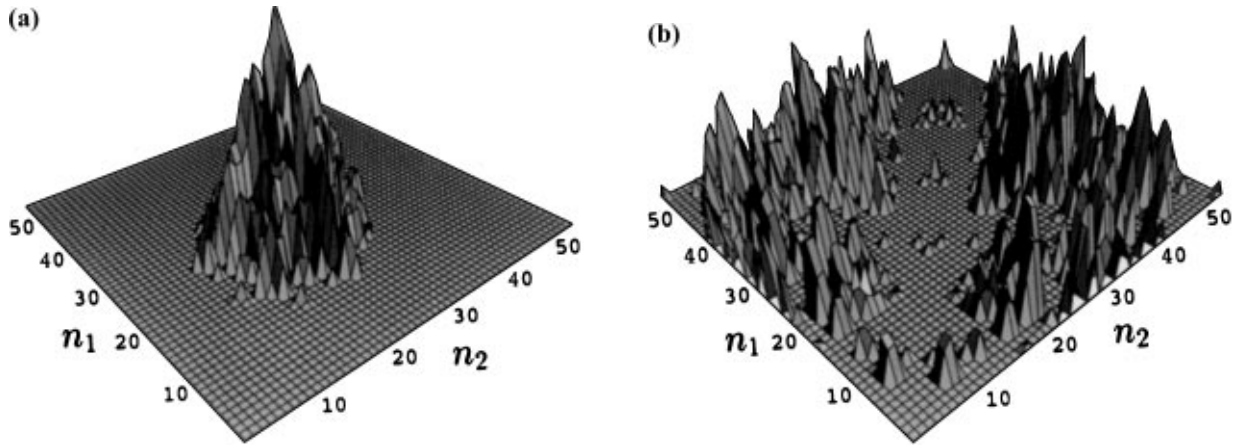

FIG. 3. Semilog plot of $W_{n_1,n_2} = |\phi_{n_1,n_2}|^2$ for localized ($E = -1.3376, -10 \leq \ln W \leq -1, \xi = 5.9, \xi_0 = 193$ [(a) left]) and delocalized ($E = -1.7368, -10 \leq \ln W \leq -3, \xi = 214, \xi_0 = 12.5$ [(b) right]) eigenstates at $U = 1, \alpha = 34/55, \beta = \sqrt{2}$.

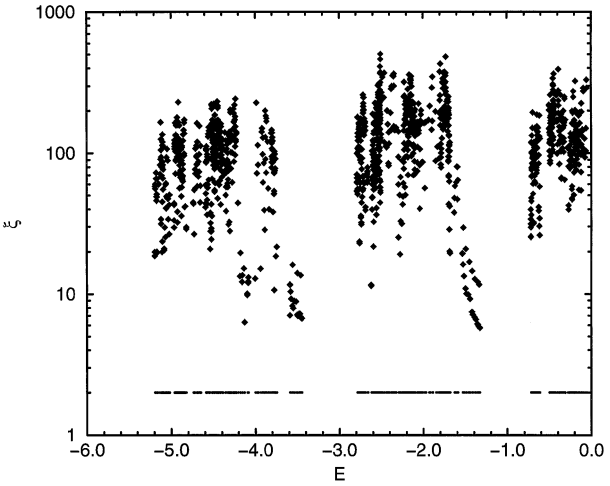

FIG. 4. Inverse participation ratios ξ vs eigenenergies E shown at $\xi = 2$; $U = 1, \alpha = 34/55, 0 \leq \beta < 2\pi$.

where χ-s are one-particle eigenfunctions. Because of this, the effective interaction becomes quite small and the unshifted butterfly at large U (TIP are in different wells) looks very similar to the one at $U = 0$. The main difference is the splitting of Landau sublevels which appears due to an effective small interaction between particles located in the same well. According to the expression for ϕ_{n_1,n_2}, such a splitting can take place only when Landau quantum numbers are different ($m_1 \neq m_2$) so that $\chi^{(1)} \neq \chi^{(2)}$. As a result the first sublevel with $m_{1,2} = 0$ is not split. For the noninteracting part, the edges are given by the same $E_{\pm}(\alpha)$ as for $U = 0$ while the U-induced shift is $\delta E(\alpha) = -8\pi\alpha/(U + 4)$ (see [24]) being in agreement with data in Fig. 2(b).

In summary, *20 years after* Hofstadter [5], our investigations of spectra and eigenstates for TIP in the Harper model (1) show that repulsive/attractive interaction leads to the appearance of localized states. Our conjecture is that due to Aubry duality breaking a localized TIP pair phase appears at an arbitrary small interaction strength. At the same time we expect that this breaking is absent for TIP on the 2D lattice with magnetic flux. However, the later model requires separate investigations [24].

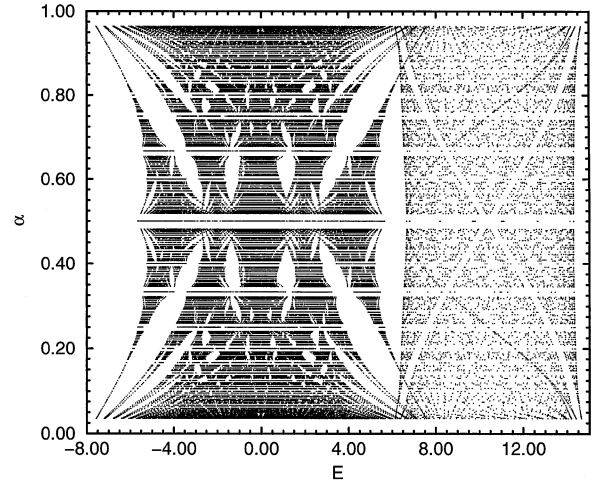

FIG. 5. Same as in Fig. 1 with $U = 10$ and $q \leq 28$.

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