# Uncertainties of clock and shift operators for an electron in one-dimensional nonuniform lattice systems*

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The clock operator $U$ and shift operator $V$ are higher-dimensional Pauli operators. Just recently, tighter uncertainty relations with respect to $U$ and $V$ were derived, and we apply them to study the electron localization properties in several typical one-dimensional nonuniform lattice systems. We find that uncertainties $\Delta U^2$ are less than, equal to, and greater than uncertainties $\Delta V^2$ for extended, critical, and localized states, respectively. The lower bound LB of the uncertainty relation is relatively large for extended states and small for localized states. Therefore, in combination with traditional quantities, for instance inverse participation ratio, these quantities can be as novel indexes to reflect Anderson localization.

**Keywords:** uncertainties, Anderson localization, nonuniform lattice systems, mobility edge

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## 1. Introduction

The Heisenberg uncertainty principle is one of the most important ideals in quantum mechanics.[1] It is often expressed by no-go statements.[2] In a general expression, two noncommuting observables do not simultaneously have well-defined values. This property has no classical analogue, so it is a basic difference between classical and quantum mechanics. As is well known, the principle plays a fundamental role in quantum theory, such as nonlocality,[3] quantum measurements,[4] and quantum phase transitions.[5] Furthermore, it has important applications in current quantum technology, for instance, entanglement detection,[6] quantum cryptography,[7] and quantum metrology.[8]

In fact, the principle was first proposed by Heisenberg,[1] and originally formulated precisely by Kennard[9] as $\Delta x\Delta p \geq \hbar/2$, where the uncertainties are quantified by standard deviations of the position and momentum. Subsequently, Robertson[10] generalized it to arbitrary pairs of noncommuting observables $A$ and $B$, which is given by $\Delta A\Delta B \geq \langle\Psi|[A,B]|\Psi\rangle/2$ in state $|\Psi\rangle$. Just recently, several uncertainty relations with respect to the clock operator $U$ and shift operator $V$ were derived.[11] The expressions of $U$ and $V$ are given by[11–14]

$$U = \sum_{j=-[\frac{d}{2}]}^{[\frac{d-1}{2}]} \mathrm{e}^{+\mathrm{i}2\pi j/d}|j\rangle\langle j|, \tag{1}$$

$$V = \sum_{k=-[\frac{d}{2}]}^{[\frac{d-1}{2}]} \mathrm{e}^{-\mathrm{i}2\pi k/d}|\tilde{k}\rangle\langle\tilde{k}|, \tag{2}$$

where $[Z]$ is the integer part of $Z$. Here, $\{|j\rangle\}_{j=-[\frac{d}{2}]}^{[\frac{d-1}{2}]}$ and $\{|\tilde{k}\rangle\}_{k=-[\frac{d}{2}]}^{[\frac{d-1}{2}]}$ are complete orthonormal bases in $d$-dimensional Hilbert space, respectively. The two bases are related by the discrete Fourier transform (DFT)

$$|j\rangle = \sum_{k=-[\frac{d}{2}]}^{[\frac{d-1}{2}]} \frac{\mathrm{e}^{-\mathrm{i}2\pi jk/d}}{\sqrt{d}}|\tilde{k}\rangle, \qquad |\tilde{k}\rangle = \sum_{j=-[\frac{d}{2}]}^{[\frac{d-1}{2}]} \frac{\mathrm{e}^{+\mathrm{i}2\pi jk/d}}{\sqrt{d}}|j\rangle.$$

Based on the DFT, the operators $U$ and $V$ can be rewritten as $U = \sum_{k=-[\frac{d}{2}]}^{[\frac{d-1}{2}]} \widetilde{|k+1\rangle}\langle\tilde{k}|$ and $V = \sum_{j=-[\frac{d}{2}]}^{[\frac{d-1}{2}]} |j+1\rangle\langle j|$. In fact, the expressions of $U$ and $V$ in Eqs. (B2) and (B4) of Ref. [11] are originally from Eqs. (5) and (7) of Ref. [14]. They should be the same. However, they are not completely the same. We have checked them and found that there exist typo errors in Eqs. (B2) and (B4) of Ref. [11]. Physically, the operators $U$ and $V$ are the non-Hermitian generalization of the traditional 2-dimensional Pauli operators to higher-dimensional ones.[12,13] The definitions of clock operator $U$ and shift operator $V$ are independent of the Hamiltonian, so it can be applied to general quantum systems.

The uncertainties of $U$ and $V$ are respectively given by[11,14]

$$\Delta U^2 = 1 - |\langle\Psi|U|\psi\rangle|^2, \tag{3}$$

$$\Delta V^2 = 1 - |\langle\Psi|V|\Psi\rangle|^2, \tag{4}$$

where $|\Psi\rangle$ is the wave function of a quantum state and $0 \leq \Delta U^2 \leq 1$ ($0 \leq \Delta V^2 \leq 1$). One of the tighter uncertainty rela-

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tions that they obey is[11]

$$\Delta U^2 + \Delta V^2 \geq 1 + |\langle \Psi_U | \Psi_V \rangle|^2 - 2\cos\Phi |\Delta^{(3)}|, \quad (5)$$

where $\Delta^{(3)} = \langle \Psi | \Psi_U \rangle \langle \Psi_U | \Psi_V \rangle \langle \Psi_V | \Psi \rangle$, $|\Psi_U\rangle = U|\Psi\rangle$, $|\Psi_V\rangle = V|\Psi\rangle$ and $\Phi = \arg \Delta^{(3)}$. We define the right side in the inequation is the lower bound

$$\mathrm{LB} = 1 + |\langle \Psi_U | \Psi_V \rangle|^2 - 2\cos\Phi |\Delta^{(3)}|. \quad (6)$$

On the other hand, Massar and Spindel pointed out that the uncertainties $\Delta U^2$ and $\Delta V^2$ can measure the localization properties of quantum states.[14] However, they do not give the corresponding explicit relation. Besides, Bagchi and Pati pointed out that LB depends on quantum states.[11] However, they did not study the relation between the values of LB and state localization properties. In this paper, we fill the gaps just mentioned. In the Anderson localization phenomenon,[15–20] a state $|\Psi\rangle$ may be localized, critical or delocalized, which depend on models and model parameters. There are many typical and extensively studied one-dimensional models, such as the slowly varying potential model,[21–23] the deterministic nearest-neighbor tight-binding models with exact mobility edges,[24] and the random-dimer potential model.[25–27] It is interesting how these quantities, including $\Delta U^2$ and $\Delta V^2$ and LB, are related to Anderson localization.

The rest of the paper is organized as follows. In Section 2, we introduce the tight-binding Hamiltonian for a single electron in one-dimensional (1D) lattice systems. In Section 3, we analyze the behaviors of $\Delta U^2$ and $\Delta V^2$, and LB in three typical models. Finally, we give a summary of our main results.

## 2. The tight-binding Hamiltonian for a single electron in one-dimensional lattice systems

A single electron in 1D lattice systems is considered. The corresponding tight-binding Hamiltonian is described by

$$H = \sum_{j=-[\frac{d}{2}]}^{[\frac{d-1}{2}]} \varepsilon_j |j\rangle\langle j| + \sum_{j=-[\frac{d}{2}]}^{[\frac{d-1}{2}]} t(|j\rangle\langle j+1| + |j+1\rangle\langle j|), \quad (7)$$

where $\varepsilon_j$ is the on-site potential on the $j$th site, $t$ is a nearest-neighbor hopping integral, and $d$ is the lattice size. Further, $|j\rangle = c_j^\dagger |0\rangle$, where $c_j^\dagger$ is the creation operator of $j$th site and $|0\rangle$ is the vacuum. Models are specified by the choice rules of $\{\varepsilon_j\}$. The system can also be described by the tight-binding equation

$$\varepsilon_j \psi_j + t(\psi_{j+1} + \psi_{j-1}) = E\psi_j. \quad (8)$$

The general wave function, i.e., eigenstate $|\Psi_\beta\rangle$ with eigenenergy $E_\beta$ for Hamiltonian in Eq. (7) can be written as the superposition

$$|\Psi_\beta\rangle = \sum_{j=-[\frac{d}{2}]}^{[\frac{d-1}{2}]} \psi_j^\beta |j\rangle, \quad (9)$$

where $\psi_j^\beta$ is the amplitude of the $\beta$th wave function at $j$th site.

## 3. Numerical results

In numerical calculations, for different models, we directly diagonalize the tight-binding equation (8) with the periodic boundary condition at finite system sizes and obtain all eigenenergies $E_\beta$ and corresponding eigenstates $|\Psi_\beta\rangle$. From Eqs. (3), (4), and (6), we obtain $\Delta U^2$ and $\Delta V^2$, as well as LB. For simplicity and convenience, based on Eqs. (3) and (4), we define a reduced relative uncertainty

$$U_\mathrm{r} = \frac{\Delta U^2 - \Delta V^2}{\Delta U^2 + \Delta V^2}. \quad (10)$$

### 3.1. Slowly varying potential model

For the slowly varying potential (SVP) model,[21–23] the on-site potential in Eq. (7) can be written as

$$\varepsilon_j = \lambda \cos(\pi\alpha j^\upsilon + \varphi). \quad (11)$$

Here, $\lambda$ is the potential strength and $\alpha$ is a real number; $\varphi$ is the original phase, which is redundant in localization. It is found that for $0 < \upsilon < 1$, there are two mobility edges (MEs) at $E_\mathrm{c} = \pm(2.0 - \lambda)t$ provided that $\lambda < 2.0t$. Extended states are in the middle of the band ($|E_\beta| < |E_\mathrm{c}|$). Localized states are at the band edges ($|E_\beta| > |E_\mathrm{c}|$); states are more localized as eigenenergies $E_\beta$ are nearer band edges. At MEs, states are critical.

We take $\lambda = 1.0t$ as an example. At the same time, $\pi\alpha = 0.2$ and $\upsilon = 0.7$ are set, which are the same as that in Refs. [21]–[23]. In this case, two MEs are $E_\mathrm{c} = \pm t$. We denote $E_\mathrm{c}^1 = -t$ and $E_\mathrm{c}^2 = t$, respectively. States are extended for $|E_\beta| < t$ and localized for $|E_\beta| > t$. Figure 1(a) shows that at extended states, uncertainties $\Delta U^2$s are near ones. At localized states, $\Delta U^2$s decrease as states vary from MEs to band edges; at the same eigenenergies $E_\beta$, the larger lattice sizes, the smaller $\Delta U^2$s are. There are sharp transitions in $\Delta U^2$s at MEs, where states are critical. Thus $\Delta U^2$s can well characterize the localization properties of the three different kinds of states in position space. At the same time, figure 1(b) shows that on the whole, uncertainties $\Delta V^2$s are decreasing as states vary from band center to band edges. There is a deep pit in $\Delta V^2$s when eigenenergies $E_\beta$ are near each ME. The values of $\Delta V^2$ are almost independent of the lattice sizes $N$s. Fortunately, figure 1(c) shows that the reduced relative uncertainty $U_\mathrm{r} > 0$ for extended states and $U_\mathrm{r} < 0$ for localized ones. For larger lattice size $N$, $U_\mathrm{r}$ almost equals to zero for critical states (seen in inset). It means that uncertainties $\Delta U^2$s are greater than, equal to, and less than uncertainties $\Delta V^2$s for extended, critical, and localized states, respectively. Therefore, different kinds of states can be distinguished from each other with the comparisons of $\Delta U^2$ and $\Delta V^2$.

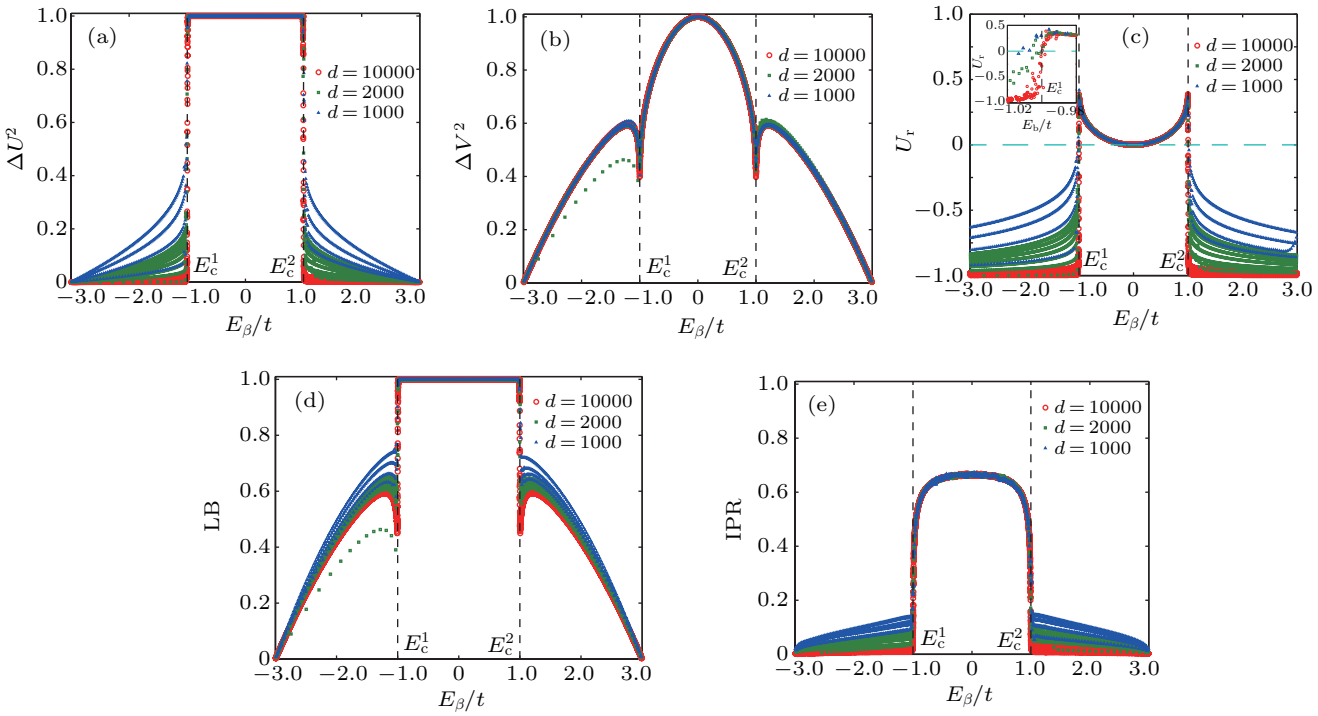



**Fig. 1.** (color online) For the slowly varying potential model, (a) $\Delta U^2$, (b) $\Delta V^2$, (c) $U_r$, (d) LB, and (e) IPR as functions of eigenenergies $E_\beta$, respectively. Here, $\lambda = 1.0t, \pi\alpha = 0.2$, and $\upsilon = 0.7$; the vertical dashed lines are for the functions $E_\beta = E_c^1 = -t$ and $E_\beta = E_c^2 = t$, respectively; the horizontal dashed line in panel (c) is for $U_r = 0$; lattice sizes $d = 1000, 2000$, and $10000$, respectively. Inset in panel (c): partial enlarger for $E_\beta$ near $E_c^1$.

Figure 1(d) shows that for extended states, LBs are near ones. For localized states, on the whole, the more localized the states are, the smaller the LBs are. There are rapid transitions in LBs as states move from the extended into the localized regime. A deep pit is in LBs when eigenenergies $E_\beta$ are near each ME, so LBs depend on states, and different kinds of states can also be distinguished from each other based on LB.

Furthermore, compared to our results intuitively, we also calculate the inverse participation ratio IPR $= (d\sum_j |\psi_j^\beta|^4)^{-1}$, which is a traditional and often used quantity to characterize localization properties of states. Roughly, it is proportional to the localization length of states.[28] Figure 1(e) shows that for extended states, IPRs are relatively large. For localized states, IPRs are relatively small, and at a fixed $E_\beta$, the larger the $d$ is, the smaller IPR is. On the whole, all our studied quantities are in good correspondence with IPR.

### 3.2. Deterministic nearest-neighbor tight-binding models with exact mobility edges

One family of the models are specified by on-site potentials[24]

$$\varepsilon_j(\tilde{\alpha}, \tilde{\phi}) = 2\lambda \frac{\cos(2\pi jb + \tilde{\phi})}{1 - \tilde{\alpha}\cos(2\pi jb + \tilde{\phi})}. \tag{12}$$

The on-site potential is a smooth function of $\tilde{\alpha}$ in the open interval $(-1, 1)$. Each value of $\tilde{\alpha}$ corresponds to a different tight-binding model. $\tilde{\phi}$ is the original phase, which is redundant in localization. For a quasiperiodic modulation, $b$ is set to be irrational. There exist self-duality points under a generalized duality transformation.[24] Based on it, the analytical critical condition about MEs when $\tilde{\alpha} \in (-1, 1)$ is

$$\tilde{\alpha}E_c = 2\mathrm{sgn}(\lambda)(|t| - |\lambda|), \tag{13}$$

where $\mathrm{sgn}(x)$ is the sign function.

In Fig. 2, we take the parameters of $\lambda = -0.9t$ and $\tilde{\alpha} = -0.6$ as examples. From Eq. (15), an ME $E_c = t/3$. In this case, all states are localized when eigenenergies $E_\beta > E_c$, and almost all states, except some states at subband edges, are extended when $E_\beta < E_c$. In calculations, the irrational number $b$ in Eq. (14) is approximated by the ratio of successive Fibonacci numbers: $F_j = F_{j-1} + F_{j-2}$, with $F_0 = F_1 = 1$. In this way, choosing $b = F_{j-1}/F_j$ and lattice size $d = F_j$, we can obtain the periodic approximant for the quasiperiodic potential.

Similar to that for the SVP model, figure 2 shows that for extended states, uncertainties $\Delta U^2$s are near ones, the reduced relative uncertainty $U_r > 0$, and LBs are near ones. For localized states, $\Delta U^2$s are near zeros, $U_r < 0$, LBs are relatively small. There are good correspondences for them with IPRs. So all these quantities can characterize the localization properties of different kinds of states in the model.

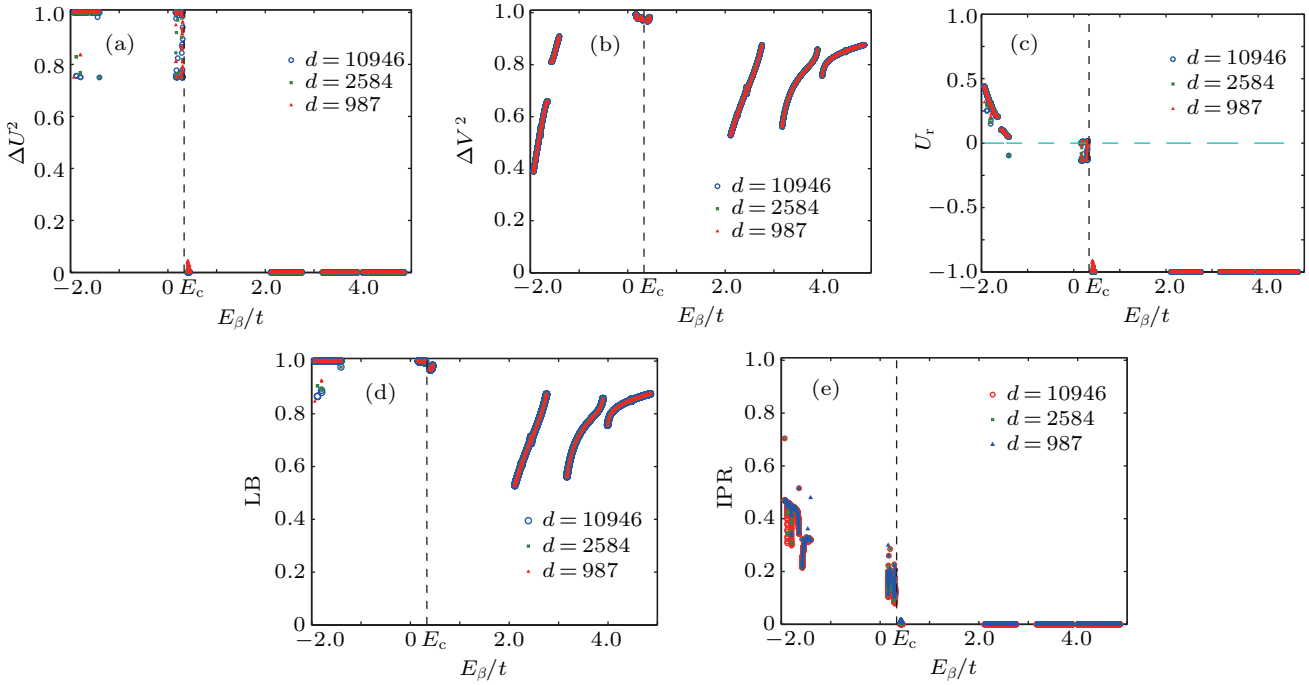



**Fig. 2.** (color online) For the deterministic nearest neighbor tight binding models with exact mobility edges, (a) $\Delta U^2$, (b) $\Delta V^2$, (c) $U_r$, (d) LB, and (e) IPR as functions of eigenenergies $E_\beta$, respectively. Here, $\lambda = -0.9t$ and $\tilde{\alpha} = -0.6$; the vertical dashed line is for the function $E_\beta = E_c = t/3$; the horizontal dashed line in panel (c) is for $U_r = 0$; lattice sizes $d = 987$, 2584, and 10946, respectively.

### 3.3. Random-dimer potential model

In the random-dimer potential (RDP) model,[25–27] the on-site potential in Eq. (7) is given by

$$\varepsilon_{2j} = \varepsilon_{2j+1} = \begin{cases} V_a, & \text{(with probability } q\text{)}, \\ V_b, & \text{(with probability } 1-q\text{)}, \end{cases} \tag{14}$$

where $V_a$ and $V_b$ are dimer energies. The potential is random but with short correlations, which is different from potentials in the above two models where potentials are determined (without disorder). It was found[25] that delocalized (extended) states exist when $|V_a - V_b| < 2.0t$ and there are only localized states when $|V_a - V_b| > 2.0t$. At finite lattice sizes $d$,

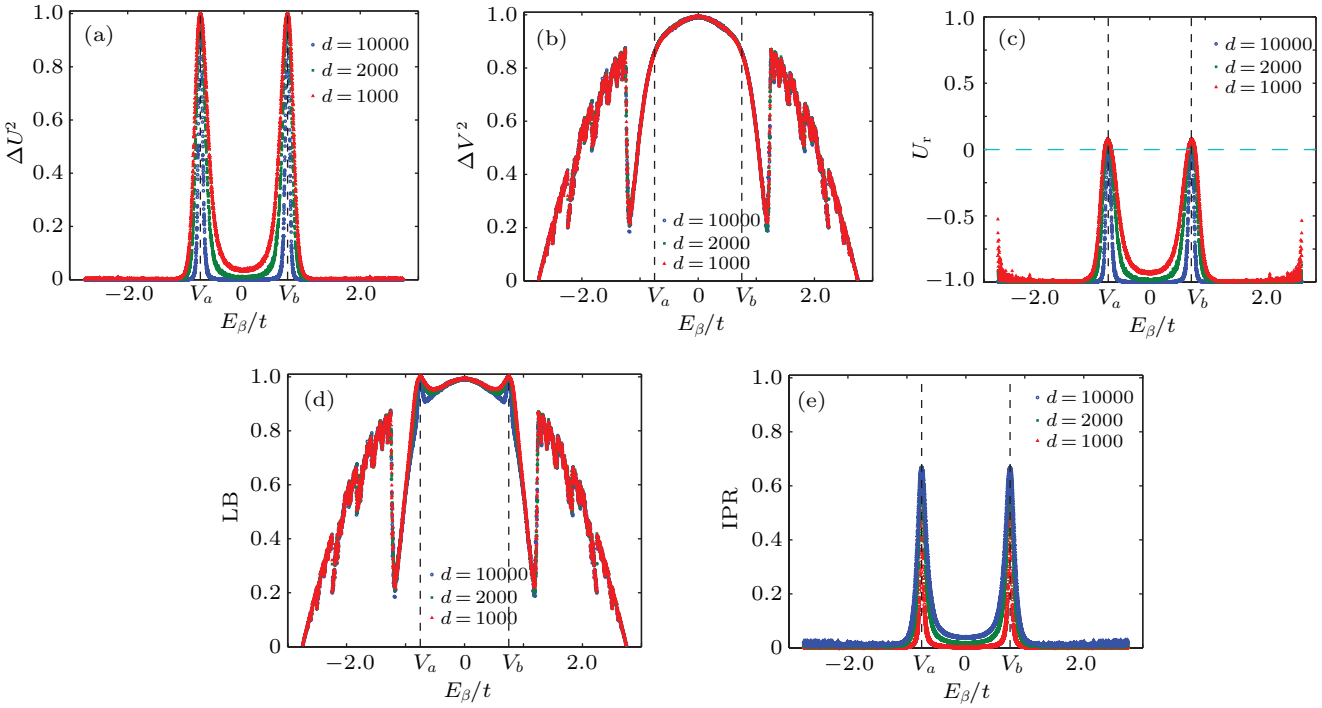



**Fig. 3.** (color online) For the random-dimer potential model, (a) $\Delta U^2$, (b) $\Delta V^2$, (c) $U_r$, (d) LB, and (e) IPR as functions of eigenenergies $E_\beta$, respectively. Here, $V_a = -V_b = -0.75t$; the vertical dashed lines are for the functions $E_\beta = V_a$ and $E_\beta = V_b$, respectively; the horizontal dashed line in panel (c) is for $U_r = 0$; lattice sizes $d = 1000, 2000$, and 10000, respectively.

the number of delocalized states is roughly proportional to $\sqrt{d}$; for infinite lattice sizes, there are only states with eigenenergy $E_\beta = V_a(V_b)$ are delocalized.[26]

In Fig. 3, we take $V_a = -V_b = -0.75t$ as examples. At the same time, we choose $q = 0.5$, which corresponds to the most random situation. In this case, states with eigenenergies $E_\beta$ near $V_a(V_b)$ are delocalized. The results of Fig. 3 are obtained for average of 500, 250, and 50 samples for lattice sizes $d = 1000$, 2000, and 10000, respectively. The averages with more samples give the same results.

Similar to that for the SVP model and the deterministic nearest-neighbor tight-binding models with exact mobility edges, figure 3 shows that for states with eigenenergies $E_\beta$ very near $V_a(V_b)$ (delocalized states), $\Delta U^2$s are near ones, $U_r > 0$, LBs are also near ones. For other states (localized ones), at the same $E_\beta$, $\Delta U^2$s decease with lattice sizes $N$s; $U_r < 0$ and LBs are relatively small. There are good correspondences between these quantities and IPRs. Thus, they can reflect the localization properties of different kinds of states in the model.

## 4. Discussion and conclusions

It is known that the operators $U$ and $V$ are the non-Hermitian generalization of the Pauli operators from two dimensions to higher dimensions. The simplest higher-dimensional quantum states may be states for an electron in lattice systems. In the three studied models, we found that $\Delta U^2$ can well characterize state localization properties. The reduced relative uncertainty $U_r$ can also do so. At the same time, Resta proposed and used a $U$-related quantity to study many-body localization.[29] Here, we found that $U$ itself can well reflect the localization properties of single electron lattice systems. Besides, Bagchi and Pati pointed out that LB [Eq. (6)] depends on states.[11] Here, we give further results that LBs are relatively large for extended states and relatively small for localized states. Therefore, all these studies present more pictures than existing works.

For the three studied models, we found that uncertainties $\Delta U^2 > \Delta V^2$, $\Delta U^2 = \Delta V^2$, and $\Delta U^2 < \Delta V^2$ for extended, critical, and localized states, respectively. A similar result has been found by contrast of Shannon information entropies of states for an electron in position and momentum space,[30] or by contrast of the distinguishability and visibility for an electron in lattice systems.[31] Thus, these quantities can be used as novel indexes to characterize Anderson localization.

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