Vol 17 No 2, February 2008
1674-1056/2008/17(02)/0674-06
Chinese Physics B
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Characterizing localization properties of two spinless electrons in a one-dimensional Harper model with concurrence*

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(Received 14 May 2007; revised manuscript received 29 June 2007)

By mapping the Fock space of many local fermionic modes isomorphically onto a many-qubit space and using the measure of concurrence, this paper studies numerically the mode entanglement of two spinless electrons with on-site interaction U moving in the one-dimensional Harper model. Generally speaking, for electrons in extended regimes (potential parameter $\lambda < 2$), the spectrum-averaged concurrence $N\langle C\rangle$ first decreases slowly as λ increases until its local minimum, then increases with λ until its peak at $\lambda = 2$, while for electrons in localized regimes ($\lambda > 2$), $N\langle C\rangle$ decreases drastically as λ increases. The functions of $N\langle C\rangle$ versus λ are different for electrons in extended and localized regimes. The maximum of $N\langle C\rangle$ occurs at the point $\lambda = 2$, which is the critical value in the one-dimensional single-particle Harper model. From these studies it can distinguish extended, localized and critical regimes for the two-particle system. It is also found for the same λ that the interaction U always induce the decreases of concurrence, i.e., the concurrence can reflect the localization effect due to the interaction. All these provide us a new quantity to understand the localization properties of eigenstates of two interacting particles.

Keywords: entanglement, two interacting particles, localization, Harper model
PACC: 7155J,7110F,0367

1. Introduction

Entanglement is an intriguing property of quantum systems. The early study of entanglement is only focused on the foundations of the quantum mechanics.[1,2] Recently due to its potential applications in quantum communications, quantum cryptography, quantum computer and quantum information, entanglement has been studied extensively.[3] As an important feature of quantum systems, entanglement naturally exists in condensed matter systems. Recently, considerable interests have been devoted to entanglement of quantum spin systems,[4−6] itinerant electron systems,[7−9] correlated fermionic systems[10] and bosonic systems,[11,12] etc.

One of the most important progress in the study of the entanglement is the quantitative measures of entanglement for a mixed state by using the entanglement of formation.[13,14] For the special case of two spin-1/2 systems, the entanglement of formation is given by the concurrence.[15−17] In the case of electron systems, a quantitative analysis in terms of quantum entanglement is also possible.[7] By mapping the Fock space of many local fermionic modes isomorphically onto a many-qubit space and using the measure of concurrence, mode entanglement sharing in single-particle states was studied in the Harper model,[18] the Frenkel–Kontorova model,[19] and other interesting one-dimensional determined and random models,[20] respectively. The connection between mode entanglement and the localization properties of the eigenstates is revealed.[18−20] Especially, very recently mode entanglement sharing in non-interacting disordered electronic systems for different band filling is also studied.[21] It is interesting to reveal whether

*Project supported by the National Nature Science Foundation of China (Grant Nos 90203009, 10175035 and 10674072), by the Specialized Research Fund for the Doctoral Program of Higher Education (Grant No 20060319007), by the Excellent Young Teacher Program of the Ministry of Education of China, by the Nature Science Foundation of Jiangsu Province of China (Grant No 06KJD140135).
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mode entanglement is suitable to exhibit the localization properties of many-particle states.

On the other hand, the problem of interacting electrons in a disordered potential is one of the important problems in condensed-matter physics.[22] In view of the complexity of the simultaneous presence of randomness and interaction, some time ago, Shepelyansky[23] proposed that it would be worthwhile to consider the simple case of two interacting particles (TIP) in a random potential. For TIP case, two models, i.e., the Anderson model[23,24] and the Harper model,[25−30] are considered extensively. There are many numerical approaches to study the interplay of disorder and interaction, e.g., a Green's function approach,[24] a transfer-matrix method,[25] a decimation method,[26] a dynamical method[23,27,28] and an exact diagonalization method.[28−30] In most of those works the focus is on the investigation of a few specific two-electron states, usually at the band centre.

In this paper, we extend the mode entanglement sharing in single-particle states to that in two-particle states. By using the measure of concurrence, we analyse the effect of quasiperiodic potential and/or particles interaction on the mode entanglement. It provides us a new quantity, i.e., concurrence, to understand the localization properties of eigenstates of TIP.

This paper is organized as follows. In next section the formalism and model are described. In Sec.3 the numerical results for two spinless electrons in the Harper model are presented. Sec.4 is devoted to conclusion.

2. Formalism and model

2.1. Concurrence

We consider two spinless electrons with antisymmetric orbital wave functions, moving in one-dimensional lattice with N sites (local fermionic modes), and interacting via a nearest-neighbour interaction U. Generally, the tight-binding Hamiltonian can be described by[31]

$$H = t\sum_{n=1}^{N}(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) + \sum_{n=1}^{N}\varepsilon_n c_n^\dagger c_n + U\sum_{n=1}^{N}(c_n^\dagger c_n)(c_{n+1}^\dagger c_{n+1}), \quad (1)$$

where t is a nearest-neighbour hopping integral, $c_n^\dagger$ (c_n) is the creation(annihilation) operator of nth site, and ε_n is the on-site potential. The site occupation basis in Fock space is

$$|n_1, n_2, \ldots, n_N\rangle = c_1^{\dagger n_1} c_2^{\dagger n_2} \ldots c_N^{\dagger n_N} |0\rangle, \quad (2)$$

where $n_i = 0, 1$, and $|0\rangle$ is the vacuum. For two particles in the system, the restriction condition is $\sum_{i=1}^{N} n_i = 2$.

It is well known that the Fock space of many local fermionic modes can be mapped isomorphically onto a many-qubit space.[7] This is easily seen by defining the mapping

$$\Lambda := \prod_{i=1}^{N} c_i^{\dagger n_i} |0\rangle \mapsto \otimes_{i=1}^{N} (\sigma_i^\dagger)^{n_i} |0\rangle, \quad (3)$$

where $\sigma_i^\dagger$ is the raising operator of ith qubit.

For N qubit system, the concurrence between qubits i and j (with $i < j$) is defined by[15,16]

$$C_{ij} = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\}, \quad (4)$$

where the λ_k's are the square roots of the eigenvalues of the matrix $R = \rho_{ij}\widetilde{\rho}_{ij}$, in descending order, here ρ_{ij} is the reduced density matrix for i and j; the spin-flipped density matrix is defined by $\widetilde{\rho}_{ij} = (\sigma_i^y \bigotimes \sigma_j^y)\rho_{ij}^*(\sigma_i^y \bigotimes \sigma_j^y)$, where σ^y is the matrix $\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$ and ρ_{ij}^* is the complex conjugate of ρ_{ij}.

For a system of spinless fermions, by the mapping (3), the reduced 4×4 density matrix ρ_{ij} is given by[18,21]

$$\rho_{ij} = \begin{pmatrix} v_{ij} & 0 & 0 & 0 \\ 0 & w_{1ij} & z_{ij}^* & 0 \\ 0 & z_{ij} & w_{2ij} & 0 \\ 0 & 0 & 0 & u_{ij} \end{pmatrix}, \quad (5)$$

with $u_{ij} = \langle \widehat{n}_i \widehat{n}_j \rangle$, $w_{1ij} = \langle (1-\widehat{n}_i)\widehat{n_j} \rangle$, $w_{2ij} = \langle \widehat{n}_i(1-\widehat{n_j}) \rangle$, $v_{ij} = \langle (1-\widehat{n}_i)(1-\widehat{n_j}) \rangle$ and $z_{ij} = \langle c_j^\dagger c_i \prod_{l=i+1}^{j-1}(1-2\widehat{n}_l) \rangle = \langle c_j^\dagger c_i \rangle$, respectively. Here $\widehat{n}_i = c_i^\dagger c_i$.

The general eigenstate of two spinless electrons is the superposition

$$|\alpha\rangle = \sum_{n_1,n_2=1}^{N} \psi_{n_1,n_2} |n_1, n_2\rangle = \sum_{n_1,n_2=1}^{N} \psi_{n_1,n_2} c_{n_1}^\dagger c_{n_2}^\dagger |0\rangle, \quad (6)$$

where ψ_{n_1,n_2} $(= -\psi_{n_2,n_1})$ is amplitude of wave function. To keep $\langle\alpha|\alpha\rangle = 1$, the normalization condition is $\sum_{n_1,n_2=1}^{N} \psi_{n_1,n_2}\psi^*_{n_1,n_2} = \frac{1}{2}$. One can show by direct calculations that,

$$u_{ij} = 4\psi_{i,j}\psi^*_{i,j}, \tag{7}$$

$$w_{1ij} = 4\sum_{k=1}^{N} \psi_{j,k}\psi^*_{j,k} - u_{ij}, \tag{8}$$

$$w_{2ij} = 4\sum_{k=1}^{N} \psi_{i,k}\psi^*_{i,k} - u_{ij}, \tag{9}$$

$$v_{ij} = 1 - (w_{1ij} + w_{2ij}) - u_{ij}. \tag{10}$$

$$z_{ij} = 4\sum_{k=1}^{N} \psi_{i,k}\psi^*_{j,k} - 8\sum_{l=i+1}^{j-1} \psi_{i,l}\psi^*_{j,l}. \tag{11}$$

From Eqs.(5) to (11), we obtain that $\lambda_{1,2,3,4} = \sqrt{w_{1ij}w_{2ij}} + |z_{ij}|$, $\left|\sqrt{w_{1ij}w_{2ij}} - |z_{ij}|\right|$, $\sqrt{u_{ij}v_{ij}}$, and $\sqrt{u_{ij}v_{ij}}$, respectively. According to Eq.(4), we can calculate the corresponding concurrence C_{ij} for two sites i and j. For nonuniform systems, the value of C_{ij} depends on the site positions i and j. At an eigenstate α, we define a site-averaged concurrence

$$\langle C^\alpha\rangle = \frac{1}{d}\sum_{i<j} C^\alpha_{ij}, \tag{12}$$

where $d = N(N-1)/2$. For examples, for a delocalized state that all $\psi_{n_1,n_2} = \frac{1}{\sqrt{2N(N-1)}}$ for all $n_1 < n_2$, $\langle C^\alpha\rangle \approx \frac{4-2\sqrt{2}}{N} = \frac{1.172}{N}$ and for a localized state that $\psi_{n_1^\circ,n_2^\circ} = \frac{1}{2}$ at given n_1° and n_2°, $\langle C^\alpha\rangle = 0$, therefore, $\langle C^\alpha\rangle$ can reflect the localization properties of eigenstates.

In order to analyse the influence of system parameters, e.g., the interaction U, on the concurrence for all eigenstates, as a further gross measure we also define a spectrum-averaged concurrence

$$\langle C\rangle = \frac{1}{M}\sum_{\alpha} \langle C^\alpha\rangle, \tag{13}$$

where M is the number of all the eigenstates.

2.2. The Harper model

The eigenvalue equation of the one-dimensional one-particle Harper model can be written as

$$\lambda\cos(2\pi\sigma n + \beta)\phi_n + t\,(\phi_{n-1} + \phi_{n+1}) = E\phi_n, \tag{14}$$

where the parameter λ characterizes the strength of the quasiperiodic potential, σ and β are a constant. Intensively analytical and numerical studies[32,33] for typical irrational values σ show that for $\lambda > 2$ the spectrum is pure-point like with gaps and all eigenstates are exponentially localized. For $\lambda < 2$ the spectrum becomes continuous with extended eigenstates corresponding to ballistic classical motion. For $\lambda = 2$ the situation is critical with a singular-continuous multifractal spectrum and power law localized eigenstates.[27]

From Eqs.(1) and (6), the eigenvalue equation for two spinless interacting electrons in the Harper model can be described by

$$\begin{aligned}&[\lambda\cos(2\pi\sigma n_1 + \beta_1) + \lambda\cos(2\pi\sigma n_2 + \beta_2)\\ &+U\delta_{|n_1-n_2|,1}]\psi_{n_1,n_2} + t(\psi_{n_1+1,n_2} + \psi_{n_1-1,n_2}\\ &+\psi_{n_1,n_2+1} + \psi_{n_1,n_2-1}) = E\psi_{n_1,n_2}.\end{aligned} \tag{15}$$

In our calculation, σ is set to $(\sqrt{5}-1)/2$, $\beta_1 = \beta_2 = 0$, t is taken as units of energy and $U > 0$, i.e., the repulsive interaction between particles is considered. In order to analyse our results, we also study the inverse participation ratio (IPR) $\xi = \left(N^2\sum_{n_1,n_2}\psi^4_{n_1,n_2}\right)^{-1}$.[29] Physically, ξ gives the number of lattice sites occupied in the TIP state. Though there is not a defined quantity to describe the localization properties for TIP, the properties of eigenstates can be analysed partially with the help of the IPR ξ.

3. Numerical results

3.1. For $U = 0$

Let ϕ^i_n be a normalized single-particle eigenstate of the eigenvalue equation (14) with eigenenergy E_i . For the nearest-neighbour interaction $U = 0$, the set of antisymmetric states

$$\psi^{\rm A}_{n_1,n_2} = \frac{1}{2}[\phi^1_{n_1}\phi^2_{n_2} - \phi^2_{n_1}\phi^1_{n_2}] \tag{16}$$

are obviously the exact eigenfunctions of Eq.(15), with the eigenenergy $E^{\rm A} = E_1 + E_2$. In our numerical calculation, we solve the eigenvalue equation (14) with open boundary and get eigenstates of TIP by Eq.(16).

The spectrum-averaged concurrence $N\langle C\rangle$ varying with parameter λ are plotted in Fig.1 for $N =$ 55, 89, and 144, respectively. Our results show that

for electrons in extended regimes ($\lambda < 2$), $N\langle C\rangle$ decreases slowly as λ increases till a local minimum, then increases and reaches its peak near $\lambda = 2.0$, while in localized regimes ($\lambda > 2$), $N\langle C\rangle$ decreases drastically as λ increases. Comparing $N\langle C\rangle$ with each other for electrons in the two regimes, we know that, on the whole, $N\langle C\rangle$ is larger for electrons in extended regimes, while smaller in localized regimes, i.e., $N\langle C\rangle$ can reflect the localization properties of two-particle states. It is similar to that for the concurrence sharing in single-particle states.[18] In detail, the values of λ, at which the $N\langle C\rangle$ is maximal, is equal to $2.05, 2.03$ and 2.015 for $N = 55, 89$ and 144, respectively. Those make us believe that $\lambda_c = 2.0$ when the size of system $N \longrightarrow \infty$, which is the critical value in the one-dimensional single-particle Harper model. It is obvious that the functions of $N\langle C\rangle$ versus λ are different for electrons in extended, critical and localized regimes, therefore from the concurrence we can distinguish extended, localized and critical regimes for the two-particle system.

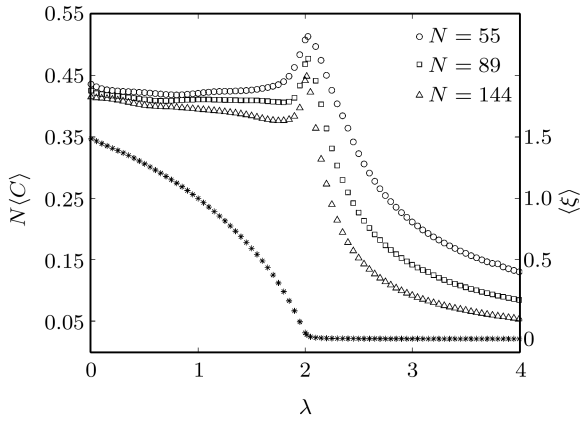


Fig.1. The spectrum-averaged concurrence $N\langle C\rangle$ varying with λ for $N = 55$ (circle), $N = 89$ (square), and $N = 144$ (up-triangle). At the same time, the spectrum-averaged IPR $< \xi >$ varying with λ for $N = 144$ (star).

The localization properties of eigenstates for TIP can be analysed partially by the IPR ξ. The $< \xi >$ varying with λ for $N = 144$ is also plotted in Fig.1. $< \xi >$ is larger when $\lambda < 2$, while very small when $\lambda > 2$. On the whole, the larger $< \xi >$ is, the larger $N\langle C\rangle$ is. There is a transition for the value of $< \xi >$ at $\lambda = 2$, at which $N\langle C\rangle$ becomes maximal. It is clear that there is a good correspondence between $N\langle C\rangle$ and $< \xi >$. Generally, the large $N\langle C\rangle$ and small $N\langle C\rangle$ correspond to delocalized and localized states, respectively, so the localization properties of eigenstates of TIP can be reflected by the concurrence.

In detail, the site-averaged concurrence $N\langle C^\alpha\rangle$ as functions of eigenenergies E and the histograms of the $N\langle C^\alpha\rangle$ are shown in Figs.2 and 3 respectively. Three examples for $N\langle C^\alpha\rangle$ versus E at $\lambda = 1, 2$ and 3 are given, respectively. For $\lambda = 1$, nearly all the values of $N\langle C^\alpha\rangle$ are in the range $[0.3, 1.25]$. Especially, majority are in the range $[0.3, 0.5]$ and a few are larger than 1.25. For $\lambda = 2$, all the value of $N\langle C^\alpha\rangle$ are almost uniformly distributed in the interval $[0.2, 0.7]$, while for $\lambda = 3$, those are distributed in a narrow interval $[0.025, 0.15]$. The properties of $N\langle C^\alpha\rangle$ for $\lambda < 2$ is similar to those for $\lambda = 1$, and for $\lambda > 2$ likes as those for $\lambda = 3$. Though the maximal value of $N\langle C^\alpha\rangle$ at small λ is larger than that at large λ, the spectrum-averaged concurrence $N\langle C\rangle$ is largest at $\lambda = 2$.

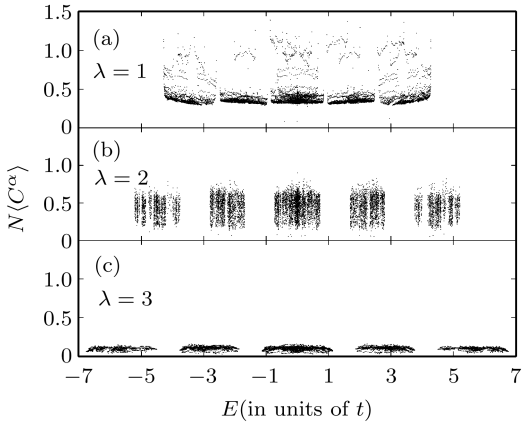


Fig.2. The site-averaged concurrence $N\langle C^\alpha\rangle$ as functions of eigenenergies for (a) $\lambda = 1$, (b) $\lambda = 2$ and (c) $\lambda = 3$, respectively. Here $N = 144$.

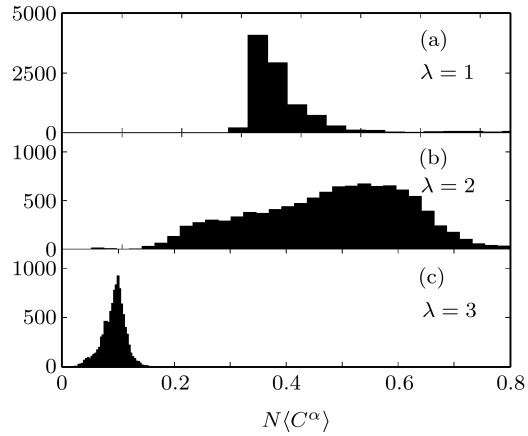


Fig.3. The histograms of the site-averaged concurrence $N\langle C^\alpha\rangle$ for (a) $\lambda = 1$, (b) $\lambda = 2$ and (c) $\lambda = 3$, respectively. Here $N = 144$.

3.2. For $U > 0$

In the presence of the nearest-neighbour interaction U, the wave functions of eigenstates for TIP

can not be simply given by the antisymmetric product of two one-particle eigenstates. At the situation, the conventional exact diagonalization method is used to obtain all two-electron eigenvalues and eigenvectors in finite systems. In Fig.4, the spectrum-averaged concurrences $N\langle C\rangle$ varying with λ are plotted for $U = 0.0, 0.1, 0.5, 4.0$ and 20.0, respectively. Here $N = 89$ and the results are similar for other system sizes. It shows that the $N\langle C\rangle$ varying with λ are similar to each other for different U. At the same λ, the $N\langle C\rangle$ for $U > 0$ is always smaller than that for $U = 0$.

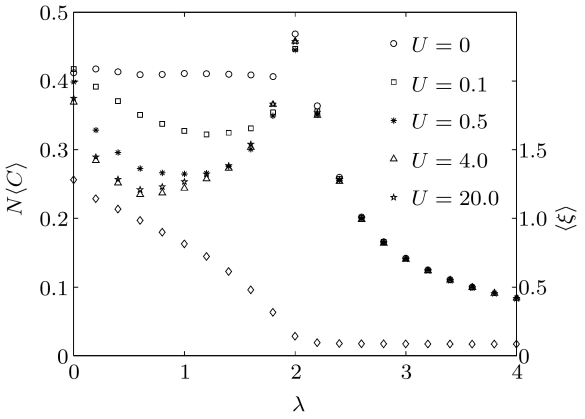


Fig.4. The spectrum-averaged concurrence $N\langle C\rangle$ varying with λ for $N = 89$ at different interaction U. At the same time, the spectrum-averaged IPR $\langle\xi\rangle$ varying with λ at $U = 4$ for $N = 89$ (diamond).

Such effect on $N\langle C\rangle$ increases with the increase of U until it is saturated at larger U, which is shown in Fig.5 for $\lambda = 0$ and $\lambda = 1$ respectively. The effect of U on $N\langle C\rangle$ in the range of $0 < \lambda < 2$ is more obvious than that in the range of $\lambda > 2$. The reason is that the interaction matrix element is small when the single-particle states are localized. We also plot the spectrum-averaged IPR as a function of λ in Fig.4 as the interaction U presents. Here the varying of $\langle\xi\rangle$ with λ is similar to that shown in Fig.1 for $U = 0$.

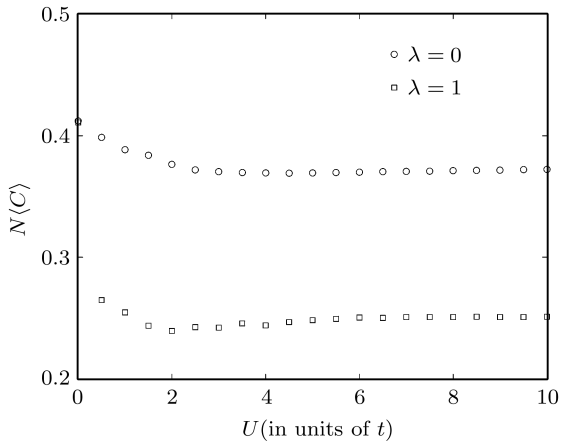


Fig.5. The spectrum-averaged concurrence $N\langle C\rangle$ varying with interaction U for $N = 89$ at $\lambda = 0$ (circle) and $\lambda = 1$ (square).

In order to study the effect of interaction U on the concurrence, the site-averaged concurrence $N\langle C^\alpha\rangle$ as functions of eigenenergies E are given in Figs.6(a) and 6(b) for $U = 0$ and $U = 4$, respectively. In the figure,

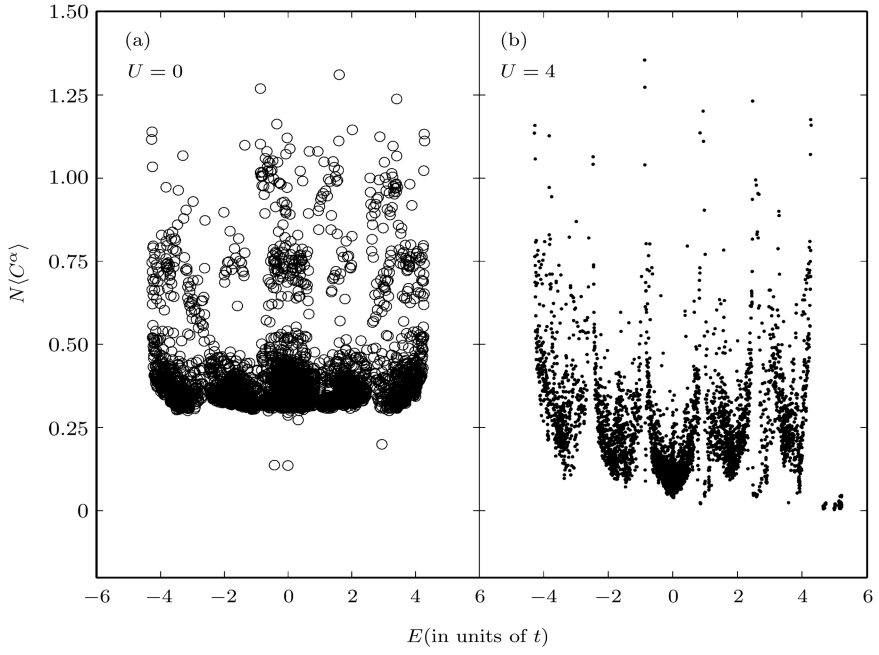


Fig.6. The site-averaged concurrence $N\langle C^\alpha\rangle$ as functions of eigenenergies at $\lambda = 1$ for (a) $U = 0$ and (b) $U = 4$, respectively. Here $N = 89$.

most of $N\langle C^{\alpha}\rangle$ for $U = 4$ are smaller than that for $U = 0$. Especially at $U > 0$, there are new-created point-like subbands above the band top of the noninteracting case.[29,30] It is interesting to note that the $N\langle C^{\alpha}\rangle$ of those eigenstates in the new subbands approximately equal to zero, which means that those eigenstates are localized. Our result that the interaction induces the decrease of concurrence is consistent with that the interaction can lead to a significant decrease in the rate of the particles propagation obtained by the dynamical method.[27]

4. Conclusions

The formalism of concurrence for two spinless electrons is obtained by mapping the Fock space of many local fermionic modes isomorphically onto a many-qubit space. By using the measure of concurrence, mode entanglement sharing in two-particle states in the one-dimensional Harper model is studied numerically. It is found that for electrons in extended regimes ($\lambda < 2$), the spectrum-averaged concurrence $N\langle C\rangle$ first decreases slowly as λ increases until its local minimum, then increases with λ until its peak at $\lambda = 2$, while for electrons in localized regimes ($\lambda > 2$), $N\langle C\rangle$ decreases drastically as λ increases. Comparing $N\langle C\rangle$ with each other for electrons in the two regimes, we know that, on the whole, $N\langle C\rangle$ is larger for electrons in extended regimes, while smaller in localized regimes. It is in accordance with the varying of the spectrum-averaged IPR $< \xi >$ versus λ, so the localization properties of eigenstates for TIP can be reflected by the concurrence. The maximum value of $N\langle C\rangle$ occurs at the point $\lambda = 2$, which is the critical value for λ in the one-dimensional single-particle Harper model. From these studies we can distinguish extended, localized and critical regimes for the two-particle system. In addition, at the same λ, $N\langle C\rangle$ for the nearest-neighbour repulsive interaction $U > 0$ is always smaller than that for $U = 0$. The effect that the interaction can induce the decrease of concurrence is consistent with that the rate of the particles propagation significantly decreases due to the interaction.[27] Therefore, with the help of concurrence, we can analyse localization properties of eigenstates for TIP.

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