Anomalously Localized States in the Anderson Model

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It is demonstrated that anomalously localized states (ALS) in the Anderson model, being lattice specific, are not related to any of the continuous theories. We identify the spatial structure of ALS on a lattice and calculate their likelihood. Analytical results explain pecularities in previous numerical simulations.

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In a weakly disordered conductor, the typical value of an eigenfunction intensity, $|\Psi_\alpha(\boldsymbol{r})|^2$, is of order L^{-d}, where L is the sample size, in d dimensions ($d = 2, 3$). However, with certain probability, the intensity can assume anomalously large values. The study of such rare events in diffusive conductors was pioneered in Ref. [1] followed by Refs. [2–4]. The "prelocalized" states, studied in Refs. [1–4], exhibit an anomalous buildup of intensity in a region of space, of a size larger than the mean-free path, l. The properties of these states are universal, in the sense that the disorder enters only via the mean-free path. Another type of rare events was identified in [5]. The corresponding eigenstates, designated as "almost localized states," are confined to small rings, of a sub-mean-free-path size. These states are nonuniversal, i.e., sensitive to the microscopic details. In particular, their likelihood sharply increases with the disorder correlation radius, R_c (for fixed value of l). Below we designate any type of an anomalously large buildup of intensity as an anomalously localized state (ALS).

The above-mentioned analytical studies of the ALS were limited to models described by a continuous (Gaussian) random potential. On the other hand, numerical studies of disordered electronic systems are necessarily performed on the lattice, most often within the Anderson model [6], with the tight-binding Hamiltonian

$$\hat{H} = \sum_{\boldsymbol{r},\boldsymbol{r}'} c_{\boldsymbol{r}}^\dagger c_{\boldsymbol{r}'} + \sum_{\boldsymbol{r}} V_{\boldsymbol{r}} c_{\boldsymbol{r}}^\dagger c_{\boldsymbol{r}}, \tag{1}$$

where $c_{\boldsymbol{r}}^\dagger$ is the creation operator of an electron at site $\boldsymbol{r}$ of a d-dimensional hypercubic lattice with lattice constant equal to 1, and $V_{\boldsymbol{r}}$ is a random on-site energy with rms $\Delta_d = \langle V_{\boldsymbol{r}}^2 \rangle^{1/2}$. The Anderson model has become a powerful tool for numerical study of various disorder-related phenomena. The early success [7] in confirmation of the scaling theory [8] was followed by recent numerical studies that have successfully addressed more delicate issues such as (i) critical exponents [9], (ii) quantitative characteristics of the quantum Hall transition [10], (iii) different aspects of the level statistics at the Anderson transition [11,12], (iv) Anderson transition in 2D [13] possible with spin-orbit coupling [14], (v) the critical conductance distribution at the transition [15,16], and (vi) verifying scaling for the full conductance distribution [17]. These successes have encouraged a number of authors [18–24] to employ the Anderson Hamiltonian for numerical study of the ALS in disordered conductors. In particular, the subject of interest is the distribution of the eigenfunction intensity, $t = |\Psi(0)|^2 L^d$, at a given energy, E, defined as

$$f_d(E, t) = \frac{1}{\nu L^d} \left\langle \sum_\alpha \delta(t - |\Psi_\alpha(0)|^2 L^d) \delta(E - E_\alpha) \right\rangle, \tag{2}$$

where Ψ_α and E_α are the eigenfunctions and eigenenergies of the Hamiltonian (1), respectively, and $\nu(E)$ is the density of states. The ALS are responsible for the large-t tail of the distribution (2). They correspond to the anomalous buildup, $t \gg 1$, of certain eigenfunctions inside the volume L^d. Simulations performed have revealed a number of unexpected peculiarities in the likelihood of the almost localized states: (i) in 2D, the behavior $f_2(E, t) \propto \exp(-C_E \ln^2 t)$, which is in accord with the theoretical prediction of Refs. [1–4], was obtained [18]. However, upon changing the disorder magnitude, Δ_2, the constant C_E did not scale with the conductance $g \sim \Delta_2^{-2}$; (ii) the magnetic field dependence of C_E in Ref. [18] turned out to be very weak. This is in contrast to the simulations [25] of the eigenfunctions intensity distribution, in which the model of the kicked rotor was studied and which demonstrated that under breaking of the time-reversal symmetry the coefficient C increases by a factor close to 2; (iii) Simulations of Ref. [24] produced $f_d(E, t)$, which *falls off* with the *correlation radius* of the random on-site energies, $V_{\boldsymbol{r}}$, for a *given* conductance, g, which is, again, in conflict with theory; (iv) Simulations in 3D [21,22] indicate that the wave function intensities, $|\Psi(m_x, m_y, m_z)|^2$, of ALS in a cube with a side L, plotted in the lexicographic order $m \to L^2(m_x - 1) + L(m_y - 1) + m_z$ (see Fig. 1), are *structured*; a typical wave function represents a system of well-defined and almost *even-spaced* spikes, each spike extending over a certain narrow interval of m. In contrast, diffusive wave

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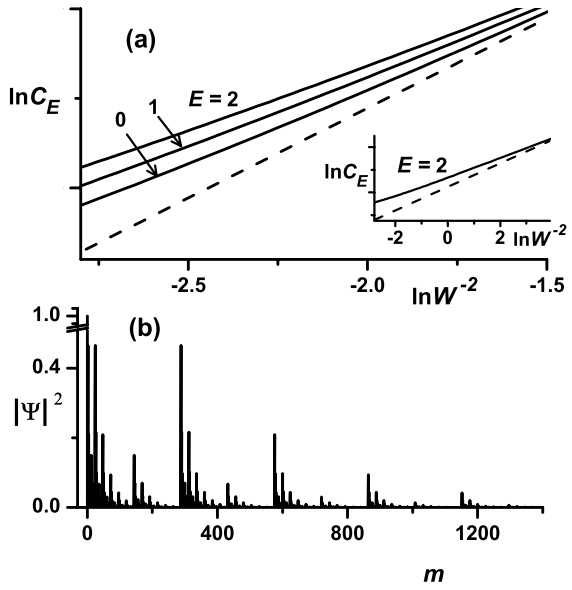

FIG. 1. (a) Numerical coefficient C_E in the dependence $|\ln f_2(E,t)| = C_E \ln^2 t$ is plotted from Eq. (11) versus the disorder strength, W, at different energies. The dotted line is a weak-disorder asymptotics, $C_E \propto W^{-2}$. Inset: $C_E(W)$ at $E = 2$ is shown in the domain of the weak disorder. (b) Wave function of an ALS with a decrement $\gamma_3 = 0.7$ in a cube with a side $L = 12$ is shown in lexicographic order $m \to L^2(m_x - 1) + L(m_y - 1) + m_z$.

functions $|\Psi(m)|^2$, plotted in the same way, do not exhibit any structure [21,22].

In the present Letter, we demonstrate that the above peculiarities stem from the fundamental difference between the ALS in continuum and on the lattice. This difference is most pronounced for energies close to the band center, $E = 0$, where all the simulations [18–24] were performed.

One should realize that the point $E = 0$ is rather special and that "continuous" theories can break down in the vicinity of this point, even if $l \gg 1$. For instance, in the 1D case, it has been noticed in Refs. [26,27] that the single parameter scaling, well established for weakly disordered continuous models, is violated near $E = 0$. Similar "nonuniversal" phenomena near $E = 0$ should persist also in 2D (3D) lattice models. In 2D with $E(\boldsymbol{k}) = 2(\cos k_x + \cos k_y)$, the center of the band corresponds to the square $k_x \pm k_y = \pm\pi$ (see Fig. 2), i.e., the dispersion law differs drastically from that in the continuum.

Below we identify a new type of ALS, specific for the lattice, and calculate their likelihood. The analytical theory allows to account for all the peculiarities (i)–(iv) uncovered in the numerics. The main idea is that the intrinsic periodicity of the Anderson model offers a possibility to localize the eigenstates by the *periodic* fluctuations, $V_{\boldsymbol{r}}$, with a period 2, which cause a "dimerization" of the underlying lattice. In 1D, such Peierls-like fluctuations [28] create a gap in the spectrum of the Hamiltonian (1). In order to "pin" the center of the

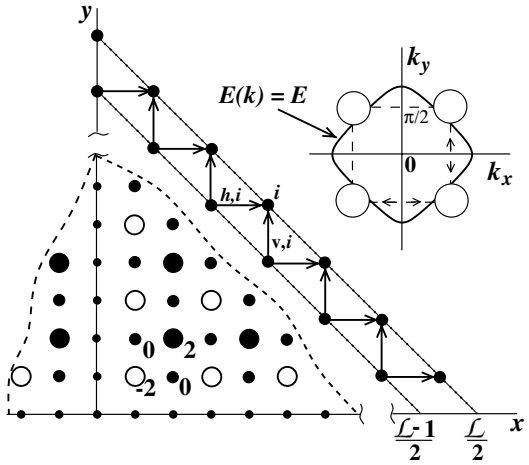

FIG. 2. Shown is one quadrant of the square with a side $\mathcal{L}/\sqrt{2}$. On-site energies in the presence of a period-doubling fluctuation are shown in the units of V_0; π-phase slip is shown only in the x direction. Inset: The solid line is a surface $E(\boldsymbol{k}) = E$. The dotted lines are regions in $\boldsymbol{k}$ space perturbed by the fluctuation.

in gap state to a certain site, a π phase shift in the periodicity should occur at this site, by analogy to the topological solitons [29]. Our prime observation is that similar fluctuations (period doubling along each axis accompanied by a π phase shift) are capable to localize tight-binding electrons in higher dimensions, *without formation of a gap*. It is still convenient pedagogically to start from the 1D case, and then generalize the theory to higher dimensions.

1D case.—As was explained above, the period-doubling fluctuation $V^{(0)}(n \neq 0) = V_0 \,\mathrm{sgn}(n) \exp(i\pi n)$ with π phase shift at $n = 0$ creates a localized state with energy, $E \in [-V_0, V_0]$. Indeed, upon introducing a vector $\chi_n = \{\Psi(2n), \Psi(2n+1)\}$, the Schrödinger equation $\hat{H}\Psi = E\Psi$ with on-site energies $V^{(0)}(n \neq 0)$ takes the form

$$[E - V_0 \,\mathrm{sgn}(n)\sigma_3 - \sigma_1]\chi_n = \sigma_- \chi_{n+1} + \sigma_+ \chi_{n-1}, \quad (3)$$

where σ_i are the Pauli matrices. The corresponding eigenvector $\chi_n \propto \exp(i\pi n - 2\gamma_1|n|)$ decays both to the left and to the right from the site $n = 0$ [29] with a decrement $\gamma_1(V_0) = \mathrm{arcsinh}\sqrt{\frac{1}{4}(V_0^2 - E^2)}$. The actual position of the localized state within the gap $[-V_0, V_0]$ is governed by the on-site energy at the origin, $V(n = 0)$. Namely, $V(n = 0)$ and E are related as $V(n = 0) = E \coth\gamma_1$.

For a 1D interval of a length, $\mathcal{L}$, the fluctuation $V^{(0)}(n)$ with $V^{(0)}(0) = V(n = 0)$ results in the buildup, $\tau = |\Psi(0)|^2/|\Psi(\mathcal{L}/2)|^2 = \exp[\gamma_1(V_0)\mathcal{L}]$, of the eigenfunction at $n = 0$. However, the statistical weight of the fluctuation $V^{(0)}(n)$ is zero. Random deviations of the on-site energies, $V(n)$, from $\pm V_0$ give rise to a certain distribution, $\mathcal{P}_{1,\mathcal{L}}(E,\tau)$, of buildups, τ. To find this distribution, we note that deviations of $V^{(0)}(n)$ from $\pm V_0$ result in the fluctuations of the *local* decrement, γ_1, so that

$$\mathcal{P}_{1,\mathcal{L}}(E,\tau)=\int_{-\infty}^{0}dV_1\int_{0}^{\infty}dV_2\ldots P(V_1)\ldots P(V_{\mathcal{L}/2})\times\delta(\tau-e^{S})\quad=\langle\delta(\tau-e^{S})\rangle_{V_n}=\frac{1}{\tau}\tilde{\mathcal{P}}_{1,\mathcal{L}}(E,\ln\tau),\tag{4}$$

where $S=2\sum_n\gamma_1(V_n)=2\sum_n\operatorname{arcsinh}\sqrt{\frac{1}{4}(V_n^2-E^2)}$, and $P(V_i)$ is the distribution of the on-site energy, V_i. The expression for S is valid for $S\gg 1$ (strong buildup). Note that continuous analog of Eq. (3) is the Dirac equation with fluctuating mass, where the expression for S via local decrements is valid for any S [30]. Now we notice that the function $\tilde{\mathcal{P}}_{1,\mathcal{L}}$ satisfies the recurrent relation

$$\tilde{\mathcal{P}}_{1,\mathcal{L}}(\ln\tau)=\int dV_1P(V_1)\tilde{\mathcal{P}}_{1,\mathcal{L}-1}[\ln\tau-2\gamma_1(V_1)].\tag{5}$$

Introducing an auxiliary function

$$I_1(\kappa,E)=\int_E^{\infty}dV\,P(V)\exp[-2i\kappa\gamma_1(V)],\tag{6}$$

we have

$$\tilde{\mathcal{P}}_{1,\mathcal{L}}(\ln\tau)=\int d\kappa e^{i\kappa\ln\tau}[I_1(\kappa)]^{\mathcal{L}/2}=e^{-\mathcal{F}_{1,\mathcal{L}}(E,\tau)}.\tag{7}$$

The analytical expression for log probability of the buildup, $\mathcal{F}_{1,\mathcal{L}}(E,\tau)$, can be obtained in the domain of $\mathcal{L}$ where the main contribution to the integral (6) comes from small κ. Then we can use the expansion $I_1(\kappa)=I_1(0)-i\langle\gamma_1\rangle\kappa-\langle\gamma_1^2\rangle\kappa^2$, where $\langle\gamma_1(E)\rangle$ and $\langle\gamma_1^2(E)\rangle$ are the average decrement γ_1 and γ_1^2, respectively. Substitution of this expansion into (7) yields

$$\mathcal{F}_{1,\mathcal{L}}=\frac{\ln^2(\tau/\mathcal{T}_1)I_1^2(0)}{\mathcal{L}[2I_1(0)\langle\gamma_1^2\rangle-\langle\gamma_1\rangle^2]}+\frac{\mathcal{L}}{2}|\ln\{I_1(0,E)\}|,\tag{8}$$

where $\ln\mathcal{T}_1=\frac{1}{2}\langle\gamma_1\rangle\mathcal{L}/I_1(0)$. The domain of applicability of Eq. (8) is $\Delta_1\mathcal{L}\gtrsim\ln(\tau/\mathcal{T}_1)\gg\Delta_1\mathcal{L}^{1/2}$. The origin of $\mathcal{T}_1$ and of the second term in Eq. (8) is the "prefactor" in the functional integral (4), which is crucial for the correct estimation of the build-up probability. The importance of the π phase slip, for our lattice specific trapping mechanism, becomes particularly clear in the 2D case, to which we now turn.

2D case.—Our main finding is that, in 2D, a straightforward extension of the 1D approach applies. Namely, the period-doubling fluctuation $V(n_x,n_y)=V_0[\operatorname{sgn}(n_x)\exp(i\pi n_x)+\operatorname{sgn}(n_y)\exp(i\pi n_y)]$ creates an ALS *without opening a gap* in $\nu(E)$. Indeed, with $V(n_x,n_y)=V(n_x)+V(n_y)$ being *additive*, the solution of the 2D tight-binding equation is *multiplicative*, i.e., $\Psi(n_x,n_y)\propto\exp[(i\pi/2-\gamma_2)(n_x+n_y)]$. The decrement $\gamma_2(V_0)=\operatorname{arsinh}\sqrt{(1/16)(4V_0^2-E^2)}$ differs from γ_1 due to the fact that, in 2D, the energy E is the sum of energies of motion along x and y. Now, analogously to the 1D case, we consider a square with a side, $\mathcal{L}/\sqrt{2}$, as shown in Fig. 2, and introduce a distribution, $\mathcal{P}_{2,\mathcal{L}}(E,\tau)$, of the probability that the buildup from the perimeter to the center along *each path* exceeds τ. The reasoning leading to a recurrent relation between $\tilde{\mathcal{P}}_{2,\mathcal{L}}(E,\ln\tau)=\tau^{\mathcal{L}}\mathcal{P}_{2,\mathcal{L}}(E,\tau)$ and $\tilde{\mathcal{P}}_{2,\mathcal{L}-1}$ goes as follows. The perimeter site, i, of the square, $\mathcal{L}$, is connected to perimeter sites of the square, $\mathcal{L}-1$, with one horizontal and one vertical link, as illustrated in Fig. 2. Denote with $\tau_i^{(\mathcal{L}-1)}$ and $\tau_{i-1}^{(\mathcal{L}-1)}$ the values of buildup from these two perimeter sites to the center. The evolution of τ along the horizontal and vertical links can be expressed as $\ln\tau_{h,i}^{(\mathcal{L})}=\ln\tau_i^{(\mathcal{L}-1)}+2\gamma_2^{(h,i)}$, and $\ln\tau_{v,i}^{(\mathcal{L})}=\ln\tau_{i-1}^{(\mathcal{L}-1)}+2\gamma_2^{(v,i)}$, respectively. This leads to the following relation:

$$\tilde{\mathcal{P}}_{2,\mathcal{L}}(\{\ln\tau_{h,i},\ln\tau_{v,i}\})=\int\ldots\int\{dV_i\,P(V_i)\}\times\tilde{\mathcal{P}}_{2,\mathcal{L}-1}(\{\ln\tau_i-2\gamma_2^{(h,i)},\ln\tau_{i-1}-2\gamma_2^{(v,i)}\}).\tag{9}$$

To make Eq. (9) closed, we recall that the actual buildup, τ_i, is the *minimal* of the horizontal and vertical values, i.e., $\tau_i=\min\{\tau_{h,i},\tau_{v,i}\}$. Taking this fact into account, the solution for $\tilde{\mathcal{P}}_{2,\mathcal{L}}$ has the form similar to Eq. (7)

$$\tilde{\mathcal{P}}_{2,\mathcal{L}}(\ln\tau)=\left(\int d\kappa\,e^{i\kappa\ln\tau}[I_2(\kappa)]^{\mathcal{L}/2}\right)^{\mathcal{L}/2}=e^{-\mathcal{F}_{2,\mathcal{L}}(E,\tau)},$$

where the function $I_2(\kappa)$ is defined by Eq. (6) with $\gamma_1(V)$ replaced by $\gamma_2(V)$. This leads to the following 2D generalization of Eq. (8):

$$\mathcal{F}_{2,\mathcal{L}}=\frac{C_E}{4}\left[\ln\tau-\frac{\langle\gamma_2\rangle\mathcal{L}}{2I_2(0)}\right]^2+\frac{\mathcal{L}^2}{4}|\ln\{I_2(0,E)\}|,\tag{11}$$

$$C_E=\frac{2I_2^2(0)}{2I_2(0)\langle\gamma_2^2\rangle-\langle\gamma_2\rangle^2}.\tag{12}$$

The remaining task is to express the intensity distribution (2) through the distribution of buildups, τ. We consider only the 2D case. For a given sample size, L, and the fluctuation size, $\mathcal{L}$, the values t and τ are related via the normalization condition for $\Psi(n)$, which can be presented as $tL^{-2}[(2\gamma_2)^{-2}+\tau^{-1}(L^2-\mathcal{L}^2)]=1$. Taking into account that $2\gamma_2\mathcal{L}=\ln\tau$, we obtain

$$\frac{\tau}{t}=1-\left(\frac{\mathcal{L}}{L}\right)^2+\left(\frac{\mathcal{L}}{L}\right)^2\frac{\tau}{\ln^2\tau}\approx 1+\left(\frac{\mathcal{L}}{L}\right)^2\frac{\tau}{\ln^2 t}.\tag{13}$$

Expressing τ from Eq. (13) and substituting into Eq. (11), we get $|\ln f_2(E,t)|=4\min_{\mathcal{L}}\mathcal{F}_{2,\mathcal{L}}$, where the factor 4 accounts for the four quadrants.

Further steps depend on the relation between L and t. For $L\gg\sqrt{t}/\langle\gamma_2\rangle\sim\sqrt{tg}$, the normalization of $\Psi(n)$ is determined by the region $L-\mathcal{L}$, i.e., outside the fluctuation. Then minimization of $\mathcal{F}_{2,\mathcal{L}}$ with respect to $\mathcal{L}$ yields $|\ln f_2(E,t)|=\eta C_E\ln^2 t$, where $\eta<1$ is a numerical

factor, which for the Gaussian $P(V)$ is equal to $\eta = \{1 + 1/[4(\pi - 2)\ln 2]\}^{-1} \approx 0.76$. In the opposite case, $L \ll \sqrt{tg}$, the smallest possible fluctuation size $\mathcal{L} \sim L \ln t/\sqrt{t}$ should be substituted into Eq. (11). Using the fact that $C_E \sim g$ and $\langle \gamma_2 \rangle \sim g^{-1/2}$, and neglecting the terms which are small in parameter $L/\sqrt{tg} \ll 1$, we arrive at $|\ln f_2| = C_E \ln^2 t$ with C_E given by Eq. (12).

Discussion.—We now return to the peculiarities in the numerical results listed earlier, and discuss them in light of the picture of ALS based on the period-doubling fluctuations. (i) The dependence of C_E on the disorder strength, calculated from Eq. (11) for Gaussian distribution with a standard notation for the rms, $\Delta_2 = \langle V^2 \rangle^{1/2} = 12^{-1/2} W$, is shown in Fig. 1(a). For the range of $2 < W < 4$, studied in Ref. [18], the slope of $\ln C_E$ versus $\ln W^{-2} \sim \ln g$ varies within the range 0.67–0.83 for the energy interval $|E| < 2$. As seen in the inset, the scaling $C_E \propto g$ is recovered from (11) at $W \lesssim 0.5$. (ii) Insensitivity of C_E to the magnetic field: For the period-doubling fluctuation along both axes, $V(n_x, n_y)$, considered above, this insensitivity is an immediate consequence of the fact that the magnetic phases in hopping matrix elements can be formally "absorbed" into the phase factors in the on-site values of the eigenfunction $\Psi(n_x, n_y)$. The underlying reason for such gauging out is that the fluctuation $V(n_x, n_y)$ is *separable*. (iii) Sensitivity of $f_d(E, t)$ to the correlation of the disorder for a given conductance: It is obvious qualitatively that for the correlation radius, R_c, exceeding the lattice constant, the likelihood of the period-doubling fluctuation, with $\sim \mathcal{L}^2$ sign changes of on-site energies at neighboring sites, is drastically suppressed. On the quantitative level, depletion of the large-t tail in $f_2(E, t)$, observed numerically in Ref. [24] can be estimated as $\{\exp[-(\gamma_2^2)/(W^2)]\}^{\mathcal{L}^2 R_c^2} \sim [f_2(E, t)]^{R_c^2}$, so that for $R_c \gg 1$ the effect is indeed dramatic. The meaning of the power $(\mathcal{L} R_c)^2$ is that maintaining the period-doubling order requires for each site to "pay the price" to all its $\sim R_c^2$ neighbors. (iv) In 3D, the corresponding period-doubling fluctuation has the form $V(n_x, n_y, n_z) = V(n_x) + V(n_y) + V(n_z)$, with $V(n) = V_0 \mathrm{sgn}(n) \exp(i\pi n)$, so that $|\Psi(n)|^2 \propto \exp[-2\gamma_3(|n_x| + |n_y| + |n_z|)]$. In lexicographic presentation [21,22], this decay manifests itself as a system of prominent quasiperiodic peaks with a period close to $2L^2$. In simulations [21,22], the side of the cube was small, $L_3 = 12$. Then the ALS extends over the entire system. In Fig. 1(b), we present the lexicographic plot of the *analytical* solution $|\Psi(n)|^2$ for $L_3 = 12$ and $\gamma_3 = 0.8$. We find that the shape of $|\Psi(n)|^2$ is remarkably close to that in numerics of Ref. [21,22].

The main message of the present Letter is that, in order to test numerically, within the Anderson model, the predictions concerning the ALS of continuous theories, simulations must be carried out not too far from the band edges ($E = \pm 4$ in 2D and $E = \pm 6$ in 3D), where the continuous description applies. Simulations performed for E close to the band center reveal *lattice-specific* ALS that do not exist in continuous models.

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