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A measure of localization properties of one-dimensional single electron lattice systems

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ABSTRACT

We propose a novel quantity to measure the degree of localization properties of various types of one-dimension single electron states. The quantity includes information about the spatial variation of probability density of quantum states. Numerical results show that it can distinguish localized states from delocalized ones, so it can be used as a fruitful index to monitor the localization–delocalization transition. Comparing with existing measures, such as geometric average density of states, inverse participation ratio, and quantum information entropies, our proposed quantity has some advantages over them.

1. Introduction

As is well known, Anderson localization is a fundamental concept in many-body physics [1]. The concept can be applied to many branches of physics, for instance, light waves, sound waves, and matter waves [2]. For electron systems, extensive studies have focused on metal–insulator transitions (MITs) or delocalization–localization transitions [2–4]. For one-dimensional (1D) Anderson model, it is well known that all eigenstates are localized and there are no mobility edges separating localized and delocalized states [5]. However, the specific delocalized states and/or mobility edges have been found in 1D systems, such as determined potential models [6–17], random potential models with short-range correlation [14–22] or long-range correlation [14,15,20,23]. Very recently, Anderson localization was experimentally observed for ultracold atomic gases in disordered optical potential systems [24] and photons in disordered superlattices [25].

How to measure the degree of localization is a challenging and important problem in the theory of Anderson localization. Until now, researchers have developed lots of quantities to characterize it, such as the Thouless exponent (or Lyapunov coefficient) [10–12,20,23], multifractal properties [4,13], dynamics of wave function [18], geometric average density of states (GADOS) [14,26], inverse participation ratio (IPR) [12,20–22,27], quantum information entropies [15–17,28], and many others [2–4]. These measures estimate localization properties from different points of view. With finite-size scaling analysis, all these quantities can distinguish localized states from delocalized ones. These quantities can be used to confirm and complement each other. Some measures may be more useful than others when using specific numerical techniques.

In this work, considering the spatial variation of probability density, we propose a novel quantity as a measure of 1D electronic localization properties. We numerically studied it for four kinds of wave functions and found that it can distinguish localized states from delocalized ones. Other standard measures, such as GADOS, IPR and quantum information entropies, do not include this position-dependent information. Comparing with them, our proposed quantity has some advantages.

The rest of the paper is organized as follows. In Section 2, we propose the measure of localization properties in single-electron systems. In Section 3, the measure is numerically tested in different models. In Section 4, the measure compares to others. Finally, results are collected in Section 5.

2. Models and formulas

We consider an electron moving in a 1D lattice with L sites [16,17]. The corresponding tight-binding Hamiltonian is described by

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$$H = \sum_{\ell=1}^{L} \varepsilon_\ell c_\ell^\dagger c_\ell - t \sum_{\ell=1}^{L} (c_\ell^\dagger c_{\ell+1} + H.c.), \tag{1}$$

where ε_ℓ is the on-site potential, t is a nearest-neighbor hopping integral, $c_\ell^\dagger$ (c_ℓ) are creation (annihilation) operators of the ℓth site. The site occupation basis is $|n_1, n_2, \ldots, n_\ell, \ldots, n_L\rangle = c_1^{\dagger n_1} c_2^{\dagger n_2} \ldots c_\ell^{\dagger n_\ell} \ldots c_L^{\dagger n_L} |0\rangle$, where $n_\ell = 0$, or 1, and $|0\rangle$ is the vacuum. For an electron, $\sum_{\ell=1}^{L} n_\ell = 1$. If we write $|\ell\rangle = |0, \ldots, 1_\ell, \ldots, 0\rangle = c_\ell^\dagger |0\rangle$, the general wave function, i.e., eigenstate $|\beta\rangle$ with eigenenergy E_β for Hamiltonian described in Eq. (1) is the superposition

$$|\beta\rangle = \sum_{\ell=1}^{L} \phi_\ell^\beta |\ell\rangle = \sum_{\ell=1}^{L} \phi_\ell^\beta c_\ell^\dagger |0\rangle . \tag{2}$$

The probability density of $|\beta\rangle$ on the ℓth site is $\rho_\ell = |\phi_\ell^\beta|^2$, and the corresponding probability density sequence $S_L^{PD} = \{\rho_1, \ldots, \rho_\ell, \ldots, \rho_L\}$.

From Eqs. (1) and (2), we suppose a quantity $P_\ell = \sum_{k=1}^{\ell} \rho_k = \sum_{k=1}^{\ell} |\phi_k^\beta|^2$, which is the local integrated DOS from the 1st site to the ℓth site. We propose a complex quantity

$$A_L^\beta = \frac{1}{L} \sum_{\ell=1}^{L} \exp(i2\pi P_\ell), \tag{3}$$

where $i = \sqrt{-1}$. For simplicity, we omit β in A_L^β unless otherwise specified. The modulus of A_L, denoted by $|A_L|$ is used to measure localization properties of 1D quantum state $|\beta\rangle$ given in Eq. (2). From the definition, A_L depends on the spatial variation of probability density sequences $S_L^{PD} = \{\rho_1, \ldots, \rho_\ell, \ldots, \rho_L\}$. To demonstrate Eq. (3) intuitively, we give some examples. For an extended state that $\phi_\ell^\beta = \frac{1}{\sqrt{L}}$ for all ℓ, $|A_L| \approx 0$ at larger L. For a localized state that $\phi_\ell^\beta = \delta_{\ell\ell_0}$ (ℓ_0 is a given site), $|A_L| = 1$. In other words, the two values of $|A_L|$ for the two specific states are as a calibration to measure the degree of localization for general quantum states. At the same time, the smaller the value $|A_L|$ is, the more delocalized the state is.

In fact, A_L in Eq. (3) is inspired by the Friedel sum rule (FSR) [29–31]. The FSR can be stated as $\theta_f(E_2) - \theta_f(E_1) \approx \pi N(E_2, E_1)$. Here the Friedel phase $\theta_f(E) = \frac{1}{2i} \ln(\det[S(E)])$, i.e., $\det[S(E)] = \exp(i2\theta_f(E))$, where S is a scattering matrix and $i = \sqrt{-1}$. $N(E_2, E_1)$ is the variation in the number of states in the energy interval $[E_1, E_2]$ due to the scatterer. That means the θ_f jumps by π when the integrated density changes by one particle. Therefore, not rigorously, A_L can be as a quantity that takes account of the contributions of the local integrated DOS to the Friedel phase.

3. Numerical results

We numerically test the conclusion that A_L can distinguish localized states from delocalized ones. First, we study it for one-electron states with an exponential shape and with a power-law ones, respectively. Then we study it for one-electron eigenstates in the Harper model and in the slowly varying potential ones, respectively. For the two models, we use the negative-eigenvalue counting method to numerically get eigenstates with relatively larger lattice sizes [32].

3.1. Quantum states with an exponential shape

We first consider quantum states with an exponential shape, i.e.,

$$\phi_\ell = Ce^{-\frac{1}{2}(\frac{\ell - L/2}{\xi})}, \tag{4}$$

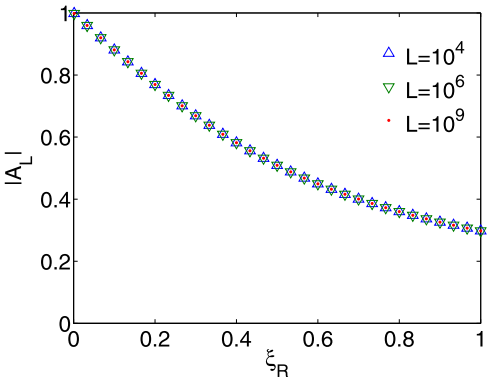

Fig. 1. (Color online.) $|A_L|$ as a function of ξ_R for quantum states with an exponential shape at $L = 10^4, 10^6$ and 10^9, respectively.

where the constant C is used to normalize states using $\sum_{\ell=1}^{L} |\phi_\ell^\beta|^2 = 1$ and $\ell = 1, 2, \ldots, L$. It is known that the states are localized and the localization length can be characterized by ξ. The more smaller ξ, the more localized the state is.

For convenience of description, we define a reduced localization length $\xi_R = 2\xi/L$. In Fig. 1, we plot $|A_L|$ versus the corresponding ξ_R at $L = 10^4, 10^6$ and 10^9, respectively. It shows that $|A_L|$ monotonously decreases with ξ_R. As $\xi_R \to 0$, $|A_L| \to 1$. For same ξ_R, $|A_L|$ is almost independent of lattice sizes L. In other words, for a certain localization length ξ, $\xi_R = 2\xi/L$ will decrease with L. It means that the state becomes more localized as it is viewed from larger lattice size L. Especially ξ_R will decreases to zero as $L \to \infty$, i.e., the state becomes most localized and the corresponding $|A_L|$ approaches to 1. Therefore, $|A_L|$ can well reflect the localization properties of quantum states with an exponential shape.

3.2. Quantum states with a power-law shape

We then consider quantum states with a power-law shape, i.e.,

$$\phi_\ell = \frac{1}{\sqrt{D}} \ell^{-\gamma/2}, \tag{5}$$

where $D = \sum_{\ell=1}^{L} \ell^{-\gamma}$ is used to normalize the quantum state. They are mathematical quantum delocalized, critical, and localized states at $0 \le \gamma < 1$, $\gamma = 1$ and $\gamma > 1$, respectively [33].

In Fig. 2(a), we plot $|A_L|$ versus γ at $L = 10^4, 10^6, 10^9$ and $L \to \infty$, respectively. At a certain γ, we use the finite size scaling to get the value of $|A_L|$ as $L \to \infty$, denoted by $|A_L^\infty|$. The scaling function $\log 10(|A_L^\infty| - |A_L|) = K \log 10(1/L)$ is chosen to fit corresponding data, where $|A_L^\infty|$ and K are two fitting parameters. Figs. 2(b), (c) and (d) give the scaling behavior of $|A_L|$ at $\gamma = 0.5, 1.0$ and 1.5, respectively. They show the scaling function can well fit corresponding data. For other γ, the results are similar. At $L \to \infty$, Fig. 2(a) shows that, in the delocalized region ($0 \le \gamma < 1$), $|A_L^\infty|$ increases from zero to almost near 1 as γ increases, while in localized region ($\gamma > 1$), $|A_L^\infty|$ are nearly equal to 1. Therefore, $|A_L|$ can well characterize the localization properties of quantum states with a power-law shape.

3.3. Eigenstates in the Harper model

For the Harper model [6–9,14,16], the on-site potential in Eq. (1) can be written as

$$\varepsilon_\ell = \lambda \cos(2\pi\sigma\ell + \varphi), \tag{6}$$

where λ is the potential strength, σ is an irrational number, and φ is an initial phase. As a typical case, $\sigma = \frac{\sqrt{5}-1}{2}$. The potential is