Statistics of spectra of disordered systems near the metal-insulator transition

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We study the nearest-level-spacing distribution function $P(s)$ in a disordered system near the metal-insulator transition. We claim that in the limit of an infinite system there are only three possible functions $P(s)$: Wigner surmise $P_W(s)$ in a metal, Poisson law $P_P(s)$ in an insulator, and a third one $P_T(s)$, exactly at the transition. The function P_T is an interesting hybrid of $P_W(s)$ and $P_P(s)$, it has the small-s behavior of the former and the large-s behavior of the latter one. A scaling theory of critical behavior of $P(s)$ in finite samples is proposed and verified numerically.

The statistical properties of the spectra of complex systems such as molecules, nuclei, and mesoscopic solids can be represented by random matrix spectra. Characteristics of such spectra are well known for the so-called Gaussian orthogonal ensemble (GOE) for which all matrix elements (diagonal and off-diagonal) have the same Gaussian distribution.[1] The probability density $P(s)$ of the nearest-neighbor spacing s is shown to be extremely close to the Wigner surmise[1]

$$P_W(s)=\frac{\pi}{2}\frac{s}{\delta^2}\exp\left[-\frac{\pi}{4}\left[\frac{s}{\delta}\right]^2\right], \tag{1}$$

where $\delta\equiv\langle s\rangle$ is the mean spacing between two adjacent levels. Equation (1) demonstrates a strong repulsion between levels. On the other hand, in the trivial case of a random matrix with zero off-diagonal elements, there is a completely random sequence of eigenvalues, and the spacing between adjacent levels has a Poisson distribution

$$P_P(s)=\frac{1}{\delta}\exp\left[-\frac{s}{\delta}\right]. \tag{2}$$

In a number of works,[2-6] the crossover between the Wigner and Poisson distributions in a disordered system was related to the localization of wave functions, which reduces the role of repulsion between levels. The conventional way to describe the localization transition is to use the Anderson Hamiltonian (AH) (Ref. 7)

$$H=\sum_i \epsilon_i a_i^\dagger a_i-\sum_{j,i} a_j^\dagger a_i, \tag{3}$$

where $a_i^\dagger$ and a_i are the electron creation and annihilation operators at site i, subscript j denotes adjacent to i, and ϵ_i is the random energy of site i in units of the overlap energy of adjacent sites and is uniformly distributed in the range from $-W/2$ to $W/2$. It is well known that eigenstates of AH in the vicinity of the energy $\epsilon=0$ experience a localization transition with increasing W. For a simple cubic lattice, the "metal-insulator" (MI) transition occurs at $W=W_C=16\pm0.5$.[8]

Numerical diagonalization of AH for simple cubic lattices $L\times L\times L$ at small $L=5$ (Refs. 3 and 4) revealed a crossover between $P_W(s)$ and $P_P(s)$, with W increasing from $W\ll W_C$ to $W\gg W_C$. However, the distribution $P(s)$ in the critical region was not studied at that time.

In this Brief Report, we (i) discuss $P(s)$ in the limit of $L\to\infty$; (ii) postulate for $L\to\infty$ a new universal $P(s)\equiv P_T(s)$ exactly at the transition point and determine it numerically; (iii) introduce a scaling hypothesis for cubes of finite L; (iv) present results of the numerical diagonalization of AH at different W and L up to 16 which confirm this scaling hypothesis; and (v) suggest a new method for the location and the analysis of the MI transition.

It is quite obvious that in an infinite system $P(s)=P_P(s)$ at any $W>W_C$. Indeed, energy levels contributing to $P(s)$ typically belong to localized states centered at very large distances of the order of L from each other. That is why if $L\to\infty$, we can neglect their repulsion even when W is close to W_C and the localization length $\xi(W)$ is much larger than the lattice constant.

Now we argue that in an infinite system everywhere on the metallic side of the transition ($W<W_C$), the function $P(s)$ coincides with $P_W(s)$. In Ref. 2, fluctuations in the number of levels inside an energy band of width ϵ were studied for metallic samples. They were shown to agree with Dyson's results[9] derived for the GOE if $\epsilon<\epsilon_C\equiv h/\tau$, where τ is the diffusion time of an electron between two opposite faces of the cube. The ratio $\epsilon_C/\delta=Gh/e^2$ (where G is the cube conductance) tends to infinity when $L\to\infty$ for any $W<W_C$. Therefore one can assume that all results known for GOE including the

Wigner surmise are valid for the metal, even for energies much larger than δ.

What happens with $P(s)$ in an infinite system exactly at $W=W_C$? We argue that there is a distribution $P_T(s)$ at $W=W_C$ which is probably universal for some class of MI transitions. At $s \gg \delta$, it should decay like $\exp(-s/\kappa\delta)$, where $\kappa \approx 0.3$.[3] The reason for such behavior is that exactly at the transition $\varepsilon_C \approx \delta$, and repulsion between levels is significant only for $s \leq \delta$.

For $s \ll \delta$, the function $P_T(s)$ should be linear in s. This follows from the general symmetry theorem proved by Dyson[9] for the case of the orthogonal ensemble which includes AH. From the point of view of this theorem, the Poisson distribution for $W > W_C$ is a result of the divergency of the slope of the linear part in the limit of $L \to \infty$, in which repulsion between adjacent levels disappears. At the transition, repulsion is important for all $s \leq \delta$, and the slope differs from the slope of $P_W(s)$ by a numerical factor only. Thus $P_T(s)$ is an interesting hybrid of $P_W(s)$ and $P_P(s)$. It has small-s behavior resembling the Wigner distribution and large-s behavior resembling the Poisson one. In Fig. 1, the curve corresponding to $W=16$ is the best approximation to $P_T(s)$ as obtained from our numerical computations (see below). It looks as expected.

At any finite L, we can expect a continuous crossover from P_W to P_P with growing W. To discuss such a crossover, we characterize $P(s)$ by one parameter, the weight of the large-s part $A \equiv \int_{2\delta}^{\infty} P(s)ds$ (P_P and P_W cross at $s=2.002$), normalized in the following way:

$$\gamma(W,L) \equiv \frac{A - A_W}{A_P - A_W} . \tag{4}$$

If $L=\infty$, then the parameter $\gamma=0$ for $W < W_C$ and $\gamma=1$ for $W > W_c$. For finite L, it is natural to expect a scaling behavior

$$\gamma(W,L) = f(L/\xi(W)) , \tag{5}$$

where $\xi(W)$ is the correlation length of the MI transition (at $W > W_C$, one calls it the localization length). The inset in Fig. 2 shows schematically the expected evolution of $\gamma(W)$ at different L. It is clear that if one obtains such a set of curves one can easily find the transition point W_C as the point where all curves cross or, in other words, the point at which the size effect changes its sign.

We have tested these predictions numerically. We constructed matrixes representing AH for the simple cubic lattice with periodic boundary conditions. The eigenvalues were obtained by diagonalizing the matrices on the Cray-YMP at the San Diego Supercomputer center and the Cray-XMP at the Minnesota Supercomputer Institute using standard library routines. We studied cubes with $L=6$, 8, 12, 16, and $W=10,12,14,15,16,17,18,20,24,30$. The number of random realizations varied with L in such a way that the number of studied eigenvalues at each combination of W and L was kept around 10^5. In order to minimize fluctuations of $P(s)$, we used levels from a band around $\epsilon=0$ containing 50% of all levels. We verified that there were no significant changes in $P(s)$ if we used 25% or 10%. This is not surprising in view of the fact that the phase trajectory of the MI transition in the (ϵ, W) plane is rather flat up to $|\epsilon|=6$ for the box distribution.[10] To take into account the very weak energy dependence of the density of states around $\epsilon=0$, we calculated dimensionless function $P_1(s/\delta) \equiv P(s)\delta$ using values for δ obtained separately for 32 energy intervals. In Fig. 1, we show $P(s)$ for lattices of size $L=12$, for various W. We note that $P(s)$ progresses from P_W to P_P as W increases. All the distributions cross near $s=2\delta$. To compare the $P(s)$ for lattices of different size, we evaluate $\gamma(W,L)$. The results are shown in Fig. 2. As expected, the transition between the Wigner ($\gamma=0$) and Poisson ($\gamma=1$) limits becomes more abrupt as L increases. The curves cross at $W=W_C=16.0\pm0.5$, which we identify as the transition point. This agrees with other determinations.[8] At $W=W_C$, we did not find any systematic dependence of the shape of $P(s)$ on L. Therefore $P(s)$ at $L=12$ and $W=16$ (see Fig. 1) indeed represents the function $P_T(s)$ at $L=\infty$ very well. To verify the scaling hypothesis [Eq. (5)] in Fig. 3, we plotted γ as a function of $L/\xi(W)$, taking values of $\xi(W)$ from Ref. 8. All

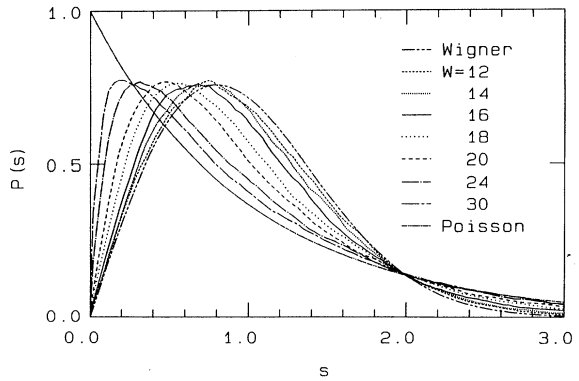

FIG. 1. Nearest-neighbor spacing function $P(s)$ for $L=12$ and different W. Wigner and Poisson functions $P_W(s)$ and $P_P(s)$ are also shown for comparison.

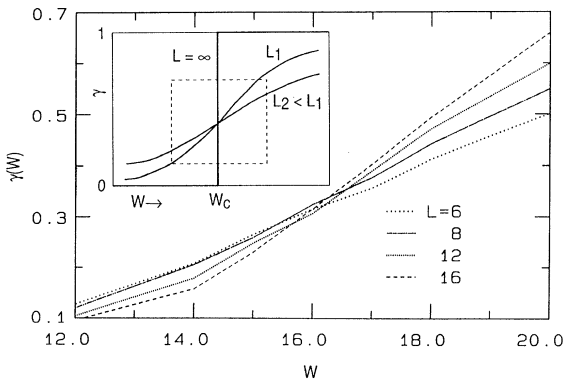

FIG. 2. The parameter γ as a function of W for different sizes of system L as obtained by numerical diagonalization. Schematic $\gamma(W)$ dependences are shown in the inset. The location of the main plot is shown by dashed lines.

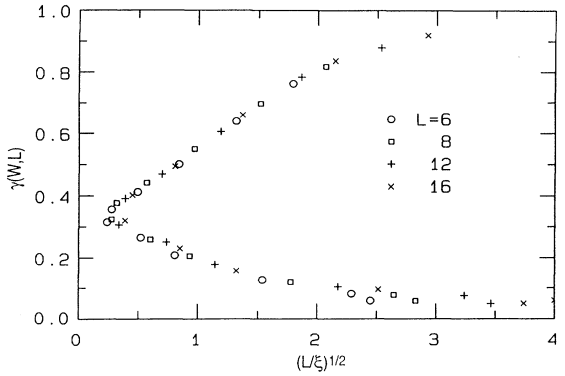

FIG. 3. Verification of the scaling hypothesis. The parameter γ as a function of $[L/\xi(W)]^{1/2}$, where $\xi(W)$ is the correlation length of the MI transition. The power $\frac{1}{2}$ is used only for the purpose of clear presentation of the data. The upper and lower sets of data are obtained from $W \geq 17$ and $W \leq 15$, respectively.

the points collapsed on two separate branches for $W < W_C$ and $W > W_C$. We consider Fig. 3 as a confirmation of the scaling theory. Using Eq. (5) and the expression

$$\xi(W) = \xi_0 \left| \frac{W}{W_C} - 1 \right|^{-\nu} \tag{6}$$

for the correlation length $\xi(W)$, we can find the exponent ν. For this purpose, we fit the data near the crossing point in Fig. 2 with the help of the expansion

$$\gamma(W,L) = \gamma(W_C,L) + C \left| \frac{W}{W_C} - 1 \right| L^{1/\nu} . \tag{7}$$

This gives $\nu = 1.50 \pm 0.15$ in agreement with Ref. 8.

We repeated the same kind of computations for the two-dimensional case and obtained γ as in Eq. (4). In this case, the curves of $\gamma(W)$ for several choices of L (as in Fig. 2) did not cross at any finite W. This means that there is no MI transition in this case. At the same time, all the data for γ collapsed into one single-valued curve when plotted against $L/\xi(W)$. Thus analysis of these spectra gives results consistent with the conventional understanding of the role of dimensionality[11,8] for the MI transition.

Returning to the shape of $P(s)$ in Fig. 2, we would like to explain the observed linear dependence $P(s) = Bs$ for $s \ll \delta$. We start from the case of the deep insulator ($W > 2W_C$). To evaluate $P(s)$ for $s \ll \delta$, we can consider the repulsion of two adjacent energy levels which most likely belong to the states localized at a distance of the order of L from each other. Solving the eigenvalue 2×2 problem for these two states, we obtain

$$s = \sqrt{(\epsilon_1 - \epsilon_2)^2 + V^2} , \tag{8}$$

where ϵ_1 and ϵ_2 are bare energies of states 1 and 2, and V is a matrix element describing tunneling from one to the other. V appears in high orders of perturbation theory as a sum over different paths from site 1 to site 2.[12] The contribution of each path has a random sign because of random signs in the perturbation-theory expansion denominators $(\epsilon_i - \epsilon_1)$. Therefore the probability density of V, $F(V)$ is finite at $V = 0$. This leads[1] to the linear behavior of $P(s)$ for $s \ll V_0 \ll \delta$, where V_0 is the typical value of $|V|$.[13]

It seems clear that if at finite L, equation $P(s) = Bs$ is valid both for $W \gg W_C$ and $W \ll W_C$, it should be valid for any W including $W = W_C$. When $L \to \infty$, coefficient B tends to infinity for $W < W_C$ and to $B_W \equiv \pi/2\delta^2$ for $W < W_C$. At $W = W_C$, it does not depend on L and is equal to B_T, the initial slope of $P_T(s)$. It follows from Fig. 1 that $B_T \simeq 1.3 B_W$.

To summarize, we have introduced and found numerically a distribution of nearest-level spacings $P_T(s)$ which occurs exactly at the MI transition. It is shown that the crossover between the Wigner and Poisson distributions for finite samples can be described by scaling theory. The MI transition point can be located as the point at which the size effect on the distribution function changes sign. We believe that this method of locating the MI transition is conceptually the simplest: it deals only with the spectrum and does not involve conductivity calculations or knowledge of eigenfunctions. At the same time, it is quite accurate and practical.

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[13]It is interesting to note that our argument for linear behavior of $P(s)$ at small s is valid only when ϵ_1 is far from the ground state of AH. Near the ground state, all denominators $\epsilon_i - \epsilon_1$ are positive. Therefore $F(V)$ peaks at positive value V_0 and $F(0)=0$. This means that near the ground state, $P(s)$ has a soft gap at $s < V_0$. We have preliminary numerical evidence of such a gap.