

Two interacting Hofstadter butterflies

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The problem of two interacting particles in a quasiperiodic potential is addressed. Using analytical and numerical methods, we explore the spectral properties and eigenstates structure from the weak to the strong interaction case. More precisely, a semiclassical approach based on noncommutative geometry techniques is used to understand the intricate structure of such a spectrum. An interaction induced localization effect is furthermore emphasized. We discuss the application of our results on a two-dimensional model of two particles in a uniform magnetic field with on-site interaction. [S0163-1829(97)02016-X]

I. INTRODUCTION

The study of crystal electrons submitted to a magnetic field has been extensive since the early works of Landau¹ and Peierls.² These studies have led to deep insights in the physics of electrons in solids (interpretation of the de Haas van Alphen effect,³ investigation of the Fermi surface . . .). The number of contributions on the subject between 1950 and 1970 reveals the importance of magnetic field effects. Twenty years ago, Hofstadter numerically computed the spectrum of the Harper model⁴ and discovered its fractal structure as a function of the normalized magnetic flux per lattice cell⁵ (Fig. 1).

The problem of a two-dimensional electron on a periodic lattice has been of special interest in solid state physics during the past fifteen years: superconducting⁶ and normal-metal networks.⁷ Harper-like models have been used to describe the quantum Hall effect⁸ in organic conductors, in Anyon superconductivity⁹ and in flux phases for the Hubbard model.¹⁰

If the lattice is given by the positions of the ions of a metal, the lattice spacing a is of the order of 1 \AA , so that even with the highest magnetic fields that can be produced now, namely $B \approx 20 \text{ T}$, we get $\alpha = \gamma/2\pi \approx 0.5 \times 10^{-4}$ which is fairly small and shows that in this situation a “semiclassical” approximation will always be relevant. As a matter of fact, an effective Planck’s constant denoted by γ proportional to the applied magnetic field naturally appears as an adjustable variable of the problem. Therefore the weak magnetic field limit $\gamma \rightarrow 0$ corresponds to the semiclassical limit $\hbar \rightarrow 0$. The corresponding classical phase space at $B=0$ is the quasimomentum space, namely, the Brillouin zone of the corresponding lattice. Topologically it is a two-torus and the appearance of the magnetic field transforms it into a noncommutative two-torus.¹¹

Whenever $\gamma = 2\pi p/q$, ($p, q \in \mathbf{N}$) the lattice Hamiltonian H recovers some periodicity and Bloch’s theory applies. We shall see then that H can be represented as a self-adjoint

$q \times q$ matrix whose entries are periodic functions of the quasimomentum components. Thus, if γ is close to any rational multiple of 2π , it is possible to compute the spectrum using semiclassical methods.

Based on these remarks, many theoretical and mathematical works were published during the past fifteen years using a renormalization group analysis¹² and pseudodifferential operators techniques.¹³ On the basis of the techniques of noncommutative geometry,¹¹ another approach was developed in order to reformulate and extend the semiclassical results.¹⁴ The algebraic semiclassical approach is justified by the simplicity of its application and its efficiency, for example, in the computation of Landau levels both in Harper-like models¹⁵ and in a model Hamiltonian on a triangular lattice.¹⁶ The comparison between semiclassical formulas and exact calculations extracted from the various spectra for $\gamma \in 2\pi\mathbf{Q}$ gives surprisingly accurate agreement even for relatively large γ ’s (namely, $\gamma/2\pi \leq 0.2$).

While in the above formulation of the problem of Bloch electrons in a magnetic field the particles are considered on a two-dimensional lattice, it is possible to map it exactly onto a one-dimensional lattice with quasiperiodic potential. The interesting property of such a lattice is the duality between momentum and spatial coordinates pointed out by Aubry and André.¹⁷ This Aubry duality results in a delocalized structure of the eigenstates characterized by an algebraic decay and a multifractal eigenspectrum. This leads to a quasidiffusive wave packet spreading on such a lattice.^{18,19}

Recently, a number of authors have followed a new path in the study of the combined effect of interaction and disorder. The *a priori* simple problem of two interacting particles in a random potential²⁰ has indeed revealed an unsuspected large interaction induced delocalization effect. However, the opposite effect has been discovered in the case of two particles in a quasiperiodic potential. In this case, the interaction leads to the emergence of a pure-point component out of the spectrum of the noninteracting problem. These facts have been firmly established by overconvincing numerical and

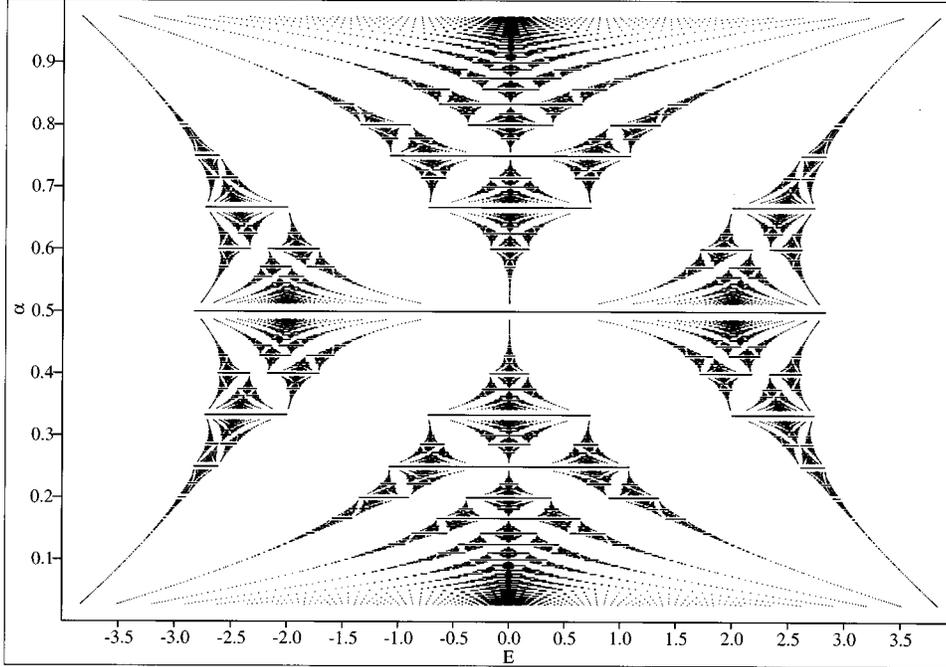


FIG. 1. Hofstadter's butterfly for rational values of $\alpha=p/q$ up to $q=29$. For each value of the magnetic flux $\alpha=p/q$, we generally have q bands. Near energies equal to ± 4 and zero flux, we observe the emergence of Landau levels.

analytical results.^{21,22} It is one of the purposes of this paper to again express these arguments in more detail.

We shall present in this work analytical and numerical results derived from the two-particle Harper problem with an on-site interaction on a one-dimensional lattice. More precisely we devote the second section to the presentation of the algebraic semiclassical approach on the noninteracting problem $U=0$. The corresponding spectrum is somehow an intricate superposition of two Hofstadter butterflies. The aim of Sec. III is to study the small interaction regime where usual perturbation theory can be applied. The evolution of the spectrum as a function of the strength of the interaction will be presented. After building the analytical framework in Sec. IV, we apply it to the computation of the levels in the strong interaction regime. We show that for very large U , the spectrum is divided into two parts: one corresponding to the noninteracting case and the second one, looking like a Mathieu spectrum corresponding to localized states strongly influenced by the interaction. Based upon Aubry's duality,¹⁷ it can be proved that all the wave functions are localized in this regime as far as the Mathieu part of the spectrum is concerned. Finally, we discuss in Sec. V the problem of two interacting particles on a two-dimensional lattice submitted to a magnetic flux.

II. NONINTERACTING MODEL

In his 1930s study of the electronic diamagnetism of metals, Landau computed the energy spectrum of a free electron subject to a uniform magnetic field.¹ If B is uniform and parallel to one axis, for example axis 3, the kinetic energy is written as

$$H_L = \frac{\hbar^2}{2m_e} (\tilde{K}_1^2 + \tilde{K}_2^2) \quad (1)$$

with $\tilde{K}_\mu = (P_\mu - q_e A_\mu)/\hbar$, $\mu=1,2$ and $A=(A_1, A_2)$ is the vector potential satisfying $\text{curl}(A)=B$, q_e the electron charge. Moreover, the quasimomenta \tilde{K}_1, \tilde{K}_2 satisfy

$$[\tilde{K}_1, \tilde{K}_2] = iq_e B/\hbar. \quad (2)$$

Let us note that this commutation rule becomes canonical when replacing \hbar by $q_e B/\hbar$. This effective Planck constant (divided by 2π) is proportional to the magnetic field B and behaves as a varying physical parameter, quite naturally.

The spectrum of H_L is $E_n = E_0 \hbar_{\text{eff}} \omega (2\nu + 1)$ with $E_0 = \hbar^2/2m_e$, $\hbar_{\text{eff}} = q_e B/\hbar$, and $\omega = 1$. Therefore

$$E_\nu = \hbar \omega_c (\nu + 1/2), \quad (3)$$

where $\omega_c = q_e B/m_e$ is the cyclotronic frequency and ν is the Landau quantum number.

When $B=0$, the electron energy $E(k)$ for each conduction band is given by Bloch's theory, where the quasimomentum components $k=(k_1, k_2)$ are defined modulo the reciprocal lattice such that for a simple square lattice in the tight-binding approximation $E(k) = 2E_0 [\cos(k_1 a_1) + \cos(k_2 a_2)]$, where a_μ is the vector of the Bravais lattice in the μ direction. The charge carriers energy is calculated by expanding $E(k)$ near its extremum, denoted by k_c , namely,

$$E(k) = E(k_c) + \hbar^2 (M^{-1})_{ij} k_i k_j / 2 + O(|k|^3), \quad (4)$$

where M stands for the effective mass matrix such that $M^{-1} = D^2 E(k_c)/\hbar^2$.

Thus Landau theory leads to a substitution $k_i a_i \rightarrow \hat{K}_i = 1/\hbar (P - q_e A) a_i$ when an external magnetic field is applied. We have the following commutation rule:

$$[\hat{K}_i, \hat{K}_j] = iq_e B a_i a_j / \hbar = 2i\pi \phi_{ij} / \phi_0 = 2i\pi \alpha = i\gamma, \quad (5)$$

where $\phi_0 = h/q_e$ is the flux quantum, ϕ_{ij} is the magnetic flux through the cell generated by (a_i, a_j) and $\alpha = \phi_{ij}/\phi_0$ is the

normalized magnetic flux. For a crystal with periodic spacing, the Peierls operator $\mathcal{P}(k)$ is represented by an effective Hamiltonian,² namely,

$$\mathcal{P}(k) = \sum_m h_m(\alpha) e^{imk}, \quad m \in \mathbf{Z}^2, \quad (6)$$

where $h_m(\alpha)$ are smooth functions of α . Thus

$$H_{\text{eff}}(\hat{K}_1, \hat{K}_2) = \sum_m h_m e^{im\hat{K}}. \quad (7)$$

If several bands intersect the Fermi level, the interband coupling due to the magnetic field is neglected and therefore

$$H_{\text{eff}} = 2t(\cos\hat{K}_1 + \cos\hat{K}_2), \quad (8)$$

where t is physically interpreted as a transfer term corresponding to the required energy for an electron to jump from one site to another (nearest neighbor) of the lattice.

For a wave function $\psi(n_1, n_2)$ defined on the two-dimensional lattice $\mathcal{L}^2(\mathbf{Z}^2)$, the magnetic field effect can be seen through the magnetic translation operators such that

$$\begin{aligned} (\mathcal{U}_1\psi)(n_1, n_2) &= e^{(-iq_e/\hbar)} \int_{(n_1-1, n_2)}^{(n_1, n_2)} \vec{A} \cdot d\vec{l} \psi(n_1-1, n_2), \\ (\mathcal{U}_2\psi)(n_1, n_2) &= e^{(-iq_e/\hbar)} \int_{(n_1, n_2-1)}^{(n_1, n_2)} \vec{A} \cdot d\vec{l} \psi(n_1, n_2-1), \end{aligned} \quad (9)$$

in an appropriate gauge we get

$$\begin{aligned} (\mathcal{U}_1\psi)(n_1, n_2) &= \psi(n_1-1, n_2), \\ (\mathcal{U}_2\psi)(n_1, n_2) &= e^{-i\gamma n_1} \psi(n_1, n_2-1). \end{aligned} \quad (10)$$

Because of the presence of the uniform magnetic field, the magnetic translation operators no longer commute, namely, in that case

$$\mathcal{U}_1\mathcal{U}_2 = e^{i\gamma}\mathcal{U}_2\mathcal{U}_1, \quad (11)$$

where γ is the normalized magnetic flux per lattice cell defined by $\gamma = 2\pi\alpha = 2\pi\phi/\phi_0$, ϕ being the flux per unit cell and $\phi_0 = h/q_e$ the flux quantum. If we set $\mathcal{U}_1 = \exp(i\hat{K}_1)$, $\mathcal{U}_2 = \exp(i\hat{K}_2)$ using the commutation rule (11), we obtain

$$[\hat{K}_1, \hat{K}_2] = \frac{iq_e B a_1 a_2}{\hbar} = 2i\pi \frac{\phi}{\phi_0} = 2i\pi\alpha = i\gamma, \quad (12)$$

which corresponds to Eq. (5) in the particular case $i=1$ and $j=2$.

Following Harper,⁴ the eigenvalue equation is written

$$\begin{aligned} E_0[\psi(n_1+a, n_2) + \psi(n_1-a, n_2) + \lambda e^{iq_e B n_1 a/\hbar} \psi(n_1, n_2+a) \\ + \lambda e^{-iq_e B n_1 a/\hbar} \psi(n_1, n_2-a)] = 2\mathcal{E}\psi(n_1, n_2). \end{aligned} \quad (13)$$

λ represents the strength of the quasiperiodic potential.

Let us assume plane-wave behavior in one direction, i.e., we set $\psi(n_1, n_2) = \int d\beta e^{i\beta n_2} \phi(n_1)$ since the coefficients in the previous equation only involve n_1 :

$$\psi(n_1, n_2) = e^{i\beta n_2} \phi(n_1)$$

and the eigenequation becomes

$$\begin{aligned} \phi(n_1+1) + \phi(n_1-1) + 2\lambda \cos(2\pi\alpha n_1 + \beta) \phi(n_1) \\ = \mathcal{E}\phi(n_1), \end{aligned} \quad (14)$$

where we included the additive energy due to the motion in the field direction in the eigenvalue \mathcal{E} and where we changed the origin of n_1 .

It is possible to characterize the properties of eigenfunctions from Eq. (14) by looking at a special regime, namely $\lambda \ll 1$. Therefore the hopping term is dominant and we can treat the quasiperiodic potential part of the eigenvalue equation as a perturbation. It is then easy to see that the solutions are given for $\lambda=0$ by Bloch waves $\phi_k(n) = \exp(ikn)$ with an energy $E = 2\cos k$. For $0 < \lambda \ll 1$, the perturbation theory allows us to perform an expansion of eigenvalues and eigenstates in λ such that

$$E(k) = 2\cos k + \sum_m \lambda^m \epsilon_m(k),$$

$$\phi_k(n) = e^{ikn} \left(1 + \sum_m \lambda^m f_m(\gamma n + \beta) \right) = e^{ikn} u_m(\gamma n + \beta). \quad (15)$$

Evaluating the first- and second-order perturbation theory contributions and replacing the expressions (15) in Eq. (14) leads to

$$\lambda(u_{m+1} + u_{m-1}) + 2\cos(\gamma m + k)u_m = E(k)u_m. \quad (16)$$

The previous equation is known as the ‘‘almost Mathieu’’ eigenvalue equation and the argument above is the Aubry duality¹⁷ between momentum and coordinate representations. As far as spectral properties are concerned one can be easily convinced that dealing with Bloch states means that the states are extended. Thanks to this duality, $\lambda \leftrightarrow 1/\lambda$ between Eqs. (14) and (16), it is quite natural to get localized states for the almost Mathieu Hamiltonian at small λ 's. More precisely, it has been proved that the almost Mathieu Hamiltonian has a pure point spectrum at small λ 's and for almost all β 's.²³ Conversely if $\lambda \gg 1$, the almost Mathieu Hamiltonian has a purely continuous spectrum for almost all β 's.²⁴

Setting $t=1$ in formula (8) and using the magnetic translation operators \mathcal{U}_1 and \mathcal{U}_2 defined on the two-dimensional square lattice by Eq. (10), the previous Harper equation can be written as the action of an effective Hamiltonian such that

$$H_{\text{eff}} = \mathcal{U}_1 + \mathcal{U}_1^{-1} + \mathcal{U}_2 + \mathcal{U}_2^{-1}. \quad (17)$$

In order to study the two interacting particles model on a quasiperiodic lattice we transform the previous eigenvalue equation (14) into ($\lambda=1$),

$$\begin{aligned} [2\cos(\gamma n_1 + \beta_1) + 2\cos(\gamma n_2 + \beta_2) + U\delta_{n_1, n_2}] \phi_{n_1, n_2} \\ + \phi_{n_1+1, n_2} + \phi_{n_1-1, n_2} + \phi_{n_1, n_2+1} + \phi_{n_1, n_2-1} = E\phi_{n_1, n_2}, \end{aligned} \quad (18)$$

where $\beta_{1,2}$ are related to the quasimomentum components of the noninteracting case. In the following we shall consider

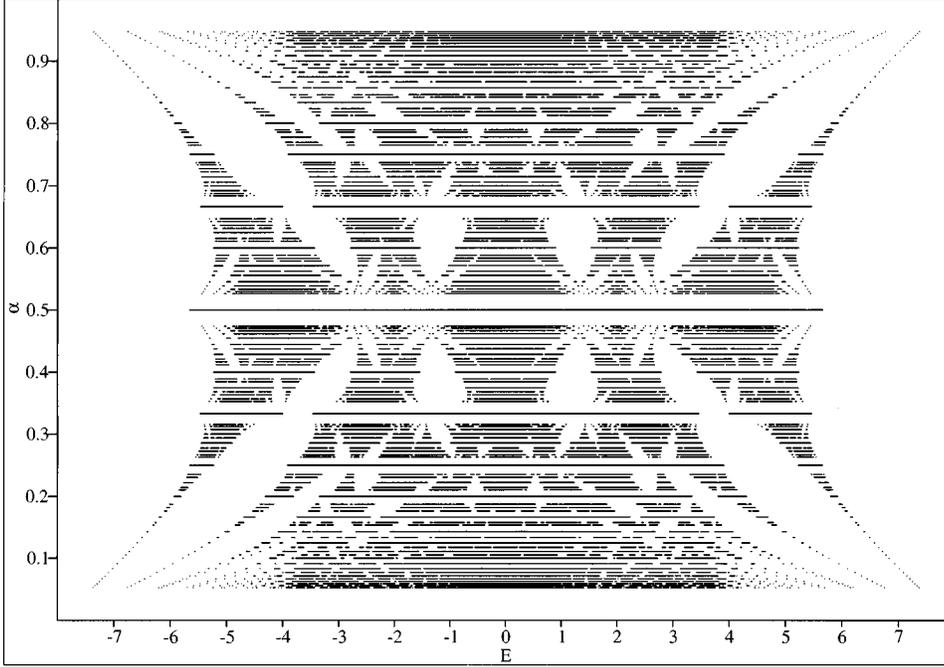


FIG. 2. Spectrum of the two-particle Harper problem with $U=0$ obtained for rational values of $\alpha=p/q$ up to $q=19$.

$\beta_{1,2}=\beta$. Here we chose the form of on-site interaction which only influences the symmetric configurations while the anti-symmetric ones remain not affected by U . Due to that, we shall only discuss symmetric configurations in the following.

In the most simple case of noninteracting particles ($U=0$), the spectrum can be computed as before and is shown in Fig. 2.

As we pointed out before, $\gamma=2\pi\alpha$ appears in our problem as an effective Planck constant since the magnetic translation operators \mathcal{U}_1 and \mathcal{U}_2 obey canonical commutation rules in γ . Therefore, we study the semiclassical limit by letting $\gamma \rightarrow 0$. It is also possible to perform calculations near a rational value of the magnetic flux, namely $\gamma' = \gamma - 2\pi p/q \rightarrow 0$. The efficiency and the accuracy of our calculations allow us to explain some features of the corresponding spectra.

When $\gamma=0$, corresponding to $B=0$, we recover the band function $E(k)$, where $k=(k_1, k_2)$. To study the Landau levels, we expand the classical symbol of the Hamiltonian around an extremum of the band function denoted by k_c :

$$\mathcal{H}(k) = \mathcal{H}(k_c) + \frac{1}{2} \partial_\mu \partial_\nu \mathcal{H}(k_c) k_\mu k_\nu + \dots \quad (19)$$

The quantization of $\mathcal{H}(k)$ consists in replacing the magnetic translation operators by¹⁴

$$\mathcal{U}_j = \exp[i(k_{c_j} + \sqrt{\gamma} K_j)], \quad j=1,2, \quad (20)$$

where k_{c_j} are the bottom well coordinates and K_j are operators satisfying Heisenberg's commutation relations $[K_1, K_2]=i$. The quantized of \mathcal{H} , denoted by H , is written as

$$H = \sum_m h(m, \gamma) e^{i(mk_c + \sqrt{\gamma} mK)},$$

with $mK = m_1 K_1 + m_2 K_2$. In the weak field limit, one formally expands H in powers of $\sqrt{\gamma}$:

$$H = \sum_m \left\{ h(m,0) e^{imk_c} + i\sqrt{\gamma} h(m,0) e^{imk_c} mK \right. \\ \left. + \gamma \left[\frac{\partial h}{\partial \gamma}(m,0) e^{imk_c} - \frac{1}{2} h(m,0) e^{imk_c} (mK)^2 \right] \right\} + O(\gamma^{3/2}), \quad (21)$$

which we rewrite as

$$H = \mathcal{H}(k_c,0) + \gamma \left(\frac{\partial \mathcal{H}}{\partial \gamma}(k_c,0) - \frac{1}{2} \partial_\mu \partial_\nu \mathcal{H}(k_c,0) K_\mu K_\nu \right) \\ + O(\gamma^{3/2}). \quad (22)$$

The $\partial \mathcal{H} / \partial \gamma$ term takes into account a possible explicit γ dependence of the classical Hamiltonian, whereas $\partial_\mu \partial_\nu \mathcal{H}$ represents the inverse effective mass matrix due to the band function curvature. By a unitary transformation, the quadratic term can be written as $\omega(K_1^2 + K_2^2)/2$ where ω is related to the determinant of the Hessian matrix $\partial_\mu \partial_\nu \mathcal{H}(k_c,0)$. We recognize here the harmonic oscillator Hamiltonian. For this reason, the energy levels denoted by E_ν are called 'Landau levels' and are equal, to that order in γ , to $\omega(\nu + 1/2)$ leading to

$$E_\nu(\gamma) = \mathcal{H}(k_c,0) + \gamma(2\nu + 1) \left(\det \frac{1}{2} D^2 \mathcal{H}(k_c,0) \right)^{1/2} \\ + \gamma \left(\frac{\partial \mathcal{H}(k_c,0)}{\partial \gamma} \right) + \dots + O(\gamma^N). \quad (23)$$

The formula (23) has been checked numerically on several models. To illustrate it, let us consider the two-particle Harper Hamiltonian on the square lattice (18) near the maximum $k_c=(0,0)$ of the band function. Using Eqs. (20) and (22) the quantized Hamiltonian is then expressed as an expansion in powers of γ :

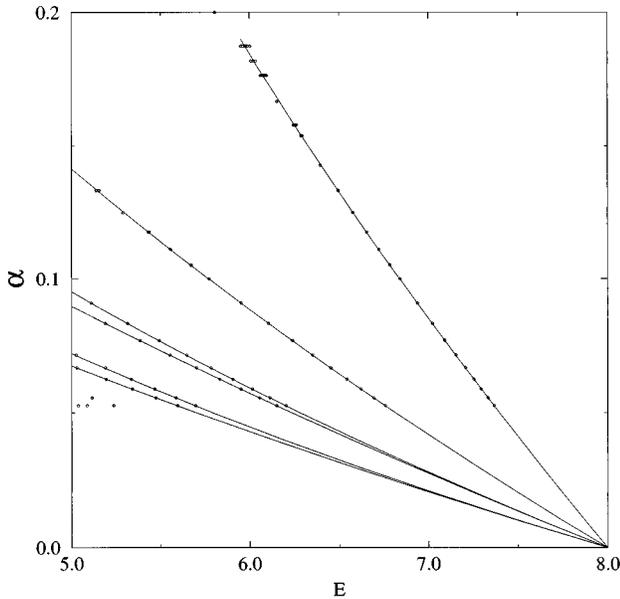


FIG. 3. Comparison between semiclassical calculations (25) (full curves) and the exact numerical spectrum (points) for Landau sublevels in the two-particle Harper model on the square lattice when $U=0$. Data are extracted in the region of energies corresponding to the maximum (0,0) of the band function.

$$H = 8 - \gamma[(K_1^{(1)})^2 + (K_2^{(1)})^2 + (K_1^{(2)})^2 + (K_2^{(2)})^2] + \frac{\gamma^2}{3}[(K_1^{(1)})^4 + (K_2^{(1)})^4 + (K_1^{(2)})^4 + (K_2^{(2)})^4] + O(\gamma^3), \quad (24)$$

where the $K^{(1,2)}$ are quasimomenta for particle 1 and 2, respectively. Finally it gives the Landau levels:

$$E_{\nu_1, \nu_2}(\gamma) = 8 - 2\gamma(\nu_1 + \nu_2 + 1) + \gamma^2[(2\nu_1 + 1)^2 + (2\nu_2 + 1)^2 + 2]/16 + O(\gamma^3), \quad (25)$$

where ν_1 and ν_2 are the Landau quantum numbers associated with particle 1 and 2, respectively. To check the accuracy of this formula, we compared it to the data extracted from the numerical spectrum obtained by exact diagonalization. Figure 3 shows the accuracy of such a semiclassical expansion in the description of the spectrum of the two-particle Harper model when $\gamma \rightarrow 0$.

III. WEAK INTERACTION REGIME

We present here a simple perturbative treatment that enables us to implement the already presented results for the weakly interacting case. The first-order contribution allows us to understand the splitting of Landau bands at sufficiently weak interaction, and describes it qualitatively well. It moreover enlightens the mechanism through which interaction affects the system. Using the representation defined by Eq. (20), we write the unperturbed Hamiltonian as

$$H_{\text{eff}} = 2\cos(\sqrt{\gamma}K_1) + 2\cos(\sqrt{\gamma}K_2). \quad (26)$$

In the semiclassical limit $\gamma \rightarrow 0$, we expand (26) in a power series around a minimum of potential

$q_N = \pi/\sqrt{\gamma} + 2\pi N/\sqrt{\gamma}$, $N \in \mathbf{Z}$. Keeping only terms up to the second order in γ we end up with a harmonic oscillator. In this approximation and in the continuous case the one-particle wave functions of the unperturbed Hamiltonian are therefore given by

$$\psi_\nu(y) = H_\nu\left(\frac{y}{\sqrt{\gamma}}\right) \exp\left(-\frac{y^2}{2\gamma}\right) / \sqrt{2^\nu \nu! \sqrt{\gamma\pi}}. \quad (27)$$

Here, $H_\nu(x)$ is a Hermite polynomial, the index ν refers to the Landau level, $y = x - q_N$ in terms of the minimum of potential q_N around which the harmonic approximation has been performed, and x is the spatial coordinate. This expression is of course valid, provided γ and $|x - q_N| \ll 1$, i.e., in the small magnetic field regime, and not too far away from a potential minimum. Extending our expansion to higher powers in γ would allow us to increase the range of validity of this expression. We could indeed write the exact normalized wave functions in an expansion in γ as

$$\varphi_\nu(y) = \exp\left(-\frac{y^2}{2\gamma}\right) \left[c_0 H_\nu\left(\frac{y}{\sqrt{\gamma}}\right) + \gamma c_1 H_\nu^{(1)}\left(\frac{y}{\sqrt{\gamma}}\right) + \dots \right]. \quad (28)$$

For the purpose of discretization, we introduce a continuous variable $\xi \in \mathbf{R}$ labeling the well, and a discrete one $l \in \mathbf{Z}$ numbering the sites. Then $y = \xi - l\sqrt{\gamma}$ since in the chosen representation, the intersite spacing is $a = \sqrt{\gamma}$. The set $\{\varphi_\nu\}$ builds a quasiorthogonal basis in the sense that for $\xi \neq \xi'$, due to the Gaussian envelop of the states we have

$$\sum_l \varphi_\nu(\xi - l\sqrt{\gamma}) \varphi_\mu(\xi' - l\sqrt{\gamma}) = O(\exp(-1/\gamma)) \delta_{\mu, \nu}. \quad (29)$$

These functions are periodic in ξ with period $1/\sqrt{\gamma}$. In the semiclassical limit the norm of φ_ν is

$$\|\varphi_\nu\|^2 = \sum_{l=-\infty}^{\infty} |\varphi_\nu(\xi - l\sqrt{\gamma})|^2 = 1/\sqrt{\gamma} \int dy |\varphi_\nu(y)|^2 = 1/\sqrt{\gamma}. \quad (30)$$

Consequently, to get normalized one-particle wave functions on the discrete lattice $\mathcal{L}(\mathbf{Z})$ we must multiply the φ 's by a factor $\gamma^{1/4}$. We thus can write the symmetrized two-particle unperturbed wave functions as

$$\begin{aligned} \phi_{\nu, \mu}^{\xi, \xi'}(l, l') &= \sqrt{\frac{\gamma}{2}} [\varphi_\nu(\xi - l\sqrt{\gamma}) \varphi_\mu(\xi' - l'\sqrt{\gamma}) \\ &\quad \pm \varphi_\mu(\xi - l\sqrt{\gamma}) \varphi_\nu(\xi' - l'\sqrt{\gamma})] \\ &\quad \times [1 - \delta_{\mu, \nu}(1 - 1/\sqrt{2})]. \end{aligned} \quad (31)$$

We are now able to compute the first-order correction for the energy. Because of the exponentially localized character of Eq. (28), two particles located on different wells have only an exponentially small overlap, and as a consequence do practically not interact. Therefore the first-order interaction induced correction to the energy is nonzero only for symmetric wave functions with $\xi = \xi'$. We have

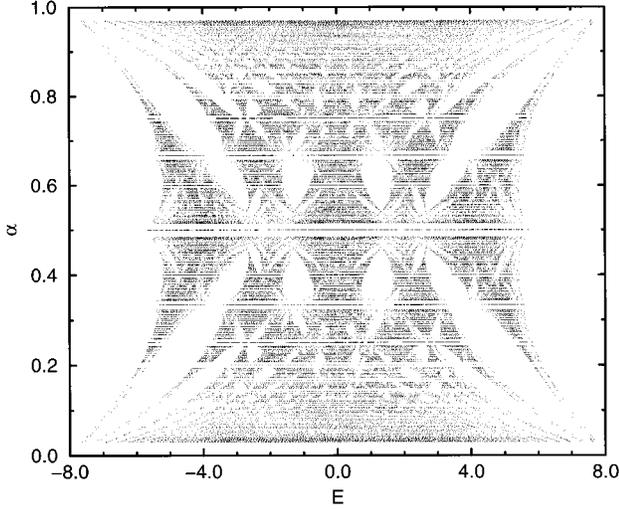


FIG. 4. Spectrum of the two-particle Harper model with on-site interaction at $U=0.4$ up to $q=23$.

$$\begin{aligned} \Delta E^{(1)} &= U \sum_l \sum_{l'} (\phi_{\nu,\mu}^{\xi,\xi'}(l,l'))^2 \delta[\xi - \xi' + (l' - l)\sqrt{\gamma}] \\ &= U \delta_{\xi,\xi'} \int dy (\varphi_\mu(y) \varphi_\nu(y))^2 (2 - \delta_{\mu,\nu}) \\ &\quad + O(\exp(-1/\gamma)). \end{aligned} \quad (32)$$

From Eq. (28), the dominant term in the last integral is of an order $O(\sqrt{\gamma})$ so that we finally have

$$\Delta E^{(1)} \sim U \delta_{\xi,\xi'} \sqrt{\gamma}. \quad (33)$$

The numerical factor can be estimated from the harmonic approximation (27) which leads to

$$\Delta E_h^{(1)} = U \delta_{\xi,\xi'} \sqrt{\frac{\gamma}{2\pi}} = U \delta_{\xi,\xi'} \sqrt{\alpha} \quad (34)$$

for states with Landau quantum numbers (0,0) and (0,1). This result shows that the interaction primarily acts on two-particle states with a high double-site occupancy. In what follows we shall call such states ‘‘pair states.’’ States for which the particles are located around different potential minima practically do not respond to the interaction. Therefore, switching on the interaction does not modify most of the spectrum as can be seen on Fig. 4.

From Eqs. (25) and (34) and for small enough interaction, the shifted part of the spectrum is given by

$$\begin{aligned} E_{\nu_1,\nu_2}(\gamma) &\sim 8 + U \sqrt{\frac{\gamma}{2\pi}} - 2\gamma(\nu_1 + \nu_2 + 1) + \gamma^2[(2\nu_1 + 1)^2 \\ &\quad + (2\nu_2 + 1)^2 + 2]/16. \end{aligned} \quad (35)$$

The amazing agreement between the numerically computed spectrum obtained by exact Lanczos diagonalization and Eq. (35) is shown in Fig. 5 where $U=0.4$. It is a confirmation of our reasoning: pair states form the shifted part of the spectrum. Because these states are much fewer than states where particles are located in different wells, the shifted spectrum is much less dense. In this sense the inter-

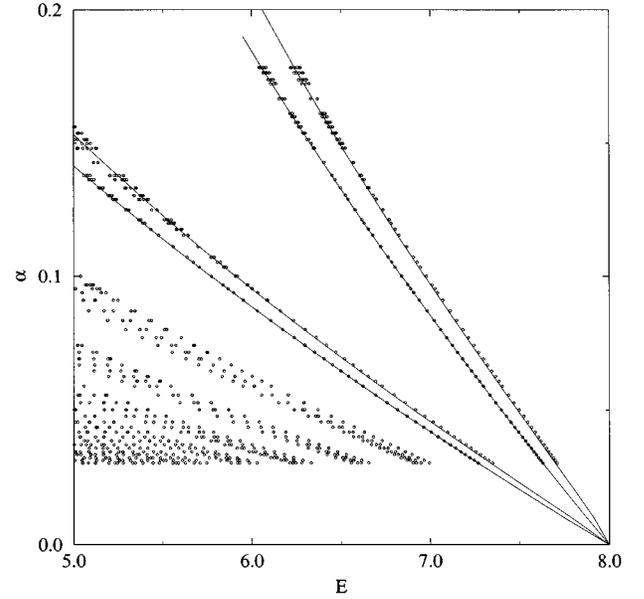


FIG. 5. Comparison between semiclassical calculations extended by perturbation theory (35) (full curves) and an exact numerical spectrum (points) for the two-particle Harper model with on-site interaction at $U=0.4$.

action splits the butterfly into two parts. One of them is practically not affected by the interaction and corresponds to the states where particles are far from each other. The second one is shifted and relates to the situation where particles form pair states. Here, the interaction results in a global shift of the spectrum. In this way, new states appear in the initial gaps of the noninteracting spectrum [see Figs. 4, 6, and Fig. 1(b) in Ref. 21]. Direct analysis of eigenstates shows that the corresponding states are exponentially localized.²¹ We shall come back to this point later on for the case of strong interaction.

IV. STRONG INTERACTION REGIME

The strongly interacting regime needs a special treatment quite analogous to the one presented in Sec. II. As we will see, Schur’s complement formula can be successfully applied to construct an effective Hamiltonian. The latter is then expanded in a power series in γ to deliver highly accurate formulas. From the weakly interacting regime we learned that particles located on different potential minima do not respond to each other: for such pairs, the interaction is suppressed by an exponentially small term of order $O(U\exp(-1/\gamma))$. Therefore, this picture remains valid even for large U ’s, the relevant parameter being the magnetic flux. Pair states on the other hand undergo an energy increase of order $\Delta E \approx U$. Therefore when the strength of the interaction $U > 0$ increases, one part of the spectrum is almost not affected. Another spectral structure appears, initially looking like a shifted butterfly (see Fig. 4 where $U=0.4$), then evolving to a shifted Mathieu spectrum as the interaction grows bigger and bigger (see Figs. 6, 7, and 8 where $U=5, 10$, and 20, respectively).

In this section, we present an analytical approach that allows us to understand completely the mechanism driving

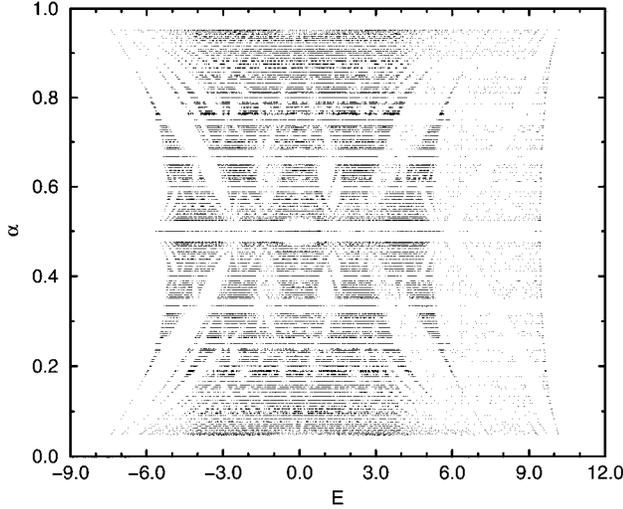


FIG. 6. Spectrum of the two-particle Harper model in the intermediate regime $U=5$ up to $q=23$.

this evolution of the spectrum. Further details like the splitting of the Landau band $\nu_1=0$, $\nu_2=1$ will also be computed, even though the physics is less transparent there (see Fig. 7). We shall concentrate our semiclassical calculation near the band function maximum $k_c=(0,0)$ corresponding to the energy $z \approx U+4$ in the spectrum. The two-particle Hamiltonian can be expressed in the following way:

$$\begin{aligned}
 H_{\text{TIP}} = & \sum_{m,n} [2\cos(\gamma m + \beta) + 2\cos(\gamma n + \beta)] \\
 & \times |m \otimes n\rangle \langle m \otimes n| + U \sum_m |m \otimes m\rangle \langle m \otimes m| \\
 & + \sum_{m \neq n} |m \otimes n\rangle [\langle m \otimes n + 1| + \langle m \otimes n - 1| \\
 & + \langle m + 1 \otimes n| + \langle m - 1 \otimes n|]. \quad (36)
 \end{aligned}$$

The strategy is based on the so-called Schur complement formula. Our Hamiltonian H_{TIP} is a self-adjoint operator act-

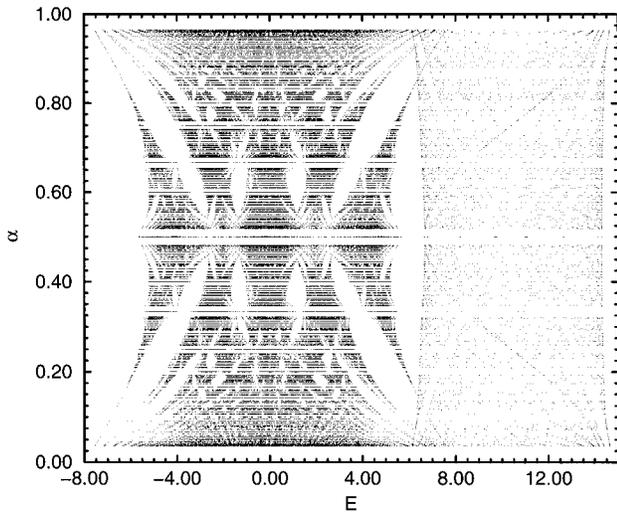


FIG. 7. Spectrum of the two-particle Harper model in the strongly interacting regime $U=10$ up to $q=23$.

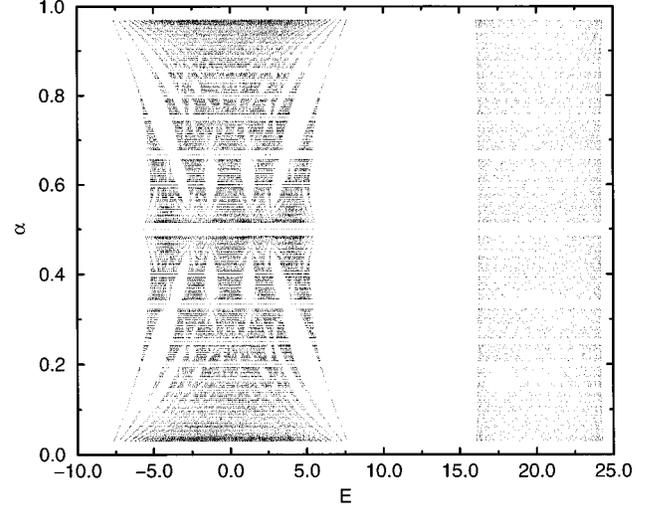


FIG. 8. Spectrum of the two-particle Harper model in the strongly interacting regime $U=20$ up to $q=23$.

ing on a Hilbert space that can be decomposed as $\mathcal{H} = \mathcal{P} \oplus \mathcal{Q}$. Let P and Q be the orthogonal projections on each subspace of that decomposition, namely,

$$P = \sum_m |m \otimes m\rangle \langle m \otimes m|,$$

$$Q = \mathbf{I} - P = \sum_{m \neq n} |m \otimes n\rangle \langle m \otimes n|.$$

In other words, P is the eigenprojection on pair states and Q is its orthogonal. If z is an eigenvalue of H_{TIP} and does not belong to the spectrum of $QH_{\text{TIP}}Q$ then it is also an eigenvalue of the following effective Hamiltonian:

$$H_{\text{TIP}}^{\text{eff}}(z) = PH_{\text{TIP}}P + PH_{\text{TIP}}Q \frac{1}{z - QH_{\text{TIP}}Q} QH_{\text{TIP}}P. \quad (37)$$

When U is large the dominant term in the effective Hamiltonian given by the Schur complement formula (37) corresponds to the pair states. The semiclassical approach we introduced in Sec. II remains valid so that $H_{\text{TIP}}^{\text{eff}}(z) = H_{\text{TIP}}^{\text{eff}}[z_0 + \gamma z_1 + \gamma^2 z_2 + O(\gamma^3)]$. The implicit equation to be solved is then

$$H_{\text{TIP}}^{\text{eff}}(z) = z_0 + \gamma z_1 + \gamma^2 z_2 + O(\gamma^3), \quad (38)$$

with

$$H_{\text{TIP}}^{\text{eff}}(z) = H_{\text{TIP}}^{(0)}(z) + \gamma H_{\text{TIP}}^{(1)}(z) + \gamma^2 H_{\text{TIP}}^{(2)}(z) + O(\gamma^3). \quad (39)$$

The expansion of the dominant term reads

$$\begin{aligned}
 PH_{\text{TIP}}P &= U + 4\cos(\sqrt{\gamma}K_2) \\
 &= U + 4 - 2\gamma K_2^2 + \frac{\gamma^2}{6} K_2^4 + O(\gamma^3), \quad (40)
 \end{aligned}$$

and if we consider U large, z is large too so that

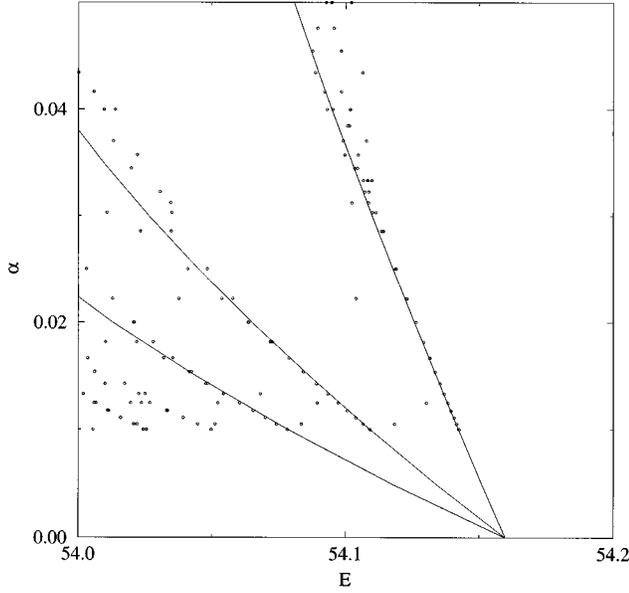


FIG. 9. Comparison between semiclassical calculations (full curves, see text) and exact numerical spectrum (points) for levels in the two-particle Harper model for $U=50$.

$$\frac{1}{z - QH_{\text{TIP}}Q} = \frac{1}{z} + \frac{QH_{\text{TIP}}Q}{z^2} + \frac{QH_{\text{TIP}}QQH_{\text{TIP}}Q}{z^3} + O(z^{-4}). \quad (41)$$

Expressing the different contributions in Schur's formula and expanding in powers of γ leads to

$$\begin{aligned} H_{\text{TIP}}^{(0)}(z) &= 4 + U + \frac{8}{z} + \frac{32}{z^2} + \frac{176}{z^3} + O(z^{-4}), \\ H_{\text{TIP}}^{(1)}(z) &= \frac{-2(z^3 + 8z + 64)}{z^3} \left[K_2^2 + \frac{z^2 + 4z + 34}{z^3 + 8z + 64} K_1^2 \right], \\ H_{\text{TIP}}^{(2)}(z) &= \frac{z^3 + 8z + 256}{z^3} \left[K_2^4 + \frac{z^2 + 4z + 70}{z^3 + 8z + 256} K_1^4 \right] \\ &\quad + 2 \frac{z+8}{z^3} (K_1^2 K_2^2 + K_2^2 K_1^2) - 8 \frac{z+8}{z^3} \\ &\quad + 16 \frac{(z+8)^2}{z^3(z^3 + 8z + 64)} (K_1^2 + K_2^2). \end{aligned} \quad (42)$$

Finally, we have to solve Eq. (38) to get the coefficients z_0 , z_1 , and z_2 . The corresponding equations for those coefficients are at most of degree four. We shall give here the equation that z_0 has to satisfy at the order $O(z^{-4})$,

$$4 + U + \frac{8}{z_0} + \frac{32}{z_0^2} + \frac{176}{z_0^3} = z_0. \quad (43)$$

In a very similar way used for the computation of z_0 , the analytical expressions of z_1 and z_2 can be derived from Eqs. (38), (42), and (43). The good agreement with the exact numerical spectrum can be seen on Fig. 9 for $U=50$. Here the numerical values for the sublevels are for $\nu_{1,2}=0$, $z(\gamma) = 54.1597 - 0.2826\gamma + 0.0356\gamma^2$, for $\nu_{1,2}=(0,1)$, $z(\gamma) = 54.1597 - 0.8480\gamma + 0.2084\gamma^2$, for $\nu_{1,2}=(1,1)$,

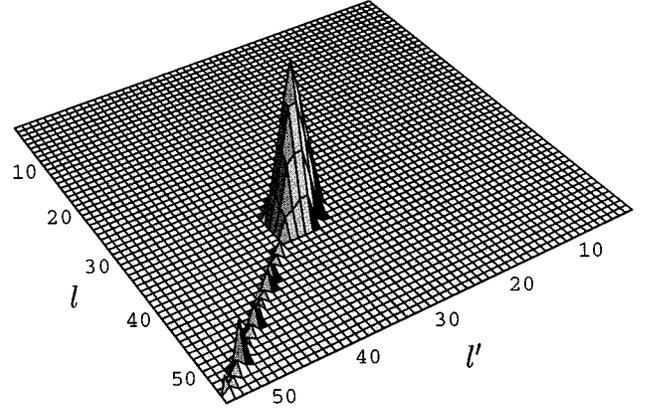


FIG. 10. Semilog plot of $W = |\phi(l, l')|^2$ for a localized state ($E=50.25$, $-30 \leq \ln W \leq -1$).

$z(\gamma) = 54.1597 - 1.4133\gamma + 0.5539\gamma^2$. A similar computation can be done near the band function minimum $k_c = (\pi, \pi)$ corresponding to the energy $z \approx U - 4$.

The structure of the pair states for $U \gg 1$ can be understood in the following way: the diagonal term corresponding to the energy of particles located on the same site is $4\lambda \cos(\gamma n + \beta) + U$. The transition amplitude on the diagonal $n_{1,2} = n$ is given by the amplitude of the hopping via virtual states with $n_1 - n_2 = \pm 1$ and energy denominator $1/U$. There are two such paths so that the effective amplitude is $V_{\text{eff}} = 2/U$. The same expression can be derived by the Schur formalism (see Sec. IV). After dividing the Hamiltonian by V_{eff} we arrive to the eigenfunctions equation in the form of Harper (14) with λ replaced by $\lambda_{\text{eff}} = U \gg 1$. Since $\lambda_{\text{eff}} \gg 1$ when $U \gg 1$, the pair states are always within the localized phase of the Harper equation showing exponential localization. In Fig. 10, we show a typical eigenstate of the Mathieu part of the spectrum for $U=50$ and $\gamma/2\pi = 34/55$. The fact that it is localized confirms the pure-point character of the corresponding spectrum.

Above we showed that in the case of strong interaction, we have $\lambda_{\text{eff}} \gg 1$. This explains the appearance of a pure-point component in the spectrum. However, we think that this pure-point component will even appear for small values of the interaction. Our argument is the following: without interaction, the system obeys Aubry's duality while the presence of the interaction introduces Aubry's duality breaking. Indeed, from Eq. (18) it is easy to see that the interaction acts in the coordinate space and the symmetry with momentum space disappears when $U \neq 0$. Formally, this argument is not sufficient to prove the existence of a pure-point spectrum at arbitrary small U . However the ensemble of numerical data we have here and in Refs. 22 and 21 confirms this conjecture.

When U is large, the unshifted part of the spectrum looks very much like the spectrum at $U=0$. The main difference can be found by looking carefully at the Landau levels (see Fig. 11). The reminiscence of the existence of the interaction is seen through the appearance of a splitting of Landau sublevels. This splitting only exists when Landau quantum numbers are different $\nu_1 \neq \nu_2$ and the two particles are located in the same well. Such a behavior is illustrated by Fig. 11. The other sublevels are described by the semiclassical formulas

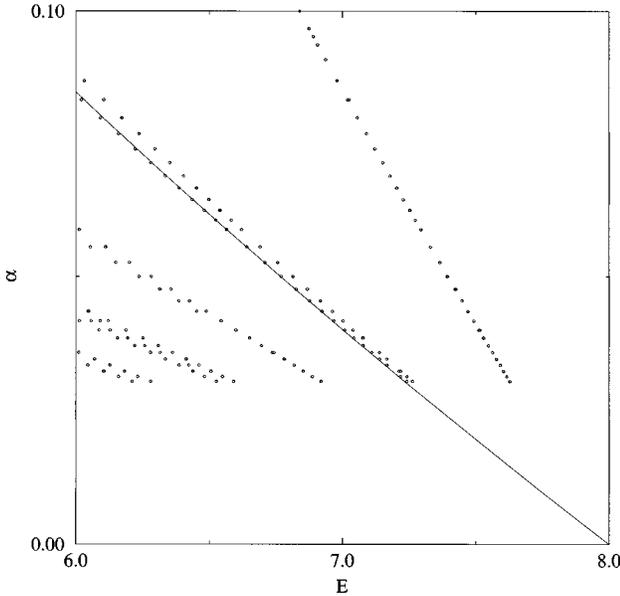


FIG. 11. Semiclassical calculations (45) (full curve) and exact numerical spectrum (points) for the splitting of the $\nu_1=0$, $\nu_2=1$ Landau sublevel in the two-particle Harper model for $U=20$.

obtained in the case $U=0$ (25). To derive this splitting using semiclassical analysis, we again apply the Schur complement formula. Dealing with the unshifted butterfly leads us to consider as the dominant term $QH_{\text{TIP}}Q$ such that Eq. (37) becomes

$$H_{\text{TIP}}^{\text{eff}}(z) = QH_{\text{TIP}}Q + QH_{\text{TIP}}P \frac{1}{z - PH_{\text{TIP}}P} PH_{\text{TIP}}Q. \quad (44)$$

Applying the same scheme as before produces an additional shift from the unperturbed energy given in first order in γ by

$$|\delta E(\gamma)| = 4 \frac{\gamma}{U+4}. \quad (45)$$

This shift is valid for the second Landau sublevel ($\nu_1=0$, $\nu_2=1$), its accuracy is shown in Fig. 11 and the two splitted subbands are given by $E(\gamma) = 8 - 4.1666\gamma$ and $E(\gamma) = 8 - 4\gamma$ up to order 1 in γ .

V. TWO INTERACTING PARTICLES ON A TWO-DIMENSIONAL LATTICE

Even though the studied model was derived from a model of two-dimensional electrons, its effective dimension is 1: as we already pointed out, Eq. (18) was derived assuming that the particle propagates as a plane wave in one direction. This assumption, though reasonable in the one-particle model, could be violated by interaction induced quantum interferences in the two-particle case. Therefore the question of the survival of interaction induced localization effect for two interacting particles in two dimensions remains an open problem. In this section we would like to discuss briefly this situation. For two interacting particles moving on a two-

dimensional square lattice submitted to a uniform magnetic flux, the eigenvalue equation reads

$$\begin{aligned} e^{i\gamma y_1} \psi_{x_1+1, y_1, x_2, y_2} + e^{-i\gamma y_1} \psi_{x_1-1, y_1, x_2, y_2} + \psi_{x_1, y_1+1, x_2, y_2} \\ + \psi_{x_1, y_1-1, x_2, y_2} + e^{i\gamma y_2} \psi_{x_1, y_1, x_2+1, y_2} \\ + e^{-i\gamma y_2} \psi_{x_1, y_1, x_2-1, y_2} + \psi_{x_1, y_1, x_2, y_2+1} + \psi_{x_1, y_1, x_2, y_2-1} \\ + \tilde{U} \delta_{x_1, x_2} \delta_{y_1, y_2} \psi_{x_1, y_1, x_2, y_2} = E \psi_{x_1, y_1, x_2, y_2}, \end{aligned} \quad (46)$$

where $(x_{1,2}, y_{1,2})$ are integers denoting the positions on the square lattice and \tilde{U} is the on-site interparticle interaction. For $\tilde{U}=0$, the previous equation can be reduced to the one-dimensional Harper equation we discussed above Eq. (18). With interaction, the same equation (18) can be obtained in the ansatz of plane waves propagating in one direction with renormalized interaction U .²² While this plane-wave approximation is a standard approach for the one-particle Harper problem, it has to be handled with care in the interacting case. Indeed this plane-wave ansatz breaks the symmetry of the original problem (46). This symmetry can be seen in the limit of strong interaction $U \gg 1$. In this case, there should be two energy bands: one corresponding to the pair states when particles are located on the same site with energy $E \approx U$ and the other with $E \approx 1$ for the states in which the two particles avoid each other. In the higher energy band, the eigenvalue equation for the pair states up to the terms of order $1/U$ has the form

$$\begin{aligned} \frac{2}{U} (e^{2i\gamma y} \phi_{x+1, y} + e^{-2i\gamma y} \phi_{x-1, y} + \phi_{x, y+1} + \phi_{x, y-1}) \\ + U \phi_{x, y} = E \phi_{x, y}. \end{aligned} \quad (47)$$

Here the term $2/U$ represents the transition amplitude for pair states. Its derivation is similar to the case of two interacting particles in the one-dimensional Harper model. Indeed if one keeps $x_1=x_2$ then the hopping term is given by $V_{\text{eff}}=2/U$ because there are two paths with virtual energy U ($y_{1,2} \rightarrow y_{1,2}+1$) which contribute to the hopping term in the y direction. Similarly the hopping in the x direction is $V_{\text{eff}}=2e^{\pm 2i\gamma}/U$.

This representation shows that the symmetry between the two directions or the Aubry duality is not broken by the interaction. The main reason is that the symmetry of the interaction is invariant under rotations on the square lattice. In the limit of large U , this property can be seen through Eq. (47). However the symmetry (Aubry's duality) should also be preserved for small interaction. Due to that, we expect that similarly to the Harper model with $\lambda=1$, the interaction will not generate a pure-point component in the spectrum. However this conjecture has to be directly checked in further analytical and numerical studies.

VI. CONCLUSIONS

In this paper we have emphasized a localizing effect due to the combined action of an on-site interaction and a quasi-periodic potential. Unlike in the random potential case,²⁰ extended unperturbed states are localized by the interaction, and this localization occurs at arbitrarily small attractive/

repulsive interaction. We successfully identified the mechanism responsible for this effect as a decoupling of a Mathieu-like model from the original two-particle Harper model in the limit of large interaction. Our conjecture is that a similar mechanism will also work for small U due to an interaction induced breaking of Aubry's duality. This breaking happens in one-dimensional incommensurate models, however in two-dimensional magnetic models, we expect that the interaction will not break the duality and that a pure-point com-

ponent in the spectrum will not arise. Further verifications of these conjectures are required.

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