Von Neumann entropy and localization properties of two interacting particles in one-dimensional nonuniform systems

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With the help of von Neumann entropy, we study numerically the localization properties for two interacting particles (TIP) with the on-site interaction in one-dimensional disordered, quasiperiodic and slowly varying potential systems, respectively. We find that for TIP in disordered and slowly varying potential systems, the spectrum-averaged von Neumann entropy \( \langle E_v \rangle \) first increases with interaction \( U \) until its peaks, then decreases as \( U \) gets larger. For TIP in the Harper model, the functions of \( \langle E_v \rangle \) versus \( U \) are different for particles in extended and localized regimes. Our numerical results indicate that for these two-particle systems, the von Neumann entropy is a suitable quantity to characterize the localization properties of particle states. Moreover, our studies propose a consistent interpretation of the discrepancies between previous numerical results.

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I. INTRODUCTION

Interacting uniform electronic systems\(^1\) and non-interacting disordered electronic systems\(^2,3\) are two of the most intriguing, albeit difficult, subjects in condensed matter physics. As a result of the complexity of the simultaneous presence of randomness and interactions, few definitive results are known.\(^4\) To understand the effects of electron interaction on the localization properties in a random potential, Shepelyansky proposed some years earlier that it would be worthwhile to consider the simple case of two interacting particles(TIP) in a one-dimensional (1D) random potential.\(^\) Subsequently, extensive efforts have been devoted to TIP in various systems.\(^7,8,9,10,11,12,14\) In particular, two interacting electrons with total spin zero in a 1D Harper model\(^8\) in Fibonacci and Thue-Morse lattices\(^9\) are studied. The behavior of TIP has been studied using the time evolution of wave packets \(^9,7,8,9\) exact diagonalization \(^8,10\) Green function\(^11,12,13\) and transfer-matrix\(^14\) etc. Due to different definitions of the localization length for TIP and different methods applied, there are discrepancies about the effect of the combination of disorder and interaction. For example, for TIP in 1D disordered potentials, Shepelyansky\(^4,5\) and others\(^11,12,13\) have found that for small interaction strengths, the two-particle interaction can enhance the Anderson localization length, while Römer and Schreiber\(^15\) found no enhancement of the localization length when the system size grows to infinity. Evangelou\(^*\) et al.\(^\) have pointed out that stronger localization occurs at large interaction when compared to the noninteracting case.\(^15\) At the same time, for TIP in a 1D Harper model, it was found that the interaction would induce localization effect\(^7,15,16\) while Evangelou and Katsanos\(^5\) found that the effects of particle interactions are different for electrons in extended and localized regimes.

On the other hand, quantum entanglement, which attracting much attention in quantum information,\(^17\) has been extensively applied in condensed matter physics.\(^18,19,20,21,22,23\) For examples, quantum entanglement measured by the von Neumann entropy was studied in the Hubbard model for the dimer case,\(^24\) in the extended Hubbard model for different band filling,\(^20\) in quantum small-world networks,\(^22\) and in low-dimensional semiconductor systems.\(^23\) It was found that the von Neumann entropy is suitable for analyzing the interplay between itinerant and localized features,\(^18\) as well as characterizing quantum phase transition \(^20,21\) and the localization-delocalization transition of electron states.\(^22\)

In this paper, we perform a detailed study of the von Neumann entropy for TIP in 1D disordered and quasiperiodic systems respectively, taking into account different on-site interactions \( U \) at various on-site potential strengths. We find that for TIP in disordered and slowly varying potential systems, the spectrum-averaged von Neumann entropy \( \langle E_v \rangle \) first increases with interaction \( U \) until its peaks, then decreases as \( U \) gets larger. For TIP in the 1D Harper model, the functions of \( \langle E_v \rangle \) versus \( U \) are different for particles in extended and localized regimes. Finally we study a two-particle system based on the slowly varying potential model.\(^24,25,26\) From these studies, we can conclude that for TIP systems, the von Neumann entropy is a suitable quantity to characterize the localization properties of particle states.

The paper is organized as follows. In the next section the von Neumann entropy is described. In Sec. III the numerical results for TIP in 1D disordered, quasiperiodic, and slowly varying potential systems are presented, respectively. And we present our conclusions and discussions in Section IV.
II. TIP MODELS AND VON NEUMANN ENTROPY

A. TIP models

Following recent literature, the eigenvalue equation for the TIP in 1D system can be written as

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

where \( \varepsilon_n \) is the on-site potential, \( t \) is a nearest-neighbor hopping integral and \( U \) characterizes the on-site interaction between particles.

Eq. (1) actually can describe the behaviors both bosons and fermions, i.e., two spinless bosons or two electrons with opposite spins.

For spinless bosons with the on-site interaction, the tight-binding Hamiltonian can generally be described by

$$H = t \sum_{n=1}^{N-1} \left( c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n \right) + U \sum_{n=1}^{N} \varepsilon_n c_n^\dagger c_n, \quad (2)$$

where \( c_n^\dagger \) \( (c_n) \) is the boson creation(annihilation) operator of the \( n \)th site. The generic eigenstate for two spinless bosons is the superposition

$$|\alpha\rangle = \sum_{n_1 \leq n_2}^{N} \psi_{n_1,n_2}^{0} |n_1, n_2\rangle = \sum_{n_1 \leq n_2}^{N} \psi_{n_1,n_2}^{0} c_{n_1}^\dagger c_{n_2} |0\rangle, \quad (3)$$

where \( |0\rangle \) is the vacuum and \( \psi_{n_1,n_2}^{0} \) is the amplitude of wave function. By making the transformation

$$\psi_{n_1,n_2}^{0} = \begin{cases} \phi_{n_1,n_2}^{\alpha} \text{ for } n_1 < n_2, \\ \sqrt{2} \phi_{n_1,n_2}^{\alpha} \text{ for } n_1 = n_2, \end{cases} \quad (4)$$

we can obtain the eigenvalue equation obtained from Eqs. (1—6) can be written as equation (1).

In the following our numerical method is described for bosons. The extension for fermions is straightforward.

B. von Neumann entropy

For the two particles in the system we are studying, there are three local states at each site, \(|2\rangle_n, |1\rangle_n, |0\rangle_n\), corresponding to the state with two, one or zero particles at the \( n \)th site, respectively. The local density matrix \( \rho_n \) is defined by

$$\rho_n = z_{2n} |2\rangle_n \langle 2| + z_{1n} |1\rangle_n \langle 1| + (1 - z_{2n} - z_{1n}) |0\rangle_n \langle 0|, \quad (7)$$

For two spinless bosons,

$$z_{2n} = \langle \alpha | c_{n}^\dagger c_{n} | \alpha \rangle = \psi_{n,n}^{\alpha} \psi_{n,n}^{*\alpha} \quad (8)$$

and

$$z_{1n} = \langle \alpha | c_{n}^\dagger c_{n} | \alpha \rangle - 2z_{2n}$$

$$z_{1n} = \sum_{m(m > n)} \psi_{n,m}^{\alpha} \psi_{n,m}^{*\alpha} + \sum_{m(m' < n)} \psi_{m',n}^{\alpha} \psi_{m',n}^{*\alpha}. \quad (9)$$

Consequently, the corresponding von Neumann entropy related to \( n \)th site is

$$E_{vn}^{\alpha} = -(1 - z_{1n} - z_{2n}) \log_2 (1 - z_{1n} - z_{2n}) - z_{1n} \log_2 z_{1n} - z_{2n} \log_2 z_{2n}. \quad (10)$$

For nonuniform systems, the value of \( E_{vn}^{\alpha} \) depends on the site position \( n \). At an eigenstate \( \alpha \), we define a site-averaged von Neumann entropy

$$E_{v}^{\alpha} = \frac{1}{N} \sum_{n=1}^{N} E_{vn}^{\alpha}. \quad (11)$$
For a delocalized state that all \( \psi_{n_1,n_2}^\alpha = \frac{1}{\sqrt{N(N+1)/2}} \) for all \( n_1 \leq n_2 \), this definition gives \( E_{\alpha}^0 \approx \frac{2}{N} \log_2 \frac{N}{2} \) at large \( N \), while for a localized state that \( \psi_{n_1,n_2}^\alpha = 1 \) at given \( n_1 \) and \( n_2 \), \( E_{\alpha}^0 = 0 \). In this paper, all the values of \( E_{\alpha}^0 \) are scaled by \( \frac{1}{V} \log_2 \frac{N}{2} \). From the two examples, we know that the scaled \( E_{\alpha}^0 \) is close to 1 for eigenstates are extended and almost vanishes for eigenstates are localized. Henceforth, we omit “scaled” for simplicity.

In order to analyze the influence of system parameters like the on-site interaction \( U \), on the von Neumann entropy for all the eigenstates, we define a spectrum-averaged von Neumann entropy as a further gross measure

\[
\langle E_{\alpha} \rangle = \frac{1}{M} \sum_{\alpha} E_{\alpha}^0,
\]

where \( M \) is the number of all the eigenstates.

### III. NUMERICAL RESULTS

From now we consider only the repulsive interaction \( (U > 0) \). We directly diagonalize the eigenvalue Eq. (1) with the periodic boundary condition at finite system sizes and obtain all eigenvalues \( E_{\alpha} \) and the corresponding eigenvectors \( |\alpha \rangle \). Without loss of generality, the hopping integral \( t \) is taken as units of energy. From the formulas (7)-(12), we then can obtain the site-averaged von Neumann entropy \( E_{\alpha} \) and the spectrum-averaged von Neumann entropy \( \langle E_{\alpha} \rangle \), respectively.

#### A. TIP in a disordered potential chain

For TIP in a disordered potential chain, the on-site potential \( \varepsilon_n \) in Eq. (3) are random variables uniformly distributed with \([-W,W]\). Here \( W \) characterizes the degree of on-site disorder as in the Anderson model. For this model, we calculate the spectrum-averaged von Neumann entropy \( \langle E_{\alpha} \rangle \) with a given set of parameters \( W \) and \( U \). For every set of parameters \( W \) and \( U \), the disorder average is taken over 100 samples. More samples simply give similar results.

For 1D Anderson model in the absence of the interaction \( (U = 0) \), it is well known that all the eigenstates are localized and the one-particle localization length is \( \xi \approx 25t^2/W^2 \) at the energy band center. Fig. 1 gives the spectrum-averaged von Neumann entropy \( \langle E_{\alpha} \rangle \) versus the disorder parameter \( W \). It shows that \( \langle E_{\alpha} \rangle \) monotonically decreases as \( W \) increases, reflecting the trivial localization effect of the on-site disorder in the model. To find the correlation between \( \langle E_{\alpha} \rangle \) and the localization properties for TIP systems, we also study the inverse participation ratio (IPR)\(^15\), defined by

\[
\xi_{\alpha} = \left( \frac{N(N+1)}{2} \sum_{n_1 \leq n_2} |\psi_{n_1,n_2}^\alpha|^4 \right)^{-\frac{1}{2}},
\]

which gives the ratio of lattice sites occupied by particles to all lattice sites at an eigenstate \( \alpha \). The larger \( \xi_{\alpha} \) is, the more delocalized the eigenstate is. In Fig. 2 we plot the site-averaged von Neumann entropy \( E_{\alpha}^0 \) versus \( \xi_{\alpha} \) at \( U = 0 \) for a typical sample with \( W = 1 \). On the whole, \( E_{\alpha}^0 \) increases logarithmically with \( \xi_{\alpha} \) as can be seen in the inset of Fig. 2 so von Neumann entropy can well reflect the localization properties of two-particle eigenstates.

For \( U > 0 \), the spectrum-averaged von Neumann entropy \( \langle E_{\alpha} \rangle \) as a function of \( U \) at \( W = 1, 2, 3 \) are plotted in Fig. 3. The results are similar for other \( W \). For all \( W \), we find that \( \langle E_{\alpha} \rangle \) first increases until its peak as \( U \) increases from zero, then decreases as \( U \) gets larger. There is a \( U^* \), at which \( \langle E_{\alpha} \rangle \) is equal to that at \( U = 0 \). When \( U \) is smaller(greater) than \( U^* \), \( \langle E_{\alpha} \rangle \) is larger(smaller) than the value of \( \langle E_{\alpha} \rangle \) at \( U = 0 \). To understand the effect of the interaction \( U \) on the von Neumann entropy, we calculate the site-averaged von Neumann entropy \( E_{\alpha}^0 \) and illustrate the results in Fig. 4 at different \( U \) for \( W = 1 \). It shows that only a small portion of the two-particle eigenstates have its value of \( E_{\alpha}^0 \) changed by the interaction \( U \). For small \( U \), most of the newly created eigenstates are

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**FIG. 1:** The spectrum-averaged von Neumann entropy \( \langle E_{\alpha} \rangle \) versus the disorder \( W \) for \( U = 0 \) at \( N = 90 \).

**FIG. 2:** The relation between the site-averaged von Neumann entropy \( E_{\alpha}^0 \) and the corresponding \( \xi_{\alpha} \) at \( W = 1 \) and \( U = 0 \) for a typical sample. The \( E_{\alpha}^0 \) versus \( \log_{10} \xi_{\alpha} \) is plotted in the inset.
in the main band and the corresponding \( E^v_0 \) are larger than that in the noninteracting case, while for large \( U \), most of them are above the top of the main band and the corresponding \( E^v_0 \) are smaller than that for particles without interaction. Therefore, the varying \( \langle E_v \rangle \) with \( U \) is not monotonic as shown in Fig. 3. These two competing effects reach an equilibrium at \( U = U^* \).

For TIP in 1D disordered potentials with \( U \leq t \) Shepelyansky\cite{S} and others\cite{S1,S2} have found that the Anderson localization length increases with \( U \). It agrees with our conclusions that for small \( U \), \( \langle E_v \rangle \) increases with \( U \). For large interaction \( U \), Evangelou et al\cite{E} have pointed out that stronger localization occurs when compared to the noninteracting case, because at \( U \gg t \) interaction can significantly modify the energy spectrum\cite{S} and the created eigenstates have the comparatively small localization lengths\cite{E}. The result is consistent with ours that for \( U > U^* \), the values of \( \langle E_v \rangle \) are smaller than that at \( U = 0 \).

B. TIP in a quasiperiodic potential chain

From Eq. (1), the eigenvalue equation for TIP in a quasiperiodic potential chain based on the Harper model can be described by\cite{S, S1, S2}

\[
[\lambda \cos(2\pi \sigma n_1 + \beta_1) + \lambda \cos(2\pi \sigma n_2 + \beta_2) + U \delta_{n_1,n_2}]\psi_{n_1,n_2} + t(\psi_{n_1+1,n_2} + \psi_{n_1-1,n_2} + \psi_{n_1,n_2+1} + \psi_{n_1,n_2-1}) = E\psi_{n_1,n_2},
\]  

where the parameter \( \lambda \) characterizes the strength of the quasiperiodic potential, \( \sigma \) and \( \beta_1, \beta_2 \) are constants. As a typical case, we set \( \sigma = (\sqrt{5} - 1)/2 \), \( \beta_1 = \beta_2 = 0 \). As is customary in the context of quasiperiodic system, the value of \( \sigma \) may in fact be approximated by the ratio of successive Fibonacci numbers—\( F_n = F_{n-2} + F_{n-1} \). In this way, choosing \( \sigma = F_{n-1}/F_n \approx (\sqrt{5} - 1)/2 \) and the system size \( N = F_n \), we can obtain the periodic approximant for the quasiperiodic potential. In our calculation, \( N \) is chosen as Fibonacci numbers 34, 55 and 89, respectively.

In the absence of the interaction \( U \) it is found\cite{S, S1, S2} that that for \( \lambda < 2 \) the spectrum becomes continuous and all eigenstates are extended. For \( \lambda > 2 \) the spectrum is pure point and all eigenstates are exponentially localized. For \( \lambda = 2 \) the situation is critical with a singular-continuous multifractal spectrum and power law localized eigenstates. Metal-insulator transition can occur at \( \lambda = 2 \). Obviously they are different from these for the
FIG. 5: (a) The spectrum-averaged von Neumann entropy $\langle E_v \rangle$ as a function of quasiperiodic potential strength $\lambda$ at $U = 0$. Here $N = 89$. (b) The $\langle E_v \rangle$ versus $\lambda$ at $U = 0$ for different $N$.

1D Anderson model where all eigenstates are localized for $W \neq 0$.

Fig. 5(a) shows the spectrum-averaged von Neumann entropy $\langle E_v \rangle$ with respect to the quasiperiodic potential strength $\lambda$ at $U = 0$. We observe that there is a sharp decrease of $\langle E_v \rangle$ near the critical value $\lambda_c = 2$. For $\lambda < \lambda_c$ which corresponds to extended states, all $\langle E_v \rangle$ are around 1, while for $\lambda > \lambda_c$ corresponding to localized states, all $\langle E_v \rangle$ are far less than 1. In Fig. 5(b) we plot $\langle E_v \rangle$ as a function of $\lambda$ at $U = 0$ for $N = 34, 55$ and 89. The curves cross at $\lambda \approx \lambda_c$. The crossing point separates the extended($\lambda < \lambda_c$) and the localized($\lambda > \lambda_c$) regimes.

For $U > 0$, the spectrum-averaged von Neumann entropy $\langle E_v \rangle$ as a function of $U$ at different $\lambda$ are shown in Fig. 6. Here we choose $\lambda = 1, 2$ and 3 as examples for extended, critical and localized regimes, respectively. At $\lambda = 1$ and $\lambda = 2$, $\langle E_v \rangle$ monotonically decreases when $U$ increases from zero. At $\lambda = 3$ $\langle E_v \rangle$ increases for small $U$ and decreases for large $U$, respectively, which is similar to that shown in Fig. 5 for TIP in a disordered potential chain. For $\lambda$ in extended and localized regimes, $\langle E_v \rangle$ as a function of $U$ are similar to that for $\lambda = 1$ and $\lambda = 3$, respectively. We also find that at the extended and critical regimes, the newly created eigenstates due to the interaction have small $E_v^0$, which will reduce the value of $\langle E_v \rangle$. At the localized regime, the effect of interaction $U$ on $\langle E_v \rangle$ is similar to that in the disordered potential system, so $\langle E_v \rangle$ increases for small $U$, decreases for large $U$, respectively.

For TIP in the 1D Harper model, Shepelyansky et al.\textsuperscript{7,15,16} found that the interaction would induce localization effect for all $\lambda$. At the same time, Evangelou and Katsanou\textsuperscript{8} found that, in the extended($\lambda < 2$) and the critical($\lambda = 2$) regimes, the velocity and the diffusion coefficient of TIP will decreases due to the localized pairing states. In the localization regime($\lambda > 2$), they found that propagation enhancement for small interaction and strong localization for large interaction, as in disorder systems. Apparently there are discrepancies in their results at the localization regime. Comparing to our results, in the extended and the critical regimes, we
find $\langle E_v \rangle$ decreases with $U$, which agrees with both of their conclusions that the interaction can induce localization effect.\cite{24,25,26} In the localized regime, we find $\langle E_v \rangle$ increases for small $U$ and decreases for large $U$, respectively, which is consistent with the results of Evangelou and Katsanó that the interaction has different effects on localization properties at small and large $U$.

C. TIP in a slowly varying potential chain

Next we study TIP moving in a 1D system based on the slowly varying potential model.\cite{24,25,26} From Eq.(1), the eigenvalue equation can be described by

$$[\lambda \cos(\pi \alpha n_1 + \beta_1) + \lambda \cos(\pi \alpha n_2 + \beta_2) + U \delta_{n_1,n_2}]\psi_{n_1,n_2} + \ell(\psi_{n_1+1,n_2} + \psi_{n_1-1,n_2} + \psi_{n_1,n_2+1} + \psi_{n_1,n_2+1}) = E\psi_{n_1,n_2},$$

(14)

here $\lambda$, $\alpha$ and $\nu$ are positive numbers. For $\alpha$ irrational with $v \geq 2$ or $v = 1$, this is equivalent to the models discussed in Sec. III (A) and (B), respectively. For $0 < v < 1$, in the absence of the interaction $U$, it is well known\cite{24} that there are two mobility edges at $E_c = \pm(2.0 - \lambda)$ provided $\lambda < 2.0$. It is found that extended states are in the middle of the band ( $|E| < 2.0 - \lambda$ ) and localized states are at the band edge ( $2.0 - \lambda < |E| < 2.0 + \lambda$ ). In other words, for $\lambda < 2.0$, the extended and localized eigenstates coexist in contrast to the models studied in Sec. III (A) and (B). For $\lambda > 2.0$, all states are found to be localized. So in this model there are always localized eigenstates at $\lambda \neq 0$. Obviously the spectrum properties are different from that for the Anderson model and the Harper model.

Fig.7 shows the spectrum-averaged von Neumann entropy $\langle E_v \rangle$ as a function of potential strength $\lambda$ at $U = 0$. The dashed line is linearly fitted for the corresponding data at $0 < \lambda \leq 2$. Here $\pi \alpha = 0.2$, $\nu = 0.7$ and $N = 89$.

![FIG. 7: The spectrum-averaged von Neumann entropy $\langle E_v \rangle$ as a function of potential strength $\lambda$ at $U = 0$. The dashed line is linearly fitted for the corresponding data at $0 < \lambda \leq 2$. Here $\pi \alpha = 0.2$, $\nu = 0.7$ and $N = 89.$](image)

IV. CONCLUSIONS AND DISCUSSIONS

With the help of von Neumann entropy, we have studied the effect of the on-site interaction $U$ on the localization properties of TIP in 1D disordered, quasiperiodic and slowly varying potential systems, respectively.

For TIP in a disordered potential chain and a slowly varying potential chain, as $U$ increases from zero, we find that at first $\langle E_v \rangle$ increases for small $U$, then decreases as $U$ gets large. It means that there are propagation enhancement for small interaction and strong localization for large interaction. For TIP in 1D Harper model with particles in the extended($\lambda < 2$) and critical($\lambda = 2$) regimes, $\langle E_v \rangle$ decreases as $U$ increases, which indicates that the interaction would induce localization effect, while in the localized regime($\lambda > 2$), the $\langle E_v \rangle$ as a function of $U$ is similar to that for TIP in the disordered potential chain. From our studies, we find that $\langle E_v \rangle$ is a suitable quantity to describe the localization properties for two-particle systems.
Summarizing all results from the three models, we can conclude that provided localized eigenstates at single-particle case exist, the delocalization (localization) effect happens for small interactions (large interactions), while single particle states are extended or critical, the interaction always induces the localization effect. According to our results, we propose a consistent interpretation of the discrepancies between previous numerical results.

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Von Neumann entropy and localization properties of two interacting particles in one-dimensional nonuniform systems

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Abstract

With the help of von Neumann entropy, we study numerically the localization properties for two interacting particles (TIP) with the on-site interaction in one-dimensional disordered, quasiperiodic and slowly varying potential systems, respectively. We find that for TIP in disordered and slowly varying potential systems, the spectrum-averaged von Neumann entropy \( \langle E_v \rangle \) first increases with interaction \( U \) until its peaks, then decreases as \( U \) gets larger. For TIP in the Harper model, the functions of \( \langle E_v \rangle \) versus \( U \) are different for particles in extended and localized regimes. Our numerical results indicate that for these two-particle systems, the von Neumann entropy is a suitable quantity to characterize the localization properties of particle states. Moreover, our studies propose a consistent interpretation of the discrepancies between previous numerical results.

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I. INTRODUCTION

Interacting uniform electronic systems\cite{1} and non-interacting disordered electronic systems\cite{2, 3} are two of the most intriguing, albeit difficult, subjects in condensed matter physics. As a result of the complexity of the simultaneous presence of randomness and interactions, few definitive results are known.\cite{4, 5} To understand the effects of electrons interaction on the localization properties in a random potential, Shepelyansky proposed some years earlier that it would be worthwhile to consider the simple case of two interacting particles(TIP) in a one-dimensional (1D) random potential.\cite{6} Subsequently, extensive efforts have been devoted to TIP in various systems.\cite{7, 8, 9, 10, 11, 12, 14} In particular, two interacting electrons with total spin zero in a 1D Harper model,\cite{8} in Fibonacci and Thue-Morse lattices\cite{9} are studied. The behavior of TIP has been studied using the time evolution of wave packets,\cite{6, 7, 8, 9} exact diagonalization,\cite{8, 10} Green function,\cite{11, 12, 13} and transfer-matrix,\cite{14} etc. Due to different definitions of the localization length for TIP and different methods applied, there are discrepancies about the effect of the combination of disorder and interaction. For example, for TIP in 1D disordered potentials, Shepelyansky\cite{6} and others\cite{11, 12} have found that for small interaction strengths, the two-particle interaction can enhance the Anderson localization length, while Römer and Schreiber\cite{14} found no enhancement of the localization length when the system size grows to infinity. Evangelou et al. have pointed out that stronger localization occurs at large interaction when compared to the noninteracting case.\cite{10} At the same time, for TIP in a 1D Harper model, it was found that the interaction would induce localization effect,\cite{7, 15, 16} while Evangelou and Katsanos\cite{8} found that the effects of particle interactions are different for electrons in extended and localized regimes.

On the other hand, quantum entanglement, which attracting much attention in quantum information\cite{17} has been extensively applied in condensed matter physics.\cite{18, 19, 20, 21, 22, 23} For examples, quantum entanglement measured by the von Neumann entropy was studied in the Hubbard model for the dimer case\cite{18}, in the extended Hubbard model for different band filling\cite{20}, in quantum small-world networks\cite{22}, and in low-dimensional semiconductor systems\cite{23}. It was found that the von Neumann entropy is suitable for analyzing the interplay between itinerant and localized features\cite{18}, as well as characterizing quantum phase transition\cite{20, 21} and the localization-delocalization transition of electron
In this paper, we perform a detailed study of the von Neumann entropy for TIP in 1D disordered and quasiperiodic systems respectively, taking into account different on-site interactions $U$ at various on-site potential strengths. We find that for TIP in disordered and slowly varying potential systems, the spectrum-averaged von Neumann entropy $\langle E_v \rangle$ first increases with interaction $U$ until its peaks, then decreases as $U$ gets larger. For TIP in the 1D Harper model, the functions of $\langle E_v \rangle$ versus $U$ are different for particles in extended and localized regimes. Finally we study a two-particle system based on the slowly varying potential model [24, 25, 26] From these studies, we can conclude that for TIP systems, the von Neumann entropy is a suitable quantity to characterize the localization properties of particle states.

The paper is organized as follows. In the next section the von Neumann entropy is described. In Sec. III the numerical results for TIP in 1D disordered, quasiperiodic, and slowly varying potential systems are presented, respectively. And we present our conclusions and discussions in Section IV.

II. TIP MODELS AND VON NEUMANN ENTROPY

A. TIP models

Following recent literature [6, 7, 12, 14, 15, 16] the eigenvalue equation for the TIP in 1D system can be written as

$$
(\varepsilon_{n_1} + \varepsilon_{n_2} + U \delta_{n_1,n_2})\psi_{n_1,n_2} + t(\psi_{n_1+1,n_2} + \psi_{n_1-1,n_2} + \psi_{n_1,n_2+1} + \psi_{n_1,n_2-1}) = E\psi_{n_1,n_2},
$$

where $\varepsilon_n$ is the on-site potential, $t$ is a nearest-neighbor hopping integral and $U$ characterizes the on-site interaction between particles.

Eq. (1) actually can describe the behaviors both bosons and fermions, i.e., two spinless bosons or two electrons with opposite spins.

For spinless bosons with the on-site interaction, the tight-binding Hamiltonian can gen-
erally be described by

\[ H = t \sum_{n=1}^{N-1} (c_{n}^{\dagger}c_{n+1} + c_{n+1}^{\dagger}c_{n}) + \sum_{n=1}^{N} \varepsilon_{n}c_{n}^{\dagger}c_{n} \]
\[ + U \sum_{n=1}^{N} (c_{n}^{\dagger}c_{n})(c_{n}^{\dagger}c_{n}), \]  

(2)

where \( c_{n}^{\dagger} (c_{n}) \) is the boson creation(annihilation) operator of the \( n \)th site. The generic eigenstate for two spinless bosons is the superposition

\[ |\alpha\rangle = \sum_{n_{1} \leq n_{2}} \psi_{n_{1},n_{2}}^{\alpha} |n_{1}, n_{2}\rangle = \sum_{n_{1} \leq n_{2}} \psi_{n_{1},n_{2}}^{\alpha} c_{n_{1}}^{\dagger}c_{n_{2}}^{\dagger} |0\rangle, \]  

(3)

where \(|0\rangle\) is the vacuum and \( \psi_{n_{1},n_{2}}^{\alpha} \) is the amplitude of wave function. From Eqs.(2) and (3) we can obtain the eigenvalue equation (1).

For electrons with the on-site interaction, the tight-binding Hamiltonian can be described by [8, 9, 10]

\[ H = t \sum_{n=1}^{N} \sum_{\sigma} (c_{n,\sigma}^{\dagger}c_{n+1,\sigma} + c_{n+1,\sigma}^{\dagger}c_{n,\sigma}) \]
\[ + \sum_{n=1}^{N} \sum_{\sigma} \varepsilon_{n}c_{n,\sigma}^{\dagger}c_{n,\sigma} + U \sum_{n=1}^{N} c_{n,\uparrow}^{\dagger}c_{n,\downarrow}^{\dagger}c_{n,\downarrow}c_{n,\uparrow}, \]

(4)

where \( c_{n,\sigma}^{\dagger} (c_{n,\sigma}) \) is the electron creation(annihilation) operator for the electron at the \( n \)th site with spin \( \sigma = \pm \frac{1}{2} \). For two electrons the Hilbert space can be conveniently divided into a singlet subspace with total spin \( S = 0 \) and a triplet subspace with total spin \( S = 1 \), respectively. Since the triplet subspace permits no double occupation, it is not affected by the on-site interaction. In order to analyze the effect of the on-site interaction \( U \), we will consider the case of the two electrons with opposite spins, i.e., the singlet subspace. In a chain with \( N \) sites the singlet subspace is spanned by \( N(N+1)/2 \) spatially symmetric basis functions

\[ |n_{1}, n_{2}\rangle \]
\[ = \begin{cases} 
\frac{1}{\sqrt{2}} (c_{n_{1},\uparrow}^{\dagger}c_{n_{2},\downarrow}^{\dagger} + c_{n_{2},\uparrow}^{\dagger}c_{n_{1},\downarrow}^{\dagger}) |0\rangle & \text{for } n_{1} < n_{2}, \\
(c_{n_{1},\uparrow}^{\dagger}c_{n_{2},\downarrow}^{\dagger}) |0\rangle & \text{for } n_{1} = n_{2}, 
\end{cases} \]

(5)

where \(|0\rangle\) is the vacuum. An eigenstate for two electrons with the spatially symmetric wave functions is in general the superposition

\[ |\alpha\rangle = \sum_{n_{1} \leq n_{2}} \phi_{n_{1},n_{2}}^{\alpha} |n_{1}, n_{2}\rangle, \]  

(6)
where $\phi_{n_1,n_2}^\alpha$ is the amplitude of wave function. By making the transformation

$$
\psi_{n_1,n_2}^\alpha = \begin{cases} 
\phi_{n_1,n_2}^\alpha & \text{for } n_1 < n_2, \\
\sqrt{2}\phi_{n_1,n_2}^\alpha & \text{for } n_1 = n_2,
\end{cases}
$$

the eigenvalue equation obtained from Eqs. [4–6] can be written as equation (1).

In the following our numerical method is described for bosons. The extension for fermions is straightforward.

## B. von Neumann entropy

For the two particles in the system we are studying, there are three local states at each site, $|2\rangle_n, |1\rangle_n, |0\rangle_n$, corresponding to the state with two, one or zero particles at the $n$th site, respectively. The local density matrix $\rho_n$ is defined [18, 20] by

$$
\rho_n = z_{2n} |2\rangle_{nn} \langle 2| + z_{1n} |1\rangle_{nn} \langle 1| + (1 - z_{1n} - z_{2n}) |0\rangle_{nn} \langle 0|.
$$

(7)

For two spinless bosons,

$$
z_{2n} = \langle \alpha | c_n^\dagger c_n c_n^\dagger c_n | \alpha \rangle = \psi_{n,n}^\alpha \psi_{n,n}^{*\alpha}
$$

(8)

and

$$
z_{1n} = \langle \alpha | c_n^\dagger c_n | \alpha \rangle - 2z_{2n} \\
= \sum_{m(m>n)} N \psi_{n,m}^\alpha \psi_{n,m}^{*\alpha} + \sum_{m'(m'<n)} N \psi_{m',n}^\alpha \psi_{m',n}^{*\alpha}.
$$

(9)

Consequently, the corresponding von Neumann entropy related to $n$th site is

$$
E_{vn}^\alpha = -(1 - z_{1n} - z_{2n}) \log_2(1 - z_{1n} - z_{2n}) \\
- z_{1n} \log_2 z_{1n} - z_{2n} \log_2 z_{2n}.
$$

(10)

For nonuniform systems, the value of $E_{vn}^\alpha$ depends on the site position $n$. At an eigenstate $\alpha$, we define a site-averaged von Neumann entropy

$$
E_{v}^\alpha = \frac{1}{N} \sum_{n=1}^{N} E_{vn}^\alpha.
$$

(11)
For a delocalized state that all $\psi_{n_1,n_2}^\alpha = \frac{1}{\sqrt{N(N+1)/2}}$ for all $n_1 \leq n_2$, this definition gives $E_v^\alpha \approx \frac{2}{N} \log_2 \frac{N}{2}$ at large $N$, while for a localized state that $\psi_{n_1,n_2}^\alpha = 1$ at given $n_1^0$ and $n_2^0$, $E_v^\alpha = 0$. In this paper, all the values of $E_v^\alpha$ are scaled by $\frac{2}{N} \log_2 \frac{N}{2}$. From the two examples, we know that the scaled $E_v^\alpha$ is close to 1 for eigenstates are extended and almost vanishes for eigenstates are localized. Henceforth, we omit “scaled” for simplicity.

In order to analyze the influence of system parameters like the on-site interaction $U$, on the von Neumann entropy for all the eigenstates, we define a spectrum-averaged von Neumann entropy as a further gross measure
\[
\langle E_v \rangle = \frac{1}{M} \sum_{\alpha} E_v^\alpha, \tag{12}
\]
where $M$ is the number of all the eigenstates.

### III. NUMERICAL RESULTS

From now we consider only the repulsive interaction ($U > 0$). We directly diagonalize the eigenvalue Eq. (1) with the periodic boundary condition at finite system sizes and obtain all eigenvalues $E_\alpha$ and the corresponding eigenvectors $|\alpha\rangle$. Without loss of generality, the hopping integral $t$ is taken as units of energy. From the formulas (7—12), we then can obtain the site-averaged von Neumann entropy $E_v^\alpha$ and the spectrum-averaged von Neumann entropy $\langle E_v \rangle$, respectively.

#### A. TIP in a disordered potential chain

For TIP in a disordered potential chain, the on-site potential $\varepsilon_n$ in Eq.(3) are random variables uniformly distributed with $[-W,W]$. Here $W$ characterizes the degree of on-site disorder as in the Anderson model. For this model, we calculate the spectrum-averaged von Neumann entropy $\langle E_v \rangle$ with a given set of parameters $W$ and $U$. For every set of parameters $W$ and $U$, the disorder average is taken over 100 samples. More samples simply give similar results.

For 1D Anderson model in the absence of the interaction ($U = 0$), it is well known that all the eigenstates are localized and the one-particle localization length is $\xi \approx \frac{25t^2}{W^2}$ at the energy band center. Fig. 1 gives the spectrum-averaged von Neumann entropy $\langle E_v \rangle$ versus
FIG. 1: The spectrum-averaged von Neumann entropy $\langle E_v \rangle$ versus the disorder $W$ for $U = 0$ at $N = 90$.

FIG. 2: The relation between the site-averaged von Neumann entropy $E^\alpha_v$ and the corresponding $\xi^\alpha$ at $W = 1$ and $U = 0$ for a typical sample. The $E^\alpha_v$ versus $\log_{10} \xi^\alpha$ is plotted in the inset.

the disorder parameter $W$. It shows that $\langle E_v \rangle$ monotonically decreases as $W$ increases, reflecting the trivial localization effect of the on-site disorder in the model. To find the correlation between $\langle E_v \rangle$ and the localization properties for TIP systems, we also study the inverse participation ratio (IPR) [15], defined by $\xi^\alpha = \left( \frac{N(N+1)}{2} \sum_{n_1 \leq n_2} |\psi^\alpha_{n_1, n_2}|^4 \right)^{-1}$, which gives the ratio of lattice sites occupied by particles to all lattice sites at an eigenstate $\alpha$. The larger $\xi^\alpha$ is, the more delocalized the eigenstate is. In Fig. 2 we plot the site-averaged von Neumann entropy $E^\alpha_v$ versus $\xi^\alpha$ at $U = 0$ for a typical sample with $W = 1$. On the whole, $E^\alpha_v$ increases logarithmically with $\xi^\alpha$ as can been seen in the inset of Fig. 2, so von Neumann entropy can well reflect the localization properties of two-particle eigenstates.

For $U > 0$, the spectrum-averaged von Neumann entropy $\langle E_v \rangle$ as a function of $U$ at $W = 1, 2, 3$ are plotted in Fig. 3. The results are similar for other $W$. For all $W$, we find that
FIG. 3: The spectrum-averaged von Neumann entropy $\langle E_v \rangle$ as a function of interaction strengths $U$ for (a) $W = 1$, (b) $W = 2$ and (c) $W = 3$, respectively. Here $N = 90$. $\langle E_v \rangle$ first increases until its peak as $U$ increases from zero, then decreases as $U$ gets larger. There is a $U^*$, at which $\langle E_v \rangle$ is equal to that at $U = 0$. When $U$ is smaller (greater) than $U^*$, $\langle E_v \rangle$ is larger (smaller) than the value of $\langle E_v \rangle$ at $U = 0$. To understand the effect of the interaction $U$ on the von Neumann entropy, we calculate the site-averaged von Neumann entropy $E^\alpha_v$ and illustrate the results in Fig. 4 at different $U$ for $W = 1$. It shows that only a small portion of the two-particle eigenstates have its value of $E^\alpha_v$ changed by the interaction $U$. For small $U$, most of the newly created eigenstates are in the main band and the corresponding $E^\alpha_v$ are larger than that in the noninteracting case, while for large $U$, most of them are above the top of the main band and the corresponding $E^\alpha_v$ are smaller than that for particles without interaction. Therefore, the varying $\langle E_v \rangle$ with $U$ is not monotonic as shown in Fig. 3. These two competing effects reach an equilibrium at $U = U^*$.

For TIP in 1D disordered potentials with $U \leq t$ Shepelyansky [6] and others [11, 12] have found that the Anderson localization length increases with $U$. It agrees with our conclusions that for small $U$, $\langle E_v \rangle$ increases with $U$. For large interaction $U$, Evangelou et al. [10] have pointed out that stronger localization occurs when compared to the noninteracting
FIG. 4: The site-averaged von Neumann entropy $E_{\alpha}$ and the corresponding eigenenergy $E_{\alpha}$ at different $U$ for a typical sample at $W = 1$. Here $N = 90$ and the spectrum-averaged von Neumann entropy $\langle E_v \rangle = 0.8431, 0.8556$ and $0.7916$ for $U = 0, 2$ and 6, respectively. This case, because at $U >> t$ interaction can significantly modify the energy spectrum \cite{6} and the created eigenstates have the comparatively small localization lengths.\cite{10} The result is consistent with ours that for $U > U^*$, the values of $\langle E_v \rangle$ are smaller than that at $U = 0$.

\section{B. Tip in a quasiperiodic potential chain}

From Eq. (11), the eigenvalue equation for TIP in a quasiperiodic potential chain based on the Harper model can be described by \cite{7, 8}

\begin{align}
[\lambda \cos(2\pi \sigma n_1 + \beta_1) + \lambda \cos(2\pi \sigma n_2 + \beta_2) + U\delta_{n_1,n_2}]\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{align}

here the parameter $\lambda$ characterizes the strength of the quasiperiodic potential, $\sigma$ and $\beta_{1,2}$ are constants. As a typical case, we set $\sigma = (\sqrt{5} - 1)/2, \beta_1 = \beta_2 = 0$. As is customary in the context of quasiperiodic system, the value of $\sigma$ may in fact be approximated by the ratio of successive Fibonacci numbers—$F_n = F_{n-2} + F_{n-1}$. In this way, choosing $\sigma = F_{n-1}/F_n \approx (\sqrt{5} - 1)/2$ and the system size $N = F_n$, we can obtain the periodic approximant for the quasiperiodic potential. In our calculation, $N$ is chosen as Fibonacci numbers 34, 55 and 89, respectively.

In the absence of the interaction $U$ it is found \cite{28, 29} that that for $\lambda < 2$ the spectrum becomes continuous and all eigenstates are extended. For $\lambda > 2$ the spectrum is pure point.
and all eigenstates are exponentially localized. For $\lambda = 2$ the situation is critical with a singular-continuous multifractal spectrum and power law localized eigenstates. Metal-insulator transition can occur at $\lambda = 2$. Obviously they are different from these for the 1D Anderson model where all eigenstates are localized for $W \neq 0$.

Fig. 5(a) shows the spectrum-averaged von Neumann entropy $\langle E_v \rangle$ with respect to the quasiperiodic potential strength $\lambda$ at $U = 0$. We observe that there is a sharp decrease of $\langle E_v \rangle$ near the critical value $\lambda_c = 2$. For $\lambda < \lambda_c$ which corresponds to extended states, all $\langle E_v \rangle$ are around 1, while for $\lambda > \lambda_c$ corresponding to localized states, all $\langle E_v \rangle$ are far less than 1. In Fig. 5(b) we plot $\langle E_v \rangle$ as a function of $\lambda$ at $U = 0$ for $N = 34$, 55 and 89. The curves cross at $\lambda \approx \lambda_c$. The crossing point separates the extended($\lambda < \lambda_c$) and the localized($\lambda > \lambda_c$) regimes.

For $U > 0$, the spectrum-averaged von Neumann entropy $\langle E_v \rangle$ as a function of $U$ at different $\lambda$ are shown in Fig. 6. Here we choose $\lambda = 1$, 2 and 3 as examples for extended, critical and localized regimes, respectively. At $\lambda = 1$ and $\lambda = 2$, $\langle E_v \rangle$ monotonically decreases when $U$ increases from zero. At $\lambda = 3$ $\langle E_v \rangle$ increases for small $U$ and decreases for large $U$, respectively, which is similar to that shown in Fig. 3 for TIP in a disordered potential chain. For $\lambda$ in extended and localized regimes, $\langle E_v \rangle$ as a function of $U$ are similar to that for $\lambda = 1$ and $\lambda = 3$, respectively. We also find that at the extended and critical regimes, the newly created eigenstates due to the interaction have small $E_v^a$, which will reduce the value of $\langle E_v \rangle$. At the localized regime, the effect of interaction $U$ on $\langle E_v \rangle$ is similar to that in the disordered potential system, so $\langle E_v \rangle$ increases for small $U$, decreases
FIG. 6: The spectrum-averaged von Neumann entropy $\langle E_v \rangle$ as a function of interaction strengths $U$ for (a) $\lambda = 1$, (b) $\lambda = 2$ and (c) $\lambda = 3$, respectively. Here $N = 89$.

For TIP in the 1D Harper model, Shepelyansky et al. [7, 15, 16] found that the interaction would induce localization effect for all $\lambda$. At the same time, Evangelou and Katsanos [8] found that, in the extended ($\lambda < 2$) and the critical ($\lambda = 2$) regimes, the velocity and the diffusion coefficient of TIP will decreases due to the localized pairing states. In the localization regime ($\lambda > 2$), they found that propagation enhancement for small interaction and strong localization for large interaction, as in disorder systems. Apparently there are discrepancies in their results at the localization regime. Comparing to our results, in the extended and the critical regimes, we find $\langle E_v \rangle$ decreases with $U$, which agrees with both of their conclusions that the interaction can induce localization effect. [7, 8, 15, 16] In the localized regime, we find $\langle E_v \rangle$ increases for small $U$ and decreases for large $U$, respectively, which is consistent with the results of Evangelou and Katsanos [8] that the interaction has different effects on localization properties at small and large $U$. 
FIG. 7: The spectrum-averaged von Neumann entropy \( \langle E_v \rangle \) as a function of potential strength \( \lambda \) at \( U = 0 \). The dashed line is linearly fitted for the corresponding data at \( 0 < \lambda \leq 2 \). Here \( \pi \alpha = 0.2 \), \( v = 0.7 \) and \( N = 89 \).

C. TIP in a slowly varying potential chain

Next we study TIP moving in a 1D system based on the slowly varying potential model.\[24, 25, 26\] From Eq.(1), the eigenvalue equation can be described by

\[
[\lambda \cos(\pi \alpha n_1^v + \beta_1) + \lambda \cos(\pi \alpha n_2^v + \beta_2) + U \delta_{n_1,n_2}]\psi_{n_1,n_2} \\
+ t(\psi_{n_1+1,n_2} + \psi_{n_1-1,n_2} + \psi_{n_1,n_2+1} + \psi_{n_1,n_2-1}) \\
= E\psi_{n_1,n_2},
\]

(14)

here \( \lambda \), \( \alpha \) and \( v \) are positive numbers. For \( \alpha \) irrational with \( v \geq 2 \) or \( v = 1 \), this is equivalent to the models discussed in Sec. III (A) and (B), respectively. For \( 0 < v < 1 \), in the absence of the interaction \( U \), it is well known [24] that there are two mobility edges at \( E_c = \pm(2.0 - \lambda) \) provided \( \lambda < 2.0 \). It is found that extended states are in the middle of the band ( \( |E| < 2.0 - \lambda \) ) and localized states are at the band edge ( \( 2.0 - \lambda < |E| < 2.0 + \lambda \) ). In other words, for \( \lambda < 2.0 \), the extended and localized eigenstates coexist in contrast to the models studied in Sec. III (A) and (B). For \( \lambda > 2.0 \), all states are found to be localized. So in this model there are always localized eigenstates at \( \lambda \neq 0 \). Obviously the spectrum properties are different from that for the Anderson model and the Harper model.

Fig.7 shows the spectrum-averaged von Neumann entropy \( \langle E_v \rangle \) as a function of \( \lambda \) at \( U = 0 \). For \( 0 < \lambda \leq 2 \) the data can be well fitted into a line. For \( \lambda > 2 \) all data points lie far away from the proposed line, i.e., there is an abrupt decrease in \( \langle E_v \rangle \) at the critical parameter \( \lambda = 2 \). The critical parameter separates the localized regime\((\lambda > 2)\)
FIG. 8: The spectrum-averaged von Neumann entropy $\langle E_v \rangle$ as functions of interaction strengths $U$ at different $\lambda$. Here $\pi\alpha = 0.2$, $v = 0.7$ and $N = 89$.

and the regime where the localized and extended eigenstates coexist ($\lambda < 2$). This result is consistent with the spectrum properties for the model, so the spectrum-averaged von Neumann entropy $\langle E_v \rangle$ can describe the localization properties for two-particle systems.

Fig. 8 shows the spectrum-averaged von Neumann entropy $\langle E_v \rangle$ versus the interaction $U$ at $\lambda \leq 2$. The results are similar to that for $\lambda > 2$. We again find that for all $\lambda$, as $U$ increases, $\langle E_v \rangle$ increases for small $U$, decreases for large $U$, respectively, similar to that shown in Fig. 3 for TIP in a disordered potential chain. It indicates that propagation enhancement for small interaction and strong localization for large interaction. In other words, as long as there are localized eigenstate at single-particle models, the effect of interaction on the localization properties of TIP is similar to that in disorder systems.

IV. CONCLUSIONS AND DISCUSSIONS

With the help of von Neumann entropy, we have studied the effect of the on-site interaction $U$ on the localization properties of TIP in 1D disordered, quasiperiodic and slowly varying potential systems, respectively.

For TIP in a disordered potential chain and a slowly varying potential chain, as $U$ increases from zero, we find that at first $\langle E_v \rangle$ increases for small $U$, then decreases as $U$ gets large. It means that there are propagation enhancement for small interaction and stronger localization for large interaction. For TIP in 1D Harper model with particles in the extended ($\lambda < 2$) and critical ($\lambda = 2$) regimes, $\langle E_v \rangle$ decreases as $U$ increases, which indicates that the interaction would induce localization effect, while in the localized regime ($\lambda > 2$),
the $\langle E_v \rangle$ as a function of $U$ is similar to that for TIP in the disordered potential chain. From our studies, we find that $\langle E_v \rangle$ is a suitable quantity to describe the localization properties for two-particle systems.

Summarizing all results from the three models, we can conclude that provided localized eigenstates at single-particle case exist, the delocaliation (localization) effect happens for small interactions (large interactions), while single particle states are extended or critical, the interaction always induces the localization effect. According to our results, we propose a consistent interpretation of the discrepancies between previous numerical results.

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