Characterizing Anderson delocalized-localized phase transition based on the response of the system to the boundary conditions

Mohammad Pouranvari
Department of Solid-State Physics, Faculty of Science, University of Mazandaran, Babolsar, Iran.

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A characterization of the Anderson phase transition has been introduced, based on the response of the system to the boundary conditions. We change the boundary conditions from periodic to anti-periodic and look for its effect on the eigenstate of the system. To characterize the effect we use overlap of the states. In particular, we numerically calculate the overlap between ground-state of the system with periodic and that with anti-periodic boundary conditions in one-dimensional models with delocalized-localized phase transitions. We observe that the overlap is close to 1 in the localized phase and it gets tangibly smaller in the delocalized phase. In addition, to characterize the entire spectrum of the models with mobility edges, we calculate also the overlaps between single-particle eigenstate with periodic and anti-periodic boundary conditions, by which we are able to locate the mobility edges.

I. INTRODUCTION

Characterizing phases and phase transition is one of the main goals of the condensed matter physics. Introducing new method to understand nature of the phases, and also to locate the phase transition point is always an important part of the current research. In general, for a non-zero phase transition, classical interpretations are usually enough to describe phases of the system and also to classify different phase transitions. Story is different for a zero-temperature phase transition, where quantum fluctuations become important and they dominate thermal fluctuations. Among quantum phase transition, Anderson phase transition between delocalized and localized phases has attracted many attentions. In this phase transition, disorder plays the central role. For an ideal clean system, where the system is translationally invariant, Bloch waves propagate through the entire system and we have and extended eigenstate, namely we are in the metallic phase. Physics will change by introducing disorder in the system; interference of the scattered waves of the disorders can be destructive and make the system localized. In one and two dimensional systems, an infinitesimal disorder make the system localized. In the three dimensional systems, we have a phase transition between delocalized and localized phases as we increase the disorder strength; for small disorders, state of the system is still delocalized, but it will become localized at a small part of the system, when disorder strength is bigger than some values, which depend on the distribution of the randomness. There are also one-dimensional models with correlated disorders, where we can see phase transition between delocalized and localized phases. Since they represent the same nature of the Anderson localization, and they are very suitable for numerical calculations.

Different quantities are introduced to characterize the phase transition between delocalized and localized phases. Since eigenstate of the system at the Fermi level is the one that shows the tendency of the material to conduct an electron, one of the obvious characterization is to measure the extent of the eigenstate at the Fermi level. To quantify how much the eigenstate of the system \( \psi \) is extended, people use the inverse participation ratio:

\[
\text{IPR} = \sum_{i=1}^{N} |\psi_i|^4,
\]

(where \( N \) is the system size) for a normalized eigenstate \( \psi \) with amplitude \( \psi_i \) at each site \( i \). In the delocalized phase, where the system is extended in the entire system, it approaches \( 1/N \) and it goes to 1 in the localized phase where it is localized at some finite sites. The next candidate would be entanglement. In the delocalized phase, where state of the system is extended, we expect larger correlation in the system than in the localized phase with a localized state; and thus amount of the entanglement is larger in the delocalized phase.

Beside the eigenstate, looking at the energy eigenvalues is also informative; level spacing (defined as \( \Delta_n = E_{n+1} - E_n \) level spacing between adjacent energy eigenstates for energy spectrum \( \{E\} \) and their distributions are another way to characterize delocalized from localized phase. In the delocalized phase energy spectrum are doubly degenerated so there is a gap between even-odd and odd-even level spacing. Moreover, ratio of the level spacing is also useful:

\[
r_n = \frac{\min(\Delta_n, \Delta_{n+1})}{\max(\Delta_n, \Delta_{n+1})},
\]

In delocalized phase, where statistics is Wigner-Dyson, the average of \( r_n \) approaches to \( \approx 0.53 \) and in the localized phase with Poisson statistics, it goes to \( \approx 0.386 \), and people use it to distinguish different phases.

To characterize the delocalized-localized phase transition, we can also look at the behavior of the system responding to the change in the boundary conditions. For an extended eigenstate, the change in the boundary condition is reflected in the corresponding eigen energy; but for a localized eigenstate, where the amplitude of the wave function is approximately non-zero for some finite
number of sites, the change in the boundary condition is not seen by the eigenstate, and thus no change in the eigen energies. In particular Ref. [22] used the shift in the eigen energy when we change the boundary condition from periodic to anti-periodic to characterize the phase transition; this idea has some other applications as well[23,24].

The response of the system to a local quench is also another characterization. A measure of this response is the overlap \( F = |\langle G'G \rangle| \) of the ground state of the system without \((G)\) and with \((G')\) a local quench. In the delocalized phase, this overlap goes to zero in a power-law fashion \((F \sim N^{-\gamma})\), the so called Anderson orthogonality catastrophe \([22]\) while it decays exponentially in the localized phase \((F \sim e^{-\beta N})\); where \(\gamma\) and \(\beta\) depend on the disorder strength \([27]\).

In this paper, we study the response of the system to the boundary conditions, by looking at the eigenstates of the system Hamiltonian. Namely, we calculate the overlap between state of the system with periodic boundary conditions (PBC) and the state of the system with anti-periodic boundary conditions (APBC) to characterize the similarity of them. When we change the boundary condition from PBC to APBC for a system, state of the system is affected in the delocalized phase, since it is extended over entire system; On the other hand, in the localized phase, state of the system is localized at some part of the space and changing the boundary condition is not seen by the state. Thus, we expect that the overlap between state of the system with PBC and with APBC becomes unity in the localized phase and becomes smaller than one in the delocalized phase. In this regard, we expect that the overlap characterizes delocalized from localized phases.

In free fermion models, to obtain the ground state of the system, by setting the Fermi energy, we fill single-particle eigenstates of the system from lowest eigen energies up to the Fermi level, and the many-body ground state of the system is the Slater determinant of these single-particle eigenstates. To understand the similarity, we can thus calculate the overlap between the many-body ground state of the system with PBC and that of the system with APBC. Beside that we can also look at the overlap of the single-particle eigenstates—those eigenstates that build the many-body state of the system.

We calculate the many-body ground states of the system with PBC and APBC, then we obtain their overlap, and we call it ground-state overlap (GSO). In addition, we calculate the single-particle eigenstates of the system with PBC and APBC, and we call their corresponding overlaps single-particle overlap (SPO). We show that the behavior of the GSO and SPO are different in delocalized and localized phases, thus we utilize them to characterize the delocalized-localized phase transition.

The reminder of the paper is as follows: In section [II] we explain the models we employ in this paper to verify our ideas, also the method to calculate the SPO and GSO are also explained. Section [III] is devoted to our numerical calculations where we present the results for the SOP and GSO for the models. We conclude the paper in section [IV] with some suggestion for the future works.

II. METHOD AND MODELS

We work with one-dimensional free fermion tight-binding models with the following Hamiltonian:

\[
H = -t \sum_{i=1}^{N} (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + \sum_{i=1}^{N} \epsilon_i c_i^\dagger c_i, \tag{3}
\]

where, \(c_i(c_i^\dagger)\) is the annihilation (creation) operator for \(i\)th site. \(N\) is the number of site in the system. The amplitude of the nearest-neighbor hopping is \(t\) and we set it to be 1 as energy scale. The models that we use in this paper are determined by their on-site energies \(\{\epsilon_i\}\). One of the models is random dimer (RD) model, where we choose \(\epsilon_i\) to be either of the two choices \(\phi_a\) and \(\phi_b\) randomly; One of them (here \(\phi_b\)) is ascribed to two successive sites (so this model is called dimer). It is shown[22] that states at the resonant energy \(E = \phi_b\) are delocalized when \(-2t < \phi_a - \phi_b < 2t\). In this study we choose \(\phi_a = 0\), thus the condition is \(-2 < \phi_b \leq 2\). States at energies other than the resonant energy are localized.

Another model is the the generalized Aubry-Andry model[33], where we choose the on-site energies \(\epsilon_i\) to be:

\[
\epsilon_i = 2\lambda \frac{\cos(2\pi ib)}{1 - \alpha \cos(2\pi ib)}, \tag{4}
\]

\(b\) is an irrational number and we set it to be the golden ratio \(b = \frac{1+\sqrt{5}}{2}\). Since \(b\) is not a rational number, system has incommensurate periodicity with respect to the lattice period which we set it to be 1. Thus, this system is not completely period nor either completely random. This model has mobility edges separating delocalized and localized eigenstates at the following eigen energies[33]

\[
E_{\text{mobility edge}} = 2s\text{gn}(|\lambda|)\frac{|t| - |\lambda|}{\alpha}. \tag{5}
\]

One special case for this model is \(\alpha = 0\), which is the Aubry-Andry model, with the following on site energies:

\[
\epsilon_i = 2\lambda \cos(2\pi ib + \theta), \tag{6}
\]

here, we added \(\theta\) as a random number that is uniformly distributed between \(-\pi\) and \(\pi\). It is shown[17] for \(\lambda < 1\) all states are delocalized and for \(\lambda > 1\) all states are localized, and thus there is a phase transition between delocalized and localized phases at \(\lambda = 1\).

Both models describe the free fermions, so we are dealing with Hamiltonians that are represented by \(N \times N\) matrices which can be diagonalized numerically. Here we use LAPACK[34] to diagonalize the matrices, and obtain its eigenvalues and its eigenvectors.
In this paper, we want to consider the overlap of the state of the system with PBC and state of the system with APBC. Here, we explain how to calculate the SPO and GSO overlaps. If we assume the following free fermion Hamiltonian with PBC and APBC:

\[ H_{\text{PBC}} = \sum_{i,j}^N h^P c_i^\dagger c_j, \]

\[ H_{\text{APBC}} = \sum_{i,j}^N h^A c_i^\dagger c_j, \]

where, \( h^P \) and \( h^A \) can be determine from the choice of the on-site energy (gAA, AA, or RD model) and the boundary condition (either PBC or APBC). We can diagonalize matrix \( h \) in the following way:

\[ h^P = U E^P U^\dagger \]

\[ h^A = V E^A V^\dagger, \]

and find the eigen energies \( E \) as well as the single-particle eigenstates \( \psi \) for each Hamiltonian (\( \psi^{\text{PBC}}_i = U_{in} \) is the \( i \)th element of the \( n \)th eigenvector, and similarly for \( \psi^{\text{APBC}}_i = V_{in} \)). To calculate the Ground-state overlap, which is the overlap between ground state of the Hamiltonian with the PBC and APBC, we use the following method. After diagonalization, we can write the both Hamiltonians as:

\[ H_{\text{PBC}} = \sum_{k=1}^N E^P b_k^\dagger b_k, \]

\[ H_{\text{APBC}} = \sum_{k=1}^N E^A c_k^\dagger c_k, \]

where \( b_k^\dagger = \sum_j U_{jk} c_j^\dagger \) and \( a_k^\dagger = \sum_j V_{jk} c_j^\dagger \). Then, GSO is:

\[ \text{GSO} = |\langle \psi_{MB}^{\text{APBC}} | \psi_{MB}^{\text{PBC}} \rangle| \]

\[ = |\langle 0 \prod_k b_k^\dagger \prod_k a_k^\dagger | 0 \rangle| \]

\[ = |\det(B)| \]

where \( B \) is a matrix build from the first \( N_F \times N_F \) part of the matrix \( U^\dagger V \) (\( N_F \) is the number of fermions).

We also use the notion of single-particle overlap, which is the overlap between corresponding single-particle eigenstates of the Hamiltonian with PBC and with APBC. To calculate it, we dot product the single-particle eigenstate \( \psi^{\text{APBC}}_n \) with the corresponding eigenstate \( \psi^{\text{PBC}}_n \) for specific \( n \)th level. We consider only its absolute values:

\[ \text{SPO} = |\langle \psi^{\text{APBC}}_F | \psi^{\text{PBC}}_F \rangle| \]

We also note that there are randomness in the AA and RD models, and thus we take disorder average of the above mentioned GSO and SPO over different random realizations.

III. RESULTS

In this section, we provide the result of the numerical calculations. First, we will study the GSO, and in the subsequent subsection, we explain and show the benefits of the SPO over GSO for models with mobility edges.

A. Ground-State Overlap

For the RD model, we calculate the GSO as we change the \( \phi_b \) and we always set \( E_F = \phi_b \). State of the system at \( E = E_F \) is delocalized for \( \phi_b < 2 \) and it is localized for \( \phi_b > 2 \). The results are plotted in the Fig. 1 for different system sizes \( N \). We can see that GSO has different behavior in delocalized and localized phases, in the delocalized phases, \( \phi_b < 2 \) the GSO is smaller than in the localized phase, \( \phi_b > 2 \). We can see that it approaches to unity deep in the localized phase. It is obvious that we can distinguish delocalized and localized phases from the behavior of the GSO. We also calculate the GSO for the AA model as well. The results are plotted in Fig. 2. The behavior of the GSO for the AA model is not as sharp as for the RD model, but still it is obvious that GSO approaches to 1 in the localized phase, \( \lambda > 1 \), and it is smaller in the delocalized phase, \( \lambda < 1 \).

B. Single-Particle Overlap

To calculate the GSO for the AA and RD model, we set a Fermi energy and based on the number of fermion that we obtain, we use Eq. 13. We saw that for both models, there is a distinction between delocalized and
localized states characterized by the GSO that we obtained. However, there are some details we would like to consider in this subsection. AA model does not have mobility edges between delocalized and localized states. In the RD model, only single-particle eigenstate at the resonant energy is delocalized and all the other states are localized. To be able to distinguish between delocalized and localized single-particle eigenstates, we use the notion of the SPO, in which we calculate the overlap between corresponding SPO rather than the GSO. For both AA and RD models, we calculated the SPO and the results are plotted in Fig. 3. For the AA model with either all delocalized or all localized states, we see that SPO is either very close to 1 (in the localized phase) or lower than 1 (in the delocalized phase). SPO for the RD model has more features; for the case of $\phi_b = 3$, where all states are localized, we see that SPO is close to 1 for the entire spectrum. On the other hand for the $\phi_b = 1$, where state at the resonant energy $E = \phi_b = 1$ is delocalized and all the other single-particle eigenstates are localized, we see that SPO is smaller than 1 around the resonant energy; and away from the resonant energy, SPO is close to 1. Thus, the SPO can be used to characterize the spectral resolution of the system for delocalized-localized phase transition.

It gets more complicated if we consider models with mobility edges between delocalized and localized phases. One example would be the gAA model with on-site energies given by Eq. (4). This model has mobility edges, separating delocalized and localized single-particle eigenstates given by Eq. (5). If we simply set the Fermi energy to $E_F = 0$ and obtain the GSO, we will obtain the plots in Fig. 4.

![Figure 2](image1.png)

**FIG. 2.** Overlap between ground state of the system with periodic boundary condition and anti-periodic boundary condition, as we change $\lambda$ for the AA model. The overlaps approaches to 1 in the localized phase, $\lambda > 1$ and it gets smaller in the delocalized phase $\lambda < 1$. We set $E_F = 0$. At each data point, disorder average is taken over 2000 random realizations.

![Figure 3](image2.png)

**FIG. 3.** Single-particle overlap between single-particle eigenstates with PBC and APBC for the entire spectrum. Left panel: SPO for the AA model. In localized phase ($\lambda = 2$) SPO is very close to 1 for the entire spectrum; in delocalized phase ($\lambda = 0.1$) SPO is lower than 1 for the entire spectrum. Right panel: SPO for the RD model. For $\phi_b = 3$ where all single-particle eigenstates are localized, SPO is close to 1 for the entire spectrum; and for the $\phi_b = 1$ with a delocalized single-particle eigenstate at the $E = 1$, SPO for points close to this energy are lower than 1.

![Figure 4](image3.png)

**FIG. 4.** Ground-state overlap for the gAA model (Eq. (4)) as we change $\alpha$ from $-1$ to 1 and for two choices of $\lambda = 0.9$ (left panel) and $\lambda = -1.1$ (right panel). We set $N = 500, E_F = 0$.

However, if we calculate the SPO, the detailed features of the mobility edges will be clear. In Fig. 5 we plotted the result of the SPO for the entire spectrum, for $-1 \leq \alpha \leq 1$ and for two choices of $\lambda = 0.9, -1.1$. Characterization of the single-particle eigenstate based on the SOP is completely in agreement with the mobility edges given by Eq. (5).

**IV. CONCLUSION**

In this paper, we studied the effect of the boundary conditions on the overlaps between ground state of the system with PBC and APBC. We observe that in the delocalized phase, the overlap is smaller than the overlap in the localized phase where it goes to unity. These observations come from the fact that state of the system in the localized phase, does not change upon changing the boundary condition. On the other hand, single-particle eigenstate is affected by the change in the boundary conditions in the delocalized phase.

This conjecture enabled us to use the notion of the GSO to distinguish delocalized from localized phases. For the AA and RD models, we saw that GSO has distinguished features in the delocalized and localized
FIG. 5. Single-particle overlap for the gAA model (Eq. (4)) for the entire spectrum of the Hamiltonian, as we change $\alpha$ from $-1$ to $1$ and for two choices of $\lambda = 0.9$ (left panel) and $\lambda = -1.1$ (right panel). The red line is the mobility edges, separating delocalized and localized phases based on Eq. (5). Color bar shows the scale of the SPO. We fix $N = 500$.

phases. In addition, we utilize the notion of the SPO, to characterize the single-particle mobility edges in models like gAA. This idea can also be used for characterizing other free fermion models with mobility edges which separate delocalized, localized, and also multifractal eigenstates\textsuperscript{[13][14][15]}. It is also possible to generalize the notion of the SPO and GSO for many-body interacting models, although some effort has been done before\textsuperscript{[12]}. 

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