The critical behaviour of three-dimensional disordered systems is investigated by analysing the spectral fluctuations of the energy spectrum. Our results suggest that the initial symmetries (orthogonal, unitary and symplectic) are broken by the disorder at the critical point. The critical behaviour, determined by the symmetry at the critical point, should therefore be independent of the previous invariances and be described by a “super” universality class. This result is strongly supported by the fact that we obtain the same critical exponent $\nu \simeq 1.35$ in the three cases: orthogonal, unitary and symplectic.

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The transport properties in three-dimensional disordered systems are a very rich topic that already has attracted considerable research. In particular the system exhibits a metal-insulator transition (MIT) as a function of the disorder. Although it seems clear now that the MIT is a second-order phase transition many points still remain unclear. One of them is the influence of the symmetry on the MIT. It is generally assumed that at the critical behaviour at the MIT can be cast into three different universality classes according to some general symmetries of the system: orthogonal (with time reversal symmetry, O(\(N\))), unitary (without time reversal symmetry, e.g. with a magnetic field, U(\(N\))) and symplectic (with spin orbit-coupling, Sp(\(N\))). One then expects different critical exponents related to the MIT for the three different universality classes. Surprisingly, in spite of the change of universality class, the same value of the critical exponent has been found, numerically, with and without a magnetic field. The MIT being a transition between a chaotic (metallic regime) and a non-chaotic system (insulating regime), a convenient way to study this problem is to resort to random matrix theory (RMT) and energy level-statistics (ELS). In RMT the statistics of the energy spectrum are generally described by three different ensembles, Gaussian orthogonal (GOE), unitary (GUE) and symplectic (GSE) ensembles depending upon the symmetries mentioned above. It has been shown, in the case without magnetic field, that besides the two expected statistics, namely the GOE for the metallic regime and the Poisson ensemble (PE) for the insulating regime, a third statistic, called the critical ensemble (CE), occurs only exactly at the critical point. The properties of the CE will reflect, in particular, the shape of the critical states, which are multifractals. It was recently proposed that a natural way to understand the critical point with the previous results being interpreted as the sign of the independence of the universality class to the breaking of time-reversal symmetry at the critical point. We think that when the system reaches the critical point, for increasing disorder, the O(\(N\)) or U(\(N\)) symmetry is spontaneously broken. The reason for this break is obvious when one considers the localised regime. If the matrix would be O(\(N\)) or U(\(N\)) invariant it would then be possible to construct delocalised states by linear combinations of the localised ones which is clearly not allowed. In RMT this phenomenon has led to the concept of a preferential basis. The distribution of the eigenvalues and the eigenvectors, which are independent for the GOE or GUE, become correlated when the disorder is increased and eventually break the O(\(N\)) or U(\(N\)) invariance. Similar results concerning the break of the O(\(N\)) invariance have been reported when studying the two-level correlation function. Considering the spacing distribution \(P(s)\) of the energy levels, previous results suggest that the term inducing the eigenvalue-eigenvector correlation and that eventually breaks the symmetry appears, at the critical point, only in the large \(s\) behaviour of \(P(s)\) and not in its small \(s\) behaviour. The symmetry of the system is therefore reflected only in its large \(s\) behaviour. However, in a recent paper, numerical evidence has been presented showing a small difference between the scaling properties of orthogonal and unitary systems using more accurate raw data. But it has been shown that an increase of the accuracy of the raw data with the transfer matrix method generates a systematic shift of the derived quantities and seems to give worse results, casting doubts about the real accuracy of them. Moreover only one distribution (box), for the site energy, was considered whereas three different (box, Gaussian and binary) were studied.

An interesting way to check this problem of symmetry is to study and to compare what happens at the critical point for the symplectic case or, in other words, to consider a system with spin-orbit coupling. It is generally as-
sumed that the critical exponent for the symplectic case should be different ($\nu \simeq 1$) from the orthogonal or unitary case ($\nu \simeq 1.35$) although some recent numerical calculations have surprisingly given a critical exponent higher than expected in the symplectic case. In this paper we would like to show that the picture with the three universality classes to describe the MIT is probably inadequate and to propose a new way to understand the MIT, shedding new light on the problem.

In order to investigate the MIT with spin-orbit coupling we consider the following spin-$\frac{1}{2}$ tight-binding Hamiltonian:

\[ H = \sum_{j,\sigma} \varepsilon_{j,\sigma}|j,\sigma\rangle\langle j,\sigma| + \sum_{j,j',\sigma,\sigma'} V_{j,j'}^{\sigma,\sigma'} |j,\sigma\rangle\langle j',\sigma' | , \tag{1} \]

with the hopping matrix elements represented by

\[ V_{j,j'}^{\sigma,\sigma'} = t^0 1 + i \mu \sum_{\gamma=1}^{3} t^\gamma \sigma_\gamma , \tag{2} \]

where the sites $j$ are distributed regularly in three-dimensional (3D) space, e.g. on a simple cubic lattice. Only interactions with the nearest neighbours are considered. The site energy $\varepsilon_{j,\sigma}$ is described by a stochastic variable. In the present investigation we use a box distribution with variance $= \sqrt{W^2/12}$. $W$ represents the disorder and is the critical parameter. $1$ and $\sigma_\gamma$ are the identity and the Pauli matrices. We choose the coupling constant $\mu = 1$, $t^0 = 1$ and $t^\gamma$ as independent random variables distributed uniformly between $[-\frac{1}{2}, \frac{1}{2}]$ for each pair of lattice sites $j$ and $j'$. The Hermiticity and the time reversal symmetry impose $V_{j,j'}^{\sigma,\sigma'} = (V_{j,j'}^{\sigma,\sigma'})^*$ and $V_{j,j'}^{\sigma',\sigma} = \sigma^\sigma (V_{j,j'}^{\sigma,\sigma'})^*$ respectively, with $\sigma, \sigma' = \pm 1$.

Based on this Hamiltonian, the MIT in the presence of spin-orbit coupling is studied by the ELS method, i.e. via the fluctuations of the energy spectrum. Starting from Eq. (1) the energy spectrum was computed by means of the Lanczos algorithm for systems of size $M \times M \times M$ with $M = 13$, $15$, $17$, $19$ and $21$ and disorder $W$ ranging from $8$ to $30$. The number of different realizations of the random site energies $\varepsilon_{j,\sigma}$ was chosen so that about $10^6$ eigenvalues were obtained for every pair of parameters $(M, W)$ for which only half of the spectrum around the band center is considered so that the results do not deteriorate due to the strongly localised states near the band edges. We checked that we obtain the same results using bands of the energy spectrum ranging from $10$ to $50\%$ (half spectrum). After unfolding the spectrum obtained, the fluctuations can be appropriately characterised by means of the spacing distribution $P(s)$ and the Dyson-Mehta statistics $\Delta_3(L)$. $P(s)$ measures the level repulsion, it is normalised, as is its first moment, because the spectrum is unfolded. $\Delta_3(L)$ measures the spectral rigidity.

Before studying what happens at the critical point we checked, for $P(s)$ and $\Delta_3(L)$, that one finds, as expected, the GSE and the PE regimes for small and large disorder respectively. This can be seen in Fig. 3 for $P(s)$ and Fig. 4 for $\Delta_3(L)$.

The next step is to find where the MIT takes place. For this, one uses that the quantities we are considering here, $P(s)$ and $\Delta_3(L)$, are scale invariant at the critical point. This is due to the fact that the MIT is a second order transition and that finite-size scaling laws apply close to the transition. So we calculate $\alpha_c(M, W) = \frac{1}{30} \int_0^{c_0} \Delta_3(L) dL$ as a function of $M$ and $W$, the critical disorder, $W_c$, being given by $W$ for which $\alpha_c(M, W)$ is independent of $M$. $\alpha_c(M, W)$ has been calculated with a step for $W$ of $0.25$ around the critical disorder and between $1$ and $2$ otherwise. But instead of using directly these data (raw data) we used the analytical properties of $\alpha_c(M, W)$ for a finite system to fit a third order polynomial between $W = 16$ and $W = 26$ for each $M$. The results ($\alpha(M, W)$) are shown in Fig. 4. The raw data ($\alpha_c(M, W)$) where used for the fit are given in the inset of Fig. 4. This method is very interesting because, as we will see later, less computational effort is required and more accurate results are obtained. We can already see that the critical disorder $W_c$ is accurately determined. One finds $W_c = 21.75 \pm 0.10$. This value is higher than in the orthogonal, $W_c \simeq 16.5$, and unitary case where it saturates, as a function of the strength of the magnetic field, around $W_c \simeq 18.75$. This is due to the weak localization, suppression of the weak localization, and antiweak localization phenomena, which take place in the orthogonal, unitary, and symplectic cases respectively. It is then more difficult to localize the states, which means an upwards shift of $W_c$. With $W_c$ it is now possible to study $P(s)$ at the critical point. The first feature we would like to consider is the small $s$ behaviour of $P(s)$. In fact for numerical reasons what we calculate is the cumulative level-spacing distribution $I(s) = \int_0^s P(s') ds'$ which allows a better study of the small $s$ behaviour of $P(s)$. The results are plotted in Fig. 5. We have $P(s) \propto a s^2$ with spin-orbit coupling, $P(s) \propto b s^2$ with magnetic field and $P(s) \propto c s$ without. The behaviour is the same as in the metallic regime except for the prefactors $a$, $b$, and $c$, which are now higher, showing a decrease of the level repulsion due to the multifractal nature of the critical states. The different small $s$ behaviours obtained has been interpreted as a sign that the disorder does not modify the symmetry of the system and that we have, indeed, three different universality classes at the critical point. We claim here that this is not necessarily the case. Considering a system with $N$ sites one sees that the $s^2$ factor, with $\beta = 1, 2, 4$, responsible for the small $s$ behaviour of $P(s)$ is, in fact, a geometrical factor related only to the size of the Hamiltonian, $N \times N$, $2N \times 2N$ and $4N \times 4N$ for orthogonal, unitary, and symplectic, respectively. In RMT, which corresponds to the metallic regime, this geometric factor certainly reflects the symmetry of the system but we do not believe it is necessarily the case for a system
with large disorder. The distribution of the eigenvalues and the eigenvectors, which are independent for the GOE, GUE, or GSE, become correlated when the disorder is increased and eventually break the O(N), U(N), or Sp(N) invariance. We think that the term introducing the eigenvalue-eigenvector correlation and which breaks the symmetry at the critical point appears first in the large s behaviour of $P(s)$. For larger disorder, in the thermodynamic limit, this term will modify the small s behaviour of $P(s)$ too, by cancelling the geometrical factor giving rise eventually to the PE. So following our argumentation what one should compare is the large s behaviour of $P(s)$ for the three different ensembles at the critical point. The results are reported in Fig. 3. As already shown [10] we see no difference between the orthogonal and the unitary case. The surprising fact is that we obtain the same results for the symplectic case too (Fig. 3). According to what we wrote above this would mean that there is only one “super” universality class at the critical point in contradiction to the fact that one expects a different critical exponent for the symplectic case. A way to check that is to calculate $\nu$ for the symplectic case. Starting with $\alpha(M, W)$ defined above, it was shown [15] that $\alpha$ can be expressed as $\alpha(M, W) = f(M/\xi_\infty(W))$ with $\xi_\infty(W) = |W - W_c|^{-\nu}$, the correlation length. $\alpha(M, W)$, being analytical for a finite system, can be written around the critical point as

$$\alpha(M, W) \simeq \alpha(M, W_c) + C|W - W_c|^{1/\nu}. \quad (3)$$

To perform the scaling procedure with the $\alpha_c(M, W)$ data, the range of $\alpha_c(M, W)$ values for various $M$ at any given disorder $W_1$ must overlap the range of $\alpha_c(M, W)$ values for various $M$ for at least one different disorder $W_2$. That would require us to compute $\alpha_c(M, W)$ for a very large number of $W$ values or for larger $M$. Using the method with the fit as described above this is not necessary because from the fit we derived all the values we need for the scaling procedure. Using the values for $\alpha(M, W)$ given in Fig. 3 we show in Fig. 4 that $\alpha(M, W)$ can be, indeed, expressed by a scaling function $f(M/\xi_\infty(W))$. In the inset of Fig. 4 the correlation length $\xi_\infty(W)$ is reported as a function of the disorder. We clearly see the divergence at $W_c \simeq 21.75$. The quality of the curves shows that using a fit to the raw data certainly improves the results. This is also reflected when using Eq. (3) the value of the critical exponent $\nu$ is derived. The tricky point is that the formula (3) is valid only in the vicinity of the critical point but, on the other hand, close to the transition the numerical inaccuracies are largest. The task is therefore to find an adequate range for $|W - W_c|$ that satisfies these two constraints. With the raw data the accuracy of the results as well as the value of $\nu$ is very sensitive to any change in the range of $|W - W_c|$. With the value of $\alpha(M, W)$ from Fig. 3 this is no longer the case. The quantities calculated are much more stable on a wider range of $|W - W_c|$ indicating a better accuracy of our results. We obtain $\nu = 1.36 \pm 0.10$ for the critical exponent which in very good agreement with $\nu = 1.35 \pm 0.15$ for the orthogonal [15, 22] and $\nu = 1.35 \pm 0.20$ for the unitary case [3]. These results seem strongly to support that the behaviour of the MIT can be cast into one “super” universality class and not into three as previously claimed. It has to be noted that recently, using a generalized version of the Ando model [24], a value of $\nu = 1.30 \pm 0.20$ has been found for the symplectic case [10] in good agreement with our results using the Evangelon-Ziman model [7]. It is interesting to note that the results at the critical point seems to be independent of the model as already noted in two dimensions [24].

Concerning $\Delta_3(L)$ the results, Fig. 3, are more difficult to interpret. We know that the shape of $\Delta_3(L)$ contains a term linear in $L$ as well as a non-linear term $L^\omega$, with $\omega < 1$ [3]. As for $P(s)$, it seems we have two different behaviours. For the non-linear term, one obtains different curves for the O(N), U(N) and Sp(N) cases. This behaviour was already observed by Batsch et al. [20] in the case with a magnetic field. If now we consider the linear term, all the curves seem to fall onto one curve. It is interesting to note that the two-point correlation function $R(s)$, from which $\Delta_3(L)$ can be obtained, has recently been calculated [22]. It was shown that $R(s)$ is composed of two terms. One of them is related to the break of the O(N) invariance and gives rise to the linear term in $\Delta_3(L)$. So as for $P(s)$ it seems that the break of the invariance and therefore the change of symmetry is only reflected in one part of $\Delta_3(L)$, namely the linear term. Numerically, even with an accuracy of 0.1 on the critical disorder, it is quite difficult to see what happens for large $L$ and more work clearly needs to be done to increase the accuracy of the results.

In conclusion we think that the picture, with the three universality classes, O(N), U(N) and Sp(N), to describe the MIT is probably inadequate. This picture comes from a field-theoretical approach using a standard $\sigma$ model [19, 25]. But we think our results are not necessarily in contradiction with the field-theoretical approach. Indeed, although these analytical results give indications as to the existence of a MIT as well as information about the weak localized regime, they say nothing about the critical regime (critical point, critical exponent). The problem comes from the $2 + \epsilon$ expansion used to solve the $\sigma$ model. This perturbative analysis is often unreliable for describing the critical regime [20] even near $D = 2$. It is now well known that the $2 + \epsilon$ expansion gives incorrect results for $D = 3$ when applied to MIT (Ref. [19]) and therefore should be used with great care. Moreover, it is far from obvious that this method is adapted for the case with magnetic field or spin-orbit coupling where the lower critical dimension is $< 2$. In particular, the multifractal character of the critical states [3], which we think plays a crucial role in the description of the critical behaviour, is up to now completely beyond the scope of the $2 + \epsilon$ expansion. In contrast, interesting progresses have recently been made applying supersymmetry techniques
to the (non linear)\(\sigma\) model to go beyond the perturbation analysis \([27]\) although the critical properties of the MIT still remain unresolved in the frame of the field theoretical approach \([23,27]\). Our results suggest that the large disorder breaks the \(O(N)\), \(U(N)\), or \(Sp(N)\) invariance at the critical point. But this break of symmetry is only reflected in some parts of \(P(s)\) or \(\Delta_3(L)\). Comparing these parts one finds that the critical behaviour of the MIT is no longer described by three different universality classes but by one “super” universality class. This result is supported by the fact that one obtains the same critical exponent \(\nu \approx 1.35\) with and without magnetic field as well as with spin-orbit coupling. Moreover, Ohtsuki and Kawarabayashi recently showed \([28]\) that the anomalous diffusion and the the fractal dimension \(D(2)\) is the same for \(O(N)\), \(U(N)\), or \(Sp(N)\) at the MIT in agreement with our results.

Finally it is interesting to note that our results are in good agreement with, at least, some experiments, for the value of the critical exponent \(\nu \approx 1.35\) as well as the the absence of influence, at the MIT, of the magnetic field \([28,29]\) and the spin-orbit coupling \([29]\). But clearly further experiments need to be done to check these points carefully, in particular to understand the different results obtained for uncompensated and compensated semiconductors.

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FIG. 1. $\alpha$ as a function of $M$ and $W$. The critical disorder is given by the point for which $\alpha$ is independent of $M$. $W_c = 21.75 \pm 0.10$. The raw data ($\alpha_r$) used for the fit to derive $\alpha$ are given in the inset.

FIG. 2. ln-ln plot of the cumulative level-spacing distribution $I(s)$ for small $s$. We have $P(s) \propto as^4$ with spin-orbit coupling ($\cdots$), $P(s) \propto bs^2$ with magnetic field ($\cdots$) and $P(s) \propto cs$ without ($\cdots$). The behaviour is the same as in the metallic regime ($\cdots$) except for the prefactors $a$, $b$, and $c$, which are now higher.

FIG. 3. Large $s$ behaviour of $P(s)$. * and + are the curves at $W = 3$ and $W = 100$, respectively, showing the metallic and the insulating regimes for $P(s)$. At the critical point the curves are independent of the presence or absence of a magnetic field as well as of the spin-orbit coupling. In the inset there is a ln plot of the tail of $P(s)$.

FIG. 4. In this figure we show that $\alpha(M, W)$ can be expressed by a scaling function $f(M/\xi_\infty(W))$. In the inset the correlation length $\xi_\infty(W)$ is reported as a function of the disorder. We clearly see the divergence at $W_c \simeq 21.75$.

FIG. 5. Dyson-Mehta statistics $\Delta_3(L)$. * is $\Delta_3(L)$ at $W = 3$ and $W = 100$. At the critical point one obtains three different sets of data which seem to merge into one linear set with increasing $L$. 
\begin{align*}
\alpha(M,W) & : M = 21 \\
\alpha_r(M,W) & : M = 19 \\
\alpha_r(M,W) & : M = 17 \\
\alpha_r(M,W) & : M = 15 \\
\alpha_r(M,W) & : M = 13
\end{align*}
\[ \log_{10}(\xi_{\infty}/M) \]

\[ \log_{10}(\alpha(M,W)) \]

- : \( M = 13 \)
- : \( M = 15 \)
+ : \( M = 17 \)
\( \circ \) : \( M = 19 \)
\( \diamond \) : \( M = 21 \)
