Does Broken Time Reversal Symmetry Modify the Critical Behavior at the Metal-Insulator Transition in 3-Dimensional Disordered Systems?

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The critical behavior of 3-dimensional disordered systems without time reversal symmetry is investigated by analyzing the spectral fluctuations of the energy spectrum. We show that in the thermodynamic limit we have two different regimes, one for the metallic side and one for the insulating side with different level statistics. The third statistics which occurs only exactly at the critical point is independent of the presence or absence of time reversal symmetry. The critical behavior which is determined by the symmetry of the system at the critical point should therefore be independent of time reversal invariance.

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It is now well known that the introduction of disorder into periodic structures has dramatic effects on the properties of the system. In particular, 3-dimensional (3D) systems exhibit a metal-insulator transition (MIT) as a function of the disorder. A lot of work [1] has already been devoted to the study of this phase transition, theoretically, numerically, as well as experimentally. While all methods seem to agree on the fact that the NIT should only be characterized by the fundamental symmetries of the system and that one can expect a second order phase transition, its description, e.g., with respect to critical disorder and critical exponents, still remains a controversial object of discussions [1].

Theoretically the standard method applied, namely the $2 + \epsilon$ expansion, for the calculation of the critical exponents turns out to be inadequate for $d = 3$ [2,3]. It seems to be a characteristic of several theories for disordered systems using perturbative methods, like the nonlinear σ model [4] or the self-consistent theory [5], to provide quantitative results in the weak localization regime (i.e., for small disorder) but to fail in the region of the critical disorder.

Because of this problem numerical investigations in the frame of the Anderson model of localization have played an important role in the description of the MIT. Based on extensive computations by means of the transfer matrix method (TMM) [6], it is now usually accepted that the critical exponent is $\nu \approx 1.4$ and is independent of the distribution chosen in the Hamiltonian [7,8]. This result has been confirmed recently [9,10] using a completely different method, namely the energy level statistics method (ELSM). Meanwhile other TMM studies have been carried out on similar models but with magnetic field, which changes the symmetry, driving the system from the orthogonal to the unitary universality class, due to the break of the time reversal invariance. Surprisingly, in spite of this change of universality class, the same value

of the critical exponent has been found with and without magnetic field and that independent of the strength of the magnetic field [11,12). In this Letter, using the ELSM which will again turn out to be very suitable for such a study, we propose to explain this surprising observation with symmetry arguments shedding new light on the problem. Our conclusions are based on our numerical results for the spacing distribution $P(s)$ and the Δ_3 statistics showing that there is a critical ensemble (CE) characteristic for the MIT irrespective of the presence or absence of time reversal symmetry which implies that the critical exponent should be independent of time reversal symmetry and then of the magnetic field.

In order to investigate the MIT with magnetic field we consider the usual Anderson Hamiltonian with an additional phase factor in the off-diagonal elements,

$$
H = \sum_{n} \epsilon_n |n\rangle\langle n| + \sum_{n \neq m} e^{i\theta_{n,m}} |n\rangle\langle m|, \qquad (1)
$$

where the sites n are distributed regularly in 3D space, e.g., on a simple cubic lattice, with periodic boundary conditions, and $\theta_{n,m} = -\theta_{m,n} = \theta$. Only interactions with the nearest neighbors are considered. The site energy ϵ_n is described by a stochastic variable. In the present investigation we use a box distribution with variance $\sigma^2 = W^2/12$. W represents the disorder and is the critical parameter. $\theta = 0$ describes the case with time reversal symmetry with a Hamiltonian invariant under orthogonal transformation, while $\theta \neq 0$ corresponds to the case with broken time reversal symmetry which is invariant under unitary transformation. In spite of the simplicity of the model, it contains all the relevant properties necessary to describe the MIT with magnetic field as far as universal values, like the critical exponents, associated to the critical behavior are concerned. A similar Hamiltonian has been proposed by Pandey and Mehta [13] and used to study, by ELSM, the transition from the Gaussian orthogonal ensemble (GOE) to the Gaussian unitary ensemble (GUE) in a metallic ring pierced by a magnetic fiux [14].

Based on this Hamiltonian, the MIT in absence of time reversal symmetry will be studied by the ELSM, i.e., via the fluctuations of the energy spectrum. This method has already given very interesting results in the case $\theta = 0$, where the MIT corresponds to a transition from the GOE to the Poisson ensemble (PE) [15,16) which refiects completely uncorrelated energy levels in the localized regime. In the thermodynamic limit one obtains two different regimes: GOE for $W < W_c$ and PE for $W > W_c$, which are separated by a CE [10,17] occurring at the critical disorder W_c . For $\theta \neq 0$ one can expect a transition between GUE and PE, but the crucial question is what happens in the vicinity of the critical point.

Before giving the results we shortly review the ELSM. Starting from Eq. (1) the energy spectrum was computed by means of the Lanczos algorithm (which is suited to diagonalize such very sparse secular matrices) for systems of size $M \times M \times M$ with $M = 13$ and 21, disorder W ranging from 3 to 80, and phase $\theta = 0.1\pi$. The number of different realizations of the random site energies ϵ_n was chosen so that about 2×10^5 eigenvalues were obtained for every pair of parameters (M, W) which means between 25 and 90 realizations, for which the full spectrum has been computed. For the subsequent investigations only half of the spectrum around the band center is considered so that the results are not deteriorated by the strongly localized states near the band edges. After unfolding the obtained spectrum the fluctuations can be appropriately characterized [18] by means of the spacing distribution $P(s)$ and the Dyson-Metha statistics Δ_3 . $P(s)$ measures the level repulsion; it is normalized. So is its first moment because the spectrum is unfolded. Δ_3 which measures the spectral rigidity is given by

$$
\Delta_3(L) = \left\langle \frac{1}{L} \min_{A,B} \int_{\epsilon'}^{\epsilon'+L} [N(\epsilon) - A\epsilon - B]^2 \, d\epsilon \right\rangle_{\epsilon'}.
$$
 (2)

where $\langle \ \rangle_{\epsilon'}$ means that we average over different parts of the spectrum.

Using the random matrix theory (RMT), it is possible to calculate $P(s)$ and Δ_3 for the two limiting cases of the spectrum, namely the GUE and the PE. For the metallic side one obtains [18]

$$
P_{\text{GUE}}(s) \simeq \frac{32}{\pi^2} s^2 \exp\left(-\frac{4}{\pi} s^2\right),\tag{3}
$$

$$
\Delta_3(L) = \frac{2}{L^4} \int_0^L (L^3 - 2L^2 r + r^3) \Sigma_{\text{GUE}}^2(r) dr , \qquad (4)
$$

where $\Sigma_{GUE}^2(r)$ is the variance of the number of levels in a spectral window of width r and is given by

$$
\Sigma_{\text{GUE}}^{2}(r) = \frac{2}{\pi^{2}} \Big[\ln(2\pi r) + \gamma + 1 - \cos(2\pi r) - \text{Ci}(2\pi r) + 2r \left(1 - \frac{2}{\pi} \text{Si}(2\pi r) \right) \Big]. \tag{5}
$$

The formula (3) for $P_{GUE}(s)$ is exact only in the case of 2×2 matrices but remains a good approximation for the other cases. For Δ_3 there is no analytical solution, and the integral (4) has to be calculated numerically.

For the localized case we have

$$
P_{\rm PE}(s) = e^{-s}.\tag{6}
$$

$$
\Delta_3(L) = \frac{L}{15} \,. \tag{7}
$$

In Fig. ¹ the results for the Dyson-Metha statistics are reported. We find, as expected, the GUE and the PE regimes for small and large disorder, respectively, as well as the continuous transition between them as a function of W . In a previous work [17] it was shown for the case $\theta = 0$ that the Δ_3 curves are functions of the system size except at the critical point where they are size independent. Moreover, the curves were shown to move with increasing M toward the GOE for $W < W_c$ and toward the PE for $W > W_c$. In Fig. 2 we observe a similar behavior for $\theta = 0.1\pi$; accordingly this time the curves move toward the GUE and the PE. The critical value of the disorder where the curves are size independent turns out to be $W_c \approx 16.5$. Correspondingly, in the thermodynamic limit we expect two different regimes with the GUE and the PE, separated by the CE at the MIT. This has now to be compared to the CE obtained in the case without magnetic field. In Fig. 3 one sees that the CE curves are identical, and thus the symmetry should be the same, too. Moreover, this was checked for $\theta = \pi/2$ which is the "most Hermitian" case, and the same results were obtained (cf. Fig. 3). Only the critical disorder, which is not a universal value, seems to be slightly shifted upward toward $W_c \approx 16.65$. Such behavior has already been noted in a different numerical approach [12], but their shift was significant. The difference might be due to the fact that our model does not contain any magnetic field within the system

FIG. 1. Dyson-Metha statistics $\Delta_3(L)$ for $M = 21$. A continuous transition from GUE to Poisson statistics occurs as a function of the disorder W (denoted on the right-hand side). The dotted line shows the GOE result for comparison.

FIG. 2. Dyson-Metha statistics $\Delta_3(L)$ for system sizes $M =$ 13 and 21 and $W = 14$, 16.5, and 19.

as in [12] but involves a vector potential due to an Aharonov-Bohm fiux. This point is still not clear, and more detailed calculations would be required in order to check if we really have a shift or not.

The CE curve seems to be proportional to $L^{3/4}$ for small L and becomes linear when increasing L . This would mean that the shape of the curve cannot solely be described either by the results of Kravtzov et al. [19] or by the results of Alt'shuler et al. [16] but rather would be in agreement with Ref. [19] for small L and with Ref. [16] for large L . Moreover, it has to be stressed again that the CE curve is completely independent of the magnetic field in contrast to Ref. [19].

The same results are derived from the study of $P(s)$ in Fig. 4. For small and large disorder we again find the GUE and the PE, respectively, while $P(s)$, at the critical point, is independent of M and θ . Another interesting point is the controversy [10,20] about the asymptotic behavior of $P(s)$. A careful analysis of the shape of $P(s)$ at the critical point gives

$$
P(s) = As \exp(-Bs^{\alpha}), \qquad (8)
$$

FIG. 3. The Dyson-Metha statistics $\Delta_3(L)$ at the critical point for different values of θ .

with $\alpha = 5/4 \pm 0.05$ and A, B the normalization constants which support the results obtained in Ref. [20]. Moreover, one notes that the value of α is in very good agreement with the formula $\alpha = 1 + 1/\nu d$ obtained by Kravtzov *et al.* [19] relating α to the critical exponent v and the dimension d of the system. Finally it has to be stressed that the dependence of the results in [19,20] on β (β = 1 for the GOE and 2 for the GUE) via some coefficients has not been derived from the calculation but assumed from the very beginning, leaving open the question whether those results, at the critical point, depend on time reversal symmetry or not. Figure 4 demonstrates that this is not the case.

As the critical behavior is determined by the fundamental symmetries of the system, one should consider the symmetry at the critical point. From the results in Figs. 3 and 4 we conclude that the break of the time reversal symmetry has no influence on the critical behavior. This means also that the critical exponent $\nu = 1.34 \pm 0.10$, which was obtained [9] for the $\theta = 0$ case, is transferable to the case without time reversal invariance

Finally we compare these results, concerning the critical exponents, with experiments. Recent measurements performed on the persistent photoconductor $Al_{0.3}Ga_{0.7}As$ [21] and on uncompensated Si:P [22] suggest, althought the situation is still not completely clear, that the MIT is effectively independent of the magnetic field. About the value of the critical exponent the situation is not really clearer but it can be mentioned that in Ref. [22], considering carefully the range of the critical behavior, a critical exponent of $\nu \approx 1.3$ has been found which would be in agreement with our results. This seems to indicate, at least in some cases, that the MIT is, in fact, driven purely by the disorder. Then it is not necessary to include interactions to characterize the critical behavior, although

FIG. 4. Spacing distribution $P(s)$ for $M = 21$, $W = 3,80$, and $\theta = 0.1\pi$. The histograms are the numerical results, and the numerical results. full lines reflect the two expected limiting ensembles, namel the GUE for the metallic side and the PE for the insulating side. The points \circ , + represent $P(s)$ at the critical point for $M = 21$ and $M = 13$. The symbol \diamond denotes the CE for the case without magnetic field ($\theta = 0$).

these can be important outside the critical regime. It has to be noted that some reserves have been made [23] about the results obtained in Ref. [22], and it will be interesting to carefully check this problem in order to clarify the situation.

In conclusion we have shown, using the statistical properties of the energy spectrum of the Anderson model of localization, that the MIT, which is determined by the symmetry of the system *at* the critical point, is not influenced by broken time reversal symmetry. This means that both cases with or without time reversal invariance belong to the same universality class, described by the CE, which opens new perspectives in the comprehension of the MIT. Although this universality class is defined only for the critical point, it is sufficient to fix the properties of the critical behavior. This is in agreement with previous numerical results [11,12] and recent experiments [21,22]. We point out that these results are valid in 3D systems and do not apply to 2D where we know that one expects no MIT with time reversal symmetry while a MIT takes place when the symmetry is broken [24].

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Noted added.—While submitting this Letter we learned [25] that the results in [19] were not completely correct and that a linear term too in the two-point correlation function has been found in agreement with the results presented here for $\Delta_3(L)$.

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