Asymptotics of Universal Probability of Neighboring Level Spacings at the Anderson Transition

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The nearest-neighbor level spacing distribution is numerically investigated by directly diagonalizing disordered Anderson Hamiltonians for systems of sizes up to $100 \times 100 \times 100$ lattice sites. The scaling behavior of the level statistics is examined for large spacings near the delocalization-localization transition and the correlation length exponent is found. By using high-precision calculations we conjecture a new interpolation of the critical cumulative probability, which has size-independent asymptotic form $\ln I(s) \propto -s^{\alpha}$ with $\alpha = 1.0 \pm 0.1$. [S0031-9007(97)03719-8]

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The statistical fluctuations in energy spectra of disordered quantum systems attract at present much attention [1–5]. It is known that by increasing the fluctuations of a random potential the one-electron states undergo a localization transition, which is the origin of the Anderson metal-insulator transition (MIT) [6]. The influence of the disorder on the wave functions is reflected by the mutual correlations between the corresponding energy levels, so that the statistics of energy levels is sensitive to the MIT. In the metallic limit the statistics of energy spectra can be described by the random-matrix theory (RMT) developed by Wigner and Dyson [7,8]. This was shown by solving the zero-mode nonlinear σ model using the supersymmetric formalism [9]. Later, perturbative corrections to the two-level correlation function obtained in the RMT were evaluated in the diffusive regime by the impurity diagram technique [10]. In the insulating regime, when the degree of disorder W is much larger than the critical value W_c, the energy levels of the strongly localized eigenstates fluctuate as independent random variables.

An important quantity for analyzing the spectral fluctuations is the nearest-neighbor level spacing distribution $P(s)$. It contains information about all of the n-level correlations. In the metallic regime $P(s)$ is very close to the Wigner surmise $P_W(s) = \pi s/2 \exp(-\pi s^2/4)$ [11] (s is measured in units of the mean level spacing Δ). In the localized regime the spacings are distributed according to the Poisson law, $P_P(s) = \exp(-s)$, because the levels are completely uncorrelated. The study of the crossover of $P(s)$ between the Wigner and the Poissonian limits which accompanies the disorder-induced MIT in a three-dimensional system (3D) was started in Ref. [12] and became the subject of several subsequent investigations [1,2,5,13,14].

It was suggested earlier [1] that $P(s)$ exhibits critical behavior and should be size independent at the MIT. Investigating the finite-size scaling properties of $P(s)$ provides not only an alternative method for locating the transition [2], but allows one also to determine the critical behavior of the correlation length [14]. A technical advantage of the method is that one needs to compute only energy spectra and not eigenfunctions and/or the conductivity. On the other hand, a large number of realizations of the random potential has to be considered. In comparison with the well-established transfer-matrix method [15] by which one approaches the MIT from the localized side, the level-statistics procedure starts from the metallic regime. Thus, the two methods can be considered to provide complementary information about the critical region.

The suggestion of the existence of a third *universal* level statistics at the MIT excited considerable interest in the explicit form of the critical spacing distribution. From general considerations for the orthogonal symmetry [8] $P(s) \propto s$ at small s. For large s, essentially two different analytical expressions were proposed [16]. One of them [1,12] assumes that $P_c(s)$ is a Poissonian for $s \gg 1$, since at the critical point the Thouless energy, which is a measure of the number of energy levels that contribute to the average conductance of the system, is of order of Δ, while level repulsion is important only for small s.

A different asymptotic form, $P_c(s) \propto \exp(-As^{\alpha})$, was proposed [4], by using an analogy between the sequence of energy levels and a classical one-dimensional gas of interacting fictitious particles. Here α is given by the dimensionality d and the localization length exponent ν,

$$\alpha = 1 + (d\nu)^{-1}. \tag{1}$$

The result is obtained in the Gibbs model by assuming the power law $s^{2-\alpha}$ for the pairwise interaction between the particles [3]. The latter distribution decays faster than the Poissonian ($\alpha = 1$), but slower than the Wigner surmise ($\alpha = 2$). Several numerical calculations for the 3D Anderson model were recently performed [5,17] in order to analyze $P_c(s)$. The results were found to be consistent with the latter of the above suggestions with an exponent $\alpha \approx 1.2$–1.3 ($\nu \approx 1.5$). However, since the rounding errors in the calculations for large s are such that $\alpha = 1$ cannot be completely ruled out, the asymptotic form of $P_c(s)$ is still an open question, and the subject of presently ongoing and controversial discussions. In this Letter we present the results of detailed high-precision numerical investigations of the critical level spacing distribution. Our findings solve the above controversy. Preliminary results have been published previously [18].

By diagonalizing the Anderson Hamiltonian with a Lanczos algorithm [14] specifically modified for systems containing up to 10^6 lattice sites, which were not achieved in previous works, we examined both the critical behavior and the finite-size scaling properties of the integrated probability distribution of neighboring spacings $I(s)$. Our main result is that the asymptotic form of critical $I_c(s)$ and, therefore, $P_c(s)$ at large s is very close to a Poissonian decay, as the leading term, thus confirming the ideas of [1,12]. In addition, by using the size independence of $I_c(s)$ at the MIT and investigating the scaling of $I(s)$ with the system sizes L and W, we estimate the correlation length exponent ν.

The Anderson model [19] is defined by $H = \sum_n \varepsilon_n a_n^\dagger a_n + \sum_{n \neq m} (a_n^\dagger a_m + \text{c.c.})$, where $a_n^\dagger$ (a_n) is the creation (annihilation) operator of an electron at a site n, with m denoting the nearest neighbors of n. The site energies ε_n are measured in units of the overlap integral between adjacent sites. They are independent random variables that are distributed around $\varepsilon = 0$ according to a box distribution of width W. A simple cubic lattice with periodic boundary conditions was used. We computed the electron spectra of cubes of linear size ranging from $L = 5$ to 100 for various W. It is known from the transfer-matrix method [20] that in the center of the band ($\varepsilon = 0$) $W_c \approx 16.4$. The spectrum was properly "unfolded" by fitting the integrated density of states around $\varepsilon = 0$ to polynomial splines. The numerical results at the MIT are summarized in Table I. It should be noted that the numerical diagonalization of giant sparse matrices of order of 10^5–10^6 is highly nontrivial.

Figure 1 shows $P(s)$ calculated at the MIT. As expected, it is L independent. To cover the whole range of spacings, the interpolation formula $P_{AKL}(s) = Bs \exp(-As^\alpha)$ has been proposed in [4]. Because of normalization $A = [\Gamma(3/\alpha)/\Gamma(2/\alpha)]^\alpha$ and $B = \alpha A^{2/\alpha}/\Gamma(2/\alpha)$. The best fit using the χ^2 criterion in the interval $0 < s < 4$ yields $\alpha = 1.48 \pm 0.08$ with a confidence level 0.95. The fitted exponent α is markedly larger than that given by (1). For $s > 3$ one observes an increasing deviation between $P_{AKL}(s)$ and the computed histogram. This shows that fitting near $s \sim 1$ does not provide reliable information about α, because the exponential tail of $P(s)$ contributes to the relative accuracy only with a very small weight. Therefore it is imperative to investigate the asymptotic behavior at large s, not including data from the region $0 < s \lesssim 2$.

In what follows, we consider the cumulative level spacing distribution function $I(s) \equiv \int_s^\infty P(s')\, ds'$. It gives the probability to find neighboring energy levels with a separation $E > s\Delta$. The integration does not change the asymptotic exponential behavior of $P(s)$. Since $s > 0$, $I(0) = 1$, and by normalization to the total number of spacings in a given interval, $\int_0^\infty I(s)\, ds = 1$. The Wigner surmise [21] and the Poisson distribution yield $I_W(s) = \exp(-\pi s^2/4)$ and $I_P(s) = \exp(-s)$, respectively. The numerical evaluation of $I(s)$ is similar to that of the density of states in unfolding the spectrum. By arranging the spacings in a descending sequence one can very accurately construct the histograms of $I(s)$ [2].

Using the common statistical hypothesis at large s

$$\ln I_c(s) = -A_c s^\alpha, \tag{2}$$

we calculated A_c and α for various L (see Table I). Independent of L the result is $\alpha = 1.0 \pm 0.1$. The numerical data of $\ln I_c(s)$ shown in Fig. 2 are better described by a *linear law* for $s > 3$, so that $I_c(s) \propto \exp(-A_c s)$ with $A_c = 1.9 \pm 0.1$. This is similar to the insulating regime, although the decay rate A_c is larger than unity due to the level repulsion. The power law with the exponent $\alpha \approx 1.2$, which was recently obtained [17] by an analysis of the shape of $P(s)$ in the range $0 < s < 5$ for system sizes $L \leq 21$, deviates from our results for $s \gtrsim 4$.

The linear asymptotic behavior of $\ln I_c(s)$ is in contrast to the power law with $\alpha \approx 1.31$ obtained numerically [5] for smaller systems $L \leq 12$. The reason for this discrepancy is the following. The energy interval E considered in [5] is so narrow that it contains only ten spacings on the average, that results in a cutoff of $P_c(s)$ at

TABLE I. Numerical parameters for various cube sizes L at $W_c = 16.4$. M: number of samples; N_s: total number of spacings; Δ: mean level spacing; $\rho = (\Delta L^3)^{-1}$: density of states; α and A_c: quantities of Eq. (2). All levels lie within the energy interval $|E| < 4.45$.

L	M	N_s	Δ ($\varepsilon = 0$)	$\rho \times 10^2$	A_c	α
5	3×10^5	18 610 321	1.42×10^{-1}	5.62	1.90	1.01 (0.02)
8	4×10^3	1 016 790	3.47×10^{-2}	5.63	1.89	0.95 (0.06)
12	3×10^3	2 576 306	1.03×10^{-2}	5.62	1.89	0.99 (0.05)
16	5×10^2	1 017 902	4.34×10^{-3}	5.62	1.88	0.98 (0.06)
20	25	99 493	2.23×10^{-3}	5.61	1.91	1.00 (0.10)
28	10	109 075	8.11×10^{-4}	5.62	1.87	1.07 (0.10)
32	10	163 097	5.40×10^{-4}	5.62	1.89	0.99 (0.08)
40	5	158 658	2.77×10^{-4}	5.62	1.91	0.97 (0.09)
64	2	260 020	6.79×10^{-5}	5.62	1.88	1.04 (0.09)
80	1	254 321	3.47×10^{-5}	5.62	1.92	1.02 (0.06)
100[a]	1	99 360	1.77×10^{-5}	5.63	1.88	0.95 (0.11)

[a]Energy interval is $|E| < 0.89$.

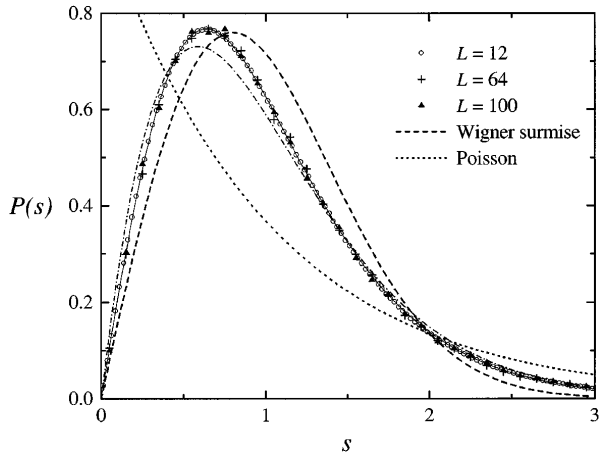

FIG. 1. Level spacing distribution $P(s)$ for various system sizes at the critical disorder W_c. Dash-dotted line is $P_{AKL}(s)$. Full line is derivative of $I_c(s)$ from interpolation formula (3).

$s \approx 10\Delta$. Thus, some fraction of the spacings $s < 10\Delta$ is not taken into account, causing the faster decay of $P_c(s)$. In our calculations the interval is wide enough, covering approximately half of all of the eigenvalues. However, such a choice of E does not lead to the undesirable mixture of the extended and the localized states. This is due to a peculiarity of the box distribution of the site energies ε_n. It follows from the localization phase diagram $\{W_c, E_c\}$ [15,22], that the critical disorder W_c is almost independent of the energy when $|E_c| < 6$. In order to investigate how the width of the energy interval influences the level statistics, we calculated $I(s)$ for $E/\Delta = 10^2$, 10^3 and 10^4, provided that all levels satisfy the critical condition $L < \xi(\varepsilon) \propto |\varepsilon/E_c - 1|^{-\nu}$. The results were practically the same within the statistical uncertainties. This implies the equivalence of averaging over the spectrum and over the random potential. Indeed, due to diminishing the spacing with the size $\Delta \propto L^3$, the averaging for smaller cubes is performed over many samples, while for our largest systems $L = 80$ and 100 a single realization without ensemble averaging is even sufficient to get similar distributions with comparable precision. For numerically describing a crossover between small and large s, we propose an explicit form of the new interpolation function

$$I_c(s) = \exp[\mu - \sqrt{\mu^2 + (A_c s)^2}] \qquad (3)$$

with a coefficient $\mu \approx 2.21$. Although we do not provide a rigorous analytical proof, it gives the excellent fit all over the range of the computed spacings. The corresponding $P(s)$ shown in Fig. 1 fulfills the both normalization conditions.

To study the finite-size scaling behavior of $I(s)$ for large s, we extended the calculations to other degrees of the disorder W close to W_c for various system sizes. The calculations were performed for an ensemble of different samples. The number of samples for each given pair of L and W was chosen such that $N_s \simeq 10^5$ spacings were obtained. We have also carefully checked the sensitivity of the results to the number of realizations. No change was observed within the error bars when increasing the system size on the expense of the number of realizations and vice versa. By increasing W the spacing distribution for fixed L changes continuously from $I_W(s)$ to $I_P(s)$ (Fig. 3). The steepness of the crossover depends on L. For larger sizes $I(s)$ changes faster between the two limiting regimes. At $W_c \simeq 16.4$ the spacing distribution has almost the same asymptotic form for all L from 5 to 100. This reflects the universality of the level statistics exactly at the MIT [1].

For finite L the distribution $I(s)$ exhibits scaling in the vicinity of W_c. Within the critical region, $L < \xi(W)$, it is reasonable to assume that the linear slope of $\ln I(s)$ is governed by the one-parameter scaling law, $A(W, L) = f[L/\xi(W)]$. Figure 4 shows the disorder dependence of

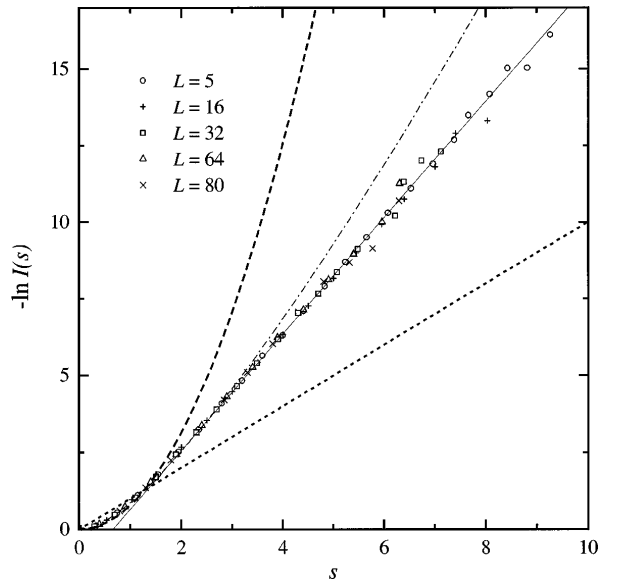

FIG. 2. Critical probability of neighboring spacings $I(s)$. Solid line is Eq. (2) with $\alpha = 1$. Dash-dotted line is the power law with $\alpha = 1.24$ from Eq. (1). Dashed and dotted lines are $I_W(s)$ and $I_P(s)$, respectively.

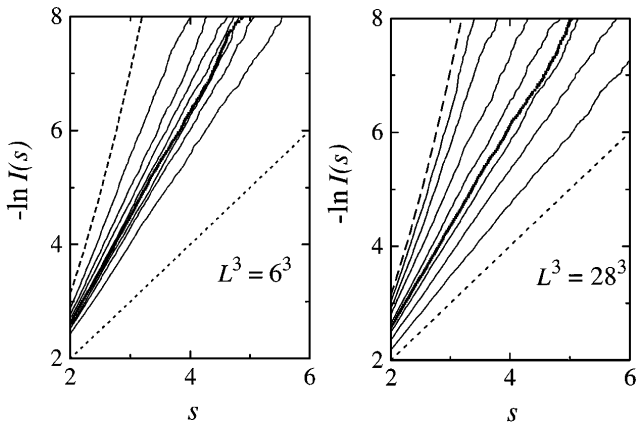

FIG. 3. Probability $I(s)$ for $L = 6$ and 28 at $W = 12$, 14, 15, 16, 16.4, 17, 18, and 20 shown consecutively from the left to the right. Dashed (dotted) line is the Wigner (Poisson) limit.

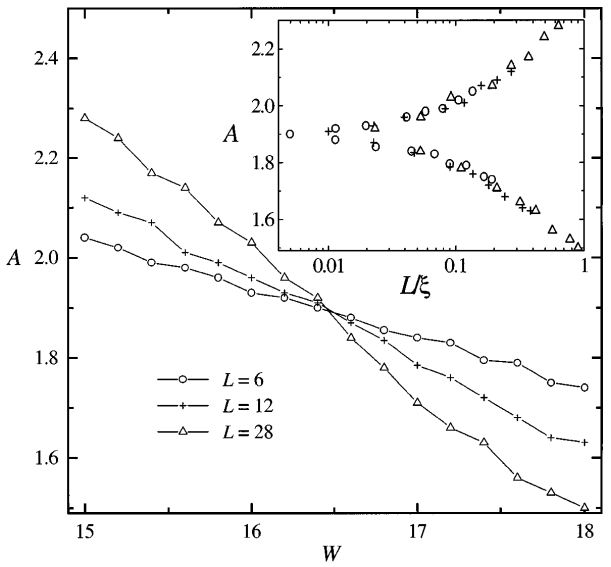

FIG. 4. Scaling variable A as a function of the disorder W for different L, showing critical behavior near the MIT. Inset: the one-parameter dependence of A on $L/\xi(W)$.

A near the critical point for various L. $A(W_c)$ does not depend on L. By introducing a scaling parameter, the correlation length $\xi(W)$ [14,15], we found a common scaling curve consisting of two branches corresponding to the delocalized and localized regimes for $A > A_c$ and $A < A_c$, respectively, as shown in the inset of Fig. 4. The critical exponent ν was determined in a similar way as done previously [14], where only the small-s part of $P(s)$ was used. We found $\nu = 1.4 \pm 0.15$ in agreement with the result obtained earlier by completely different methods [2,15,20].

In conclusion, we present the first large-scale numerical results on the statistics of the energy levels near the disorder-induced MIT for systems of sizes up to $L^3 = 100^3$ sites. A comparative analysis with results obtained from various analytical approaches and other numerical studies is performed. At the critical point the asymptotic universal probability of energy level spacings has a Poisson-like form $I_c(s) \propto \exp(-A_c s)$. We believe that the simple exponential asymptotics of the critical level spacing distributions are valid not only for the orthogonal symmetry (with spinless electrons and without magnetic field), but also for other universality classes: the unitary (in the presence of the magnetic field) and the symplectic (in the presence of spin-orbit coupling) classes. Recent computer simulations [23] corroborate that the decay rate A_c is almost insensitive to the fundamental symmetry. However, it could depend on the physical dimensionality. Finally, we have determined the influence of the disorder of the system on the exponential tail of $I(s)$, and constructed numerically the corresponding scaling function. The critical exponent of the correlation length was calculated, $\nu \approx 1.4$.

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