Anomalously localized states and multifractal correlation of critical wavefunctions in two-dimensional electron systems with spin-orbital interactions

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Anomalously localized states (ALS) at the critical point of the Anderson transition are studied for the SU(2) model belonging to the two-dimensional symplectic class. Giving a quantitative definition of ALS to clarify statistical properties of them, the system-size dependence of a probability to find ALS at criticality is presented. It is found that the probability increases with the system size and ALS exist with a finite probability even in an infinite critical system, though the typical critical states are kept to be multifractal. This fact implies that ALS should be eliminated from an ensemble of critical states when studying critical properties from distributions of critical quantities. As a demonstration of the effect of ALS to critical properties, we show that the distribution function of the correlation dimension $D_2$ of critical wavefunctions becomes a delta function in the thermodynamic limit only if ALS are eliminated.

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I. INTRODUCTION

The disorder induced metal-insulator transition, namely, the Anderson transition corresponds to a fixed point in a real-space renormalization transformation. Approaching the critical point from an insulating phase, the localization length $\xi$ increases and diverges at the critical point. Since the length $\xi$ is a unique characteristic length near the transition point, there is no length scale characterizing the critical state. This implies that the wavefunction at the Anderson transition point (the critical wavefunction) is scale invariant. In fact, Aoki and Wegner have demonstrated that critical wavefunctions have multifractal properties which can be described by an infinite set of exponents. These exponents are quite important because they define not only spatial distribution of wavefunction amplitudes but also dynamical properties of the electron system at criticality.

Among various works in which exponents characterizing multifractality of critical wavefunctions have been extensively studied, numerical multifractal analyses based on the box-counting method give the most reliable values of exponents at the present stage, except for a few exactly-solvable problems. However, values of exponents reported so far widely fluctuate. For example, the correlation dimension $D_2$ for the three-dimensional Anderson model takes values ranging from 1.45 to 1.68. These fluctuations result mainly from the following reasons. One is a finite-size effect which can be excluded in principle by a finite-size scaling. Another reason is related to anomalously localized states (ALS) at the critical point. Statistical properties of ALS in a metallic phase have been studied well. Specific local configurations of disorder in a finite spatial region may lead to electron states localized within this region, while the average disorder is weak compared to the critical disorder. Although such ALS induced by statistical fluctuations of disorder configurations remain even if the system is infinite, they do not contribute to ensemble-averaged properties of amplitude distributions of wavefunctions or transport properties in the metallic phase. This is because ALS have point-like spectra, while metallic (extended) states have continuous ones.

ALS also appear at the critical point. The localization length of a multifractal wavefunction diverges in an infinite system at the critical point, while sizes of ALS are finite. In contrast to the case of metallic phases, it is not obvious that ALS can be neglected in infinite systems at the critical point. The effect of ALS is much stronger than that in metallic phases. However, fundamental knowledge on, e.g., a probability to find ALS or influences of ALS to critical properties, are still unclear because of the lack of a quantitative definition of ALS. It is important to clarify how strong ALS affect critical properties by defining ALS quantitatively and revealing their fundamental features.

In the present paper, we give a quantitative and practical definition of ALS at criticality suitable for numerical investigations. In order to define ALS, it is natural to evaluate spatial extent of wavefunctions. Quantum states with localization lengths less than the system size are regarded as ALS in a finite system. This definition is, however, not appropriate for precise and systematic calculations, because we cannot determine which wavefunctions are more multifractal if localization lengths of two wavefunctions are both close to the system size. We show that the correlation function of box-measures of multifractal critical wavefunctions works quite well for the definition of ALS. In order to demonstrate how ALS influence critical properties of the Anderson transition, we examine the distribution function of the correlation dimension $D_2$ of critical wavefunctions. Results presented here urge us to reconsider our picture of ALS.

The efficiency of our definition of ALS is demonstrated by applying them to critical wavefunctions in two-dimensional electron systems with spin-orbit interactions (symplectic systems), which exhibit the Anderson metal-insulator transition. For ensuring the multifractality of typical critical wavefunctions even in a short-range scale,
we adopt the SU(2) model in which scaling corrections due to irrelevant scaling variables are negligible.

This paper is organized as follows. In Sec. II we propose a quantitative definition of ALS based on the correlation function of box-measures of wavefunction amplitudes. Some quantities and exponents appearing in the multifractal analysis are defined in this section. In Sec. III we briefly explain the SU(2) model for which our definition of ALS works via concrete examples of ALS in the model. We display how well our definition of ALS estimates the correlation of box measures. This will be demonstrated by showing an example in Sec. IV.

**II. DEFINITION OF ANOMALOUSLY LOCALIZED STATES**

In this section, we propose a quantitative definition of ALS based on a multifractal analysis. For this purpose, we give some definitions of basic quantities and exponents used in the multifractal analysis. At first, we introduce a quantity $Z_q(l)$ defined by

\[ Z_q(l) = \sum_b \mu^q_b(l), \]

where $\mu_b(l) = \sum_{i \in b(l)} \langle |\psi_i|^2 \rangle$ or $\mu_b(l) = \int_{b(l)} |\psi(r)|^2 dr$ in continuous systems is the box measure of wavefunction amplitudes. The summation $\sum_{i \in b(l)}$ (or the integral $\int_{b(l)} dr$) is taken over sites $i$ (or the spatial region) within a small box $b$ of size $l$, and the summation in Eq. (1) is taken over such boxes. The quantity $q$ is the order of the moment $Z_q(l)$. For a multifractal wavefunction, $Z_q(l)$ obeys a power law

\[ Z_q(l) \propto l^{\tau(q)}, \]

where $\tau(q)$ is called the mass exponent. From Eq. (2), the mass exponent is given by

\[ \tau(q) = \lim_{l \to 0} \frac{\ln Z_q(l)}{\ln l}. \]

Since ALS are not multifractal, it seems possible to define ALS by calculating deviations of the moment $Z_q(l)$ from the power law Eq. (2). However, the moment $Z_q(l)$ represents simply the average of $\mu^q_b(l)$ [except for a trifling prefactor $(L/l)^q$], and does not describe the multifractal correlation of box measures. Thus, the quantity $Z_q(l)$ is not sensitive to ALS and Eq. (2) is insufficient for the definition of ALS. This will be demonstrated by showing an example in Sec. IV.

The correlation function $G_q(l, L, r)$ defined below can describe the box-measure correlations and can be expressed as

\[ G_q(l, L, r) = \frac{1}{N_b N_r} \sum_{b} \sum_{r} \mu^q_{b(l)} \mu^q_{b(r)}, \]

where $\mu_{b(l)}$ is the box measure of a box $b(l)$ of size $l$ fixed distance $r - l$ away from the box $b(l)$, $N_b$ (or $N_r$) is the number of boxes $b(l)$ (or $r(l)$), and the summation over all such boxes $b(l)$ and $r(l)$. The correlation function $G_q(l, L, r)$ is a generalized quantity of the $q$th moment $Z_q(l)$. For a multifractal wavefunction, $G_q(l, L, r)$ should behave as

\[ G_q(l, L, r) \propto I^{(q)} L^{-y(q)} r^{-z(q)}, \]

where $x(q)$, $y(q)$, and $z(q)$ are exponents in multifractal correlations. This proportionality relation is sensitive to ALS and then suitable for defining ALS. Our purpose is to examine multifractality of individual wavefunctions by using Eq. (5), the system size $L$ is always fixed. To find the $l$ and $r$ dependences of $G_q(l, L, r)$, we concentrate on the following functions,

\[ Q_l(l) = G_{2}(l, L, r = l) \propto I^{(2)} r^{-(2)}, \]

and

\[ R_{l}(r) = G_{2}(l = 1, L, r) \propto r^{-z(2)}. \]

In order to quantify non-multifractality of a specific wavefunctions, it is convenient to introduce variances $\text{Var}(\log_{10} Q_l)$ and $\text{Var}(\log_{10} R_l)$ from the linear functions of $\log_{10} l$ and $\log_{10} r$. $\log_{10} Q_{l}(l) = [x(2) - z(2)] \log_{10} l + c_Q$ and $\log_{10} R_{l}(r) = -z(2) \log_{10} r + c_R$, respectively, calculated by the least-square fit. From these variances, a quantity $\Gamma$ is defined by

\[ \Gamma(L, \lambda) = \lambda \text{Var}(\log_{10} Q_{L}) + \text{Var}(\log_{10} R_{L}), \]

where $\lambda$ is a factor to compensate the difference between average values of $\text{Var}(\log_{10} Q_{L})$ and $\text{Var}(\log_{10} R_{L})$. Using $\Gamma$ given by Eq. (8), the quantitative and exponential definition of ALS at criticality is presented by

\[ \Gamma > \Gamma^*, \]

where $\Gamma^*$ is a critical value of $\Gamma$ to distinguish ALS from multifractal states and chosen appropriately as demonstrated later.

**III. MODEL**

In this paper, the efficiency of the above definition of ALS and the effect of ALS will be demonstrated for an ensemble of wavefunctions at the Anderson metal-insulator transition. For this purpose, the effect of scaling corrections due to irrelevant fields which is a finite-size effect and independent of the ALS should be reduced as
much as possible. Therefore, considering the advantage of system sizes, we focus our attention on the Anderson transition in two-dimensional electron systems with strong spin-orbit interactions, in which systems have no spin-rotational symmetry but have the time-reversal one. Hamiltonians describing these systems belong to the symplectic ensemble. Several models\cite{30,31,32} have been proposed so far to represent the symplectic systems. Although the Ando model\cite{28} has been most extensively studied, relatively large scaling corrections make it difficult to distinguish the ALS effect. Recently, Asada et al.\cite{29} proposed the SU(2) model belonging to the symplectic class, for which scaling corrections are negligibly small. While the SU(2) model is rather mathematical, we believe that presented results are qualitatively the same with those for other systems exhibiting the Anderson transition.

The Hamiltonian of the SU(2) model is compactly written in a quaternion representation as

\[ H = \sum_i \varepsilon_i c_i^\dagger c_i - V \sum_{i,j} R_{ij} c_i^\dagger c_j, \tag{10} \]

where \( c_i^\dagger (c_i) \) is the creation (annihilation) operator acting on a quaternion state vector, \( R_{ij} \) is the quaternion-real hopping matrix element between the sites \( i \) and \( j \), and \( \varepsilon_i \) denotes the on-site random potential distributed uniformly in the interval \([-W/2, W/2]\). The strength of the hopping \( V \) is taken to be the unit of energy. Hereafter, we denote quaternion-real quantities by bold symbols. A quaternion-real number \( x \) can be written in the form

\[ x = \sum_{\mu=0}^3 x_\mu \tau^\mu, \tag{11} \]

where \( x_\mu \) is a real number and the primitive elements \( \tau^\mu (\mu = 0, 1, 2, 3) \) define the quaternion algebra as

\[ \tau^0 \tau^0 = - \tau^n \tau^n = \tau^0 \quad (n = 1, 2, 3), \tag{12} \]

\[ \tau^0 \tau^n = \tau^n \tau^0 = \tau^n \quad (n = 1, 2, 3), \tag{13} \]

\[ \tau^l \tau^m = - \tau^m \tau^l = \tau^n \quad (l, m, n = 1, 2, 3 \text{ and any cyclic permutation}). \tag{14} \]

In the Hamiltonian Eq. (10), the matrix element \( R_{ij} \) is defined by

\[ R_{ij} = \cos \alpha_{ij} \cos \beta_{ij} \tau^0 + \sin \gamma_{ij} \sin \beta_{ij} \tau^1 - \cos \gamma_{ij} \sin \beta_{ij} \tau^2 + \sin \alpha_{ij} \cos \beta_{ij} \tau^3, \tag{15} \]

where \( \alpha_{ij} \) and \( \gamma_{ij} \) are distributed uniformly in the range of \([0, 2\pi]\), and \( \beta_{ij} \) is distributed according to the probability density \( P(\beta) d\beta = \sin(2\beta) d\beta \) for \( 0 \leq \beta \leq \pi/2 \).

We have calculated eigenvectors of the Hamiltonian Eq. (10) by using the forced oscillator method (FOM)\cite{29}. The FOM is an efficient algorithm to solve quickly an eigenvalue problem with saving memory spaces, in which an eigenvector belonging to the eigenenergy \( E \) is extracted as a resonant mode of the classical dynamical system described by the same Hamiltonian to an external periodic force with the angular frequency \( \sqrt{E} \). The FOM can be extended to the eigenvalue problem of quaternion-real matrices. The corresponding dynamical system is described by

\[ \frac{d^2}{dt^2} x_i(t) = - \sum_j H_{ij} x_j(t) + F_i \cos(\Omega t), \tag{16} \]

where \( H_{ij} \) is the quaternion-real matrix element of the Hamiltonian Eq. (10), \( x_i(t) \) is the displacement vector, and \( F_i \) is the site-dependent amplitude of a quaternion-real external force. Decomposing the displacement \( x_i(t) \) into quaternion normal modes \( e_i(\lambda) \) as \( x_i(t) = \sum_\lambda e_i(\lambda) Q_\lambda(t) \), the quaternion coefficient \( Q_\lambda(t) \) with \( \lambda \) for which \( E_\lambda \) is the closest eigenenergy to \( \Omega^2 \) enlarges compared to other coefficients after a long time. We should note the order of normal modes \( e_i(\lambda) \) and \( Q_\lambda(t) \) in the decomposition of \( x_i(t) \) reflecting the non-commutative property of quaternion numbers. An iterative procedure can accelerate the enhancement of \( Q_\lambda(t) \). Finally, we can obtain the eigenvector of the quaternion-real matrix \( H \) as \( x_i(t) \sim e_i(\lambda) \). The obtained quaternion-real eigenvector represents two physical states simultaneously, which correspond to the Kramers doublet belonging to \( E_\lambda \). Denoting \( e_i(\lambda) = \sum_\mu e_i^\mu (\lambda) \tau^\mu \), the \( \mu \)th elements of the two complex vectors \( |f(\lambda)\rangle \) and \( |g(\lambda)\rangle \) corresponding to the Kramers doublet are given by

\[ f_{2\lambda-1}(\lambda) = e_i^0 (\lambda) + i e_i^1 (\lambda), \quad f_{2\lambda}(\lambda) = -e_i^0 (\lambda) + i e_i^1 (\lambda), \]

\[ g_{2\lambda-1}(\lambda) = e_i^0 (\lambda) + i e_i^1 (\lambda), \quad g_{2\lambda}(\lambda) = e_i^0 (\lambda) - i e_i^1 (\lambda), \]

respectively. As we expected, \( |g(\lambda)\rangle \) is the time-reversal vector of \( |f(\lambda)\rangle \), namely, \( |g(\lambda)\rangle = -i\sigma_y |f(\lambda)\rangle \), where \( \sigma_y \) is the \( y \)-component of the Pauli matrix.

**IV. ANOMALOUSLY LOCALIZED STATES FOR THE SU(2) MODEL AT THE CRITICAL POINT**

In this section, we demonstrate by showing critical wavefunctions of the SU(2) model that ALS can be discriminated by examining the box-measure correlation function defined by Eq. (4). Critical wavefunctions are calculated by the FOM for the SU(2) model with \( W = 5.952 \) for which the eigenstate with \( E = 1 \) is known to be critical\cite{28}. All wavefunctions calculated in this paper have their eigenenergies closest to \( E = 1 \). This implies that we extract only one critical state from a system. In numerical calculations, the periodic boundary conditions are employed for both directions. Figure 1 shows squared amplitudes of critical wavefunctions in systems of \( L = 120 \) with different realizations of on-site random potentials. The wavefunctions shown in Fig. 1a seems to be strongly localized with a single peak of large amplitudes even for the critical conditions (\( W = 5.952 \) and \( E \approx 1 \)). We can regard this eigenstate as an ALS. In order to exclude a possibility that the critical energy is
shifted due to finite-size effects, it has been confirmed that eigenstates belonging to adjacent energy levels are not localized. The wavefunction shown in Fig. 1(b) is also localized with a relatively long localization length. In this case, we see two peaks of large amplitudes in the spatial distribution of squared amplitudes. On the contrary, the wavefunction shown in Fig. 1(c) seems to be multifractal. The existence of localized wavefunctions at criticality are not peculiar to the SU(2) model. We have obtained localized wavefunctions also for the Ando model at criticality.

In order to distinguish systematically ALS from wavefunctions shown in Fig. 1 by the box-measure correlation function, we calculate $Q_L(l)$ and $R_L(r)$ for these three wavefunctions. Results are shown in Fig. 2 by filled circles $[Q_L(l)]$ and open circles $[R_L(r)]$. Figures 2(a), 2(b), and 2(c) correspond to the wavefunctions in Figs. 1(a), 1(b), and 1(c), respectively. Dashed lines are just guide to the eye. The quantity $Q_L(l)$ gives the averaged value over different ways to divide the system into small boxes of size $l$. It is found that $Q_L(l)$ and $R_L(r)$ for the wavefunction Fig. 2(a) do not obey power laws as shown in Fig. 2(a), which implies that the wavefunction is not multifractal. The function $R_L(r)$ shown in Fig. 2(b) does not follow a power law, while $Q_L(l)$ seems to be fit to a straight line. This is because the wavefunction shown in Fig. 2(b) has two peaks of large amplitudes and bears resemblance to the multifractal wavefunction [Fig. 2(c)] in a local view. There exists, however, a distinct characteristic length scale, namely, a distance between two peaks. This fact prevents $R_L(r)$ from obeying a power law. Since $Q_L(l)$ is the same with $N_b^{-1} Z_4(l)$, Fig. 2(b) shows that $Z_4(l)$ is not sensitive to ALS. On the contrary, both $Q_L(l)$ and $R_L(r)$ depicted in Fig. 2(c) well follow power laws. This means that the wavefunction shown in Fig. 2(c) is multifractal as we expected.

We calculate the distribution function of the quantity $\Gamma$ defined by Eq. 8 for ensembles of critical wavefunc-
Thus, the function \( F(\Gamma, L) \) is characterized only by the (arithmetic) average value of \( \Gamma \), and is a function independent of \( L \), and

\[
F(\Gamma, L) = F_0(\bar{\Gamma}) f(\Gamma/\bar{\Gamma})
\]

where \( \bar{\Gamma} \) is the average value of \( \Gamma \) and is a function of the system size \( L \), \( f \) is a function independent of \( L \), and

\[
F_0 \text{ is a normalization factor. The } L \text{ dependence of } \bar{\Gamma} \text{ is shown in Fig. 4. We see from Fig. 4 that } \bar{\Gamma} \text{ converges to a finite value } \Gamma_\infty \text{ for } L \to \infty, \text{ which implies that the probability to find ALS in an infinite system remains to be finite. The fact that } F(\Gamma, L) \text{ can be scaled only by } \bar{\Gamma} \text{ would be an important statistical property of ALS. These results were obtained for the SU(2) model. However, we believe that similar qualitative features will be obtained for other systems at the Anderson transition point.}

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distribution functions of \( D_2 \) for the same ensembles as for Fig. 3 are shown in Fig. 5. The correlation dimension fluctuates over samples in finite systems whereas the width of the distribution function \( P(D_2) \) becomes narrow as the system size increases. This fluctuation results from the existence of ALS and some scaling corrections due to a finite system-size. The fluctuation of \( D_2 \) due to ALS remains even in infinite systems. In order to obtain the distribution function of \( D_2 \) for typical critical wavefunctions, we eliminate ALS defined by \( \Gamma > \Gamma^* \) from the original ensembles. To this end, we choose the value of \( \Gamma^* \) appeared in the definition of ALS [Eq. (9)] as \( \Gamma^* = 0.03 \). We study the system-size dependence of the standard deviation \( \sigma(L) \) of the distribution function \( P(D_2) \).

Figure 6 shows the standard deviations \( \sigma(L) \) for the original ensembles and the refined ensembles (i.e., the ensembles in which ALS are eliminated). Error bars of \( \sigma \) estimated by the bootstrap method are smaller than their marks. According to a standard scaling analysis that the \( L \)-dependence of a statistical quantity at the critical point is scaled by an irrelevant length, we can write \( \sigma(L) \) as

\[
\sigma(L) = \sigma_\infty + cL^{-y},
\]

where \( y \) is an irrelevant exponent and \( \sigma_\infty \) is the standard deviation for \( L \to \infty \). Fitting data for the original ensembles to Eq. (10), we obtain \( \sigma_\infty = 0.032 \pm 0.018 \) and \( y = 0.39 \pm 0.12 \). The value of \( \sigma_\infty \) is positive finite even though its error bar is taken into account. More precisely, \( \sigma_\infty \) is not zero with the confidence coefficient 93\%. This implies that \( D_2 \) fluctuates even in the thermodynamic limit as shown by Ref. 35. On the contrary, fitting data for the refined ensembles gives \( \sigma_\infty = 0.005 \pm 0.013 \) and \( y = 0.42 \pm 0.08 \). In this case, \( \sigma_\infty \) is very close to zero, and the error bar of \( \sigma_\infty \) is larger than its mean value. Therefore, it is natural to deduce that \( \sigma_\infty \) is zero. We can then conclude that the correlation dimension \( D_2 \) for typical critical wavefunctions does not fluctuate in the thermodynamic limit. It should be noted that ALS were also eliminated in the numerical work of Ref. 11 which supports the non-fluctuating \( D_2 \) for \( L \to \infty \).

Finally, we consider the exponent \( y \) in Eq. (10). In the SU(2) model, the scaling correction due to a spin-relaxation length is quite small. What is the origin of the irrelevant exponent \( y \) in this case? We emphasize that the value of \( y \) is close to \( d - D_2 \) within the numerical error, where \( D_2 = 1.66 \pm 0.05 \) estimated for the refined ensemble for \( L = 120 \). The relation \( y = d - D_2 \) has been analytically predicted by Polyakov,\textsuperscript{38} where \( y \) is the exponent describing the correction related to the quantum return probability. Thus, we claim that the exponent \( y \) describing the system-size dependence of the standard deviation \( \sigma(L) \) for the refined ensembles is nothing but the irrelevant exponent predicted by Polyakov, which is independent of microscopic details of systems.

VI. CONCLUSIONS

We have studied statistical properties of anomalously localized states (ALS) at the Anderson transition point by defining ALS quantitatively. In our definition, a wavefunction is regarded as ALS when the functions \( Q_L(l) \) and \( R_L(r) \) which are the special cases of the box-measure correlation functions \( G_q(l, r) \) do not follow the power laws Eqs. (9) and (10). Applying the definition of ALS to ensembles of critical wavefunctions of the SU(2) model which describes a two-dimensional electron system with strong spin-orbit interactions, it has been revealed that the probability to find ALS at criticality increases with the system size, while typical states are multifractal. This result suggests that ALS should be eliminated from an ensemble of critical wavefunctions if we study critical
properties from distributions of critical quantities. We also found that the distribution function of $\Gamma$ is characterized only by its average value $\bar{\Gamma}$, where $\Gamma$ quantifies non-multifractality of a wavefunction. The influence of ALS to critical properties in infinite systems has been demonstrated by investigating the distribution of the correlation dimension $D_2$. While the distribution function of $D_2$ has a finite width in the thermodynamic limit if ALS are not eliminated from an ensemble of critical wavefunctions, $D_2$ takes a definite value for $L \to \infty$ if ALS are eliminated.

The existence of ALS at the critical point gives crucial influences also for transport properties at the Anderson transition point. The value of conductance for ALS is small, while it is relatively large for multifractal states. The fluctuation of critical conductance is deeply related to the ALS distribution such as Fig. 3. Furthermore, the frequency dependence of ac conductivity is affected by ALS as well, because strongly localized ALS contribute only to high-frequency ac transport. Our numerical works have been performed for the SU(2) model. We believe, however, that properties of ALS are essentially the same for systems belonging to other universality classes which exhibit the Anderson transition. Further quantitative investigations of ALS reveal concrete relations between the nature of ALS and physical phenomena.

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