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 non interacting problem. Our numerical studies allow to understand the global structure of the spectrum. Analytical approach developed permits to understand the origin of localized states in the limit of strong interaction $U$ and fine spectral structure for small $U$.

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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 2). 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. 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 has been performed in 1985 using superconducting networks 3 and more recently experiments with superlattices also allowed to observe the first hierarchical steps of multifractal butterfly structure 4.

The deep understanding of such an intricate spectral structure attracted interest of mathematicians and physicists who developed new approaches for its investigation such as non commutative geometry 5, pseudodifferential operators 6, functional analysis 7, renormalization group approach 8,9, thermodynamical formalism 10. All these tools allowed 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 11, it is possible to prove rigorously the existence of localized or delocalized states 12. It was also found that quantum systems which are chaotic in the classical limit may have quite unusual properties in the presence of underly- ing quasiperiodic structure 12,13,14.

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 rôle. Therefore it is natural to address the question of the influence of inter-action on multifractal spectrum. The most simple example of such a case is an interaction between two particles. Recently it has been found that in the case of random potential even such simple model has a number of unexpected properties 13. For example repulsive/attractive short range interaction leads to 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 14. 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 13 allowed 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 diagonalisation based upon 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

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

where the parameter $\gamma$ characterizes the quasiperiodic lattice for the one-particle problem. 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 $\alpha$ plays the role of an effective Planck’s constant so that $\alpha \rightarrow 0$ corresponds to the semiclassical limit. The two parameters $\beta_{1,2}$ are related to the quasimomentum components in the non interacting problem. The parameter $\lambda$ characterizes the strength of the quasiperiodic potential and for the case
of electrons on a square lattice $\lambda = 1$ [3]. However from mathematical point of view it is also interesting to study the different regimes with $\lambda < 1$ and $\lambda > 1$. 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 [14,10,1,20]. The strength of the short range on-site interaction is characterized by $U$. In the absence of interaction, the corresponding two particle spectra of the Harper model and is shown in Fig. 1 (a). Comparing with the one-particle spectrum (Hofstadter’s butterfly), we can remark that the spectrum becomes much more dense near the centers of the bands and subbands but still the gaps in the spectrum survive on all energy scales.

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

The main features which can be immediately observed in this figure 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 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 $E_{\pm}(\alpha) = \pm 8 + 4\pi a(m_1 + m_2 + 1) + \pi^2 n^2 (2 + (2m_1 + 1)^2 + (2m_2 + 1)^2)/4 + O(\alpha^3)$, which is superposition of two Hofstadter butterflies in semiclassical regime [3]. 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 non shifted 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 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 on Fig. 2 (a). This shows that the shifted butterfly corresponds to the case when the 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.

**Fig. 1**: Spectrum of 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.

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 it can be seen with the typical 3-D plot of Fig. 3.

The properties of eigenstates can also be analyzed with the help of the inverse participation ratio (IPR) \( \xi = (\sum |W_{n_1,n_2}|^2)^{-1/2} \). Its value for different energies is shown in Fig. 4 for \( \alpha = 34/55 \). In agreement with the above discussion, the localized states with small \( \xi \) correspond to the part of the shifted butterfly with less dense spectrum while the unshifted butterfly is associated to large \( \xi \) with delocalized states. It is interesting to determine the IPR \( \xi_0 \) in the non interacting eigenstates basis. Such approach has been quite useful for TIP in a random potential. It is interesting to note that the situation for TIP in the Harper model is quite different. Namely, the delocalized states have very small value of \( \xi_0 \) while the localized ones are delocalized in the non interacting eigenstates basis and have very large \( \xi_0 \) (see Fig. 3). This result once more shows that delocalized states correspond to almost non interacting particle propagation while localized states appear only due to interaction which can be even repulsive (Fig. 3a).

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

**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 \( \xi \) vs eigenenergies \( E \) shown at \( \xi = 2; U = 1, \alpha = 34/55, 0 \leq \beta < 2\pi \).

**Fig. 5**: Same as in Fig. 1 with \( U = 10 \) and \( q \leq 28 \).

The physical reason for the appearance of such 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:

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

(2)

Here \( V_{\text{eff}} \) 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 Harper equation with \( \lambda_{\text{eff}} = 2\lambda/V_{\text{eff}} \gg 1 \). Due to that 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 pair of particles. For strong $U$, the renormalized $\lambda_{\text{eff}}$ is much larger than 1 that, according to the Aubry duality $[\text{14}]$, leads to localization of TIP pairs in quasiperiodic potential. Our conjecture is that in a sense $\lambda_{\text{eff}}$ remains larger than 1 even for moderate values of $U \sim 1$. In a sense interaction breaks Aubry duality leading to appearence of 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 accurate expressions for the TIP energy edges of shifted spectral band can be found using semiclassical analysis at small flux values by methods developed in $[\text{23}]$. The details of computations will be given elsewhere $[\text{24}]$. For the case of Fig. 2 (b), they give $E = 6.0 + 0.59 \times 2\pi\alpha + O(\alpha^2)$ that is in good agreement with numerical data (Fig. 2 (b)).

For the part of the spectrum represented by unshifted butterfly at $U \gg 1$, the eigenstates become more and more similar to asymmetric TIP configuration i.e. $\phi_{n_1,n_2} = \text{sign}(n_1 - n_2) \left( \chi^{(1)}_{n_1} \chi^{(2)}_{n_2} - \chi^{(1)}_{n_2} \chi^{(2)}_{n_1} \right) / \sqrt{2}$, where $\chi$s are one-particle eigenfunctions. Due to that, 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 effective small interaction between particles located in the same well. According to the expression for $\phi_{n_1,n_2}$, such splitting can take place only when Landau quantum numbers are different $(n_1 \neq n_2)$ so that $\chi^{(1)} \neq \chi^{(2)}$. As the result the first sublevel with $m_{1,2} = 0$ is not splitted. For non interacting part, the edges are given by the same $E_{\pm}(\alpha)$ as for $U = 0$ (see above) while for interacting case, the additional shift is $\delta E(\alpha) = -8\pi\alpha/(U + 4)$ (see $[\text{24}]$). These analytical expressions are in good agreement with numerical results as shown in Fig. 2 (b).

In summary, 20 years after $[\text{3}]$ our investigations of spectra and eigenstates for TIP in the Harper model (1) show that repulsive/attractive interaction leads to appearence of localized states. Our conjecture is that due to Aubry duality breaking a localized TIP pair phase appears at 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 $[\text{24}]$.

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