Scaling of the Level Compressibility at the Anderson Metal-Insulator Transition

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1. Introduction

In a recent paper,[1)] henceforth it shall be called P1, we have successfully been able to characterize the metal-insulator transition (MIT) of the three dimensional (3D) anisotropic Anderson[2)] model (AM) via scaling of the level compressibililty. The existence of an MIT for this model even in the presence of very strong anisotropy was previously demonstrated by the use of transfer-matrix methods,[3)] multifractal analysis[4)] and energy level statistics.[5)] The presence of a disorder induced MIT in 3D and the absence of such in 2D and in 1D was shown via scaling arguments[6)] (FSS). In the 3D AM we have the metallic, the critical and the insulating phases for low, critical and high disorder, respectively. At the MIT the localization length ξ diverges as a function of, say, disorder W, $\xi \sim |W - W_c|^{-\nu}$, where W_c is the critical disorder and ν is the localization length critical exponent.[7)]

2. Spectral Statistics and Level Compressibility

The localization properties of wave functions of disordered single-electron systems are closely related to the statistical properties of the corresponding spectra.[8)] In the insulating regime localized states, even if they are close in energy, have an exponentially small overlap and their levels are completely uncorrelated. Accordingly, in the thermodynamic limit the normalized distribution of spacing s between neighboring energy levels follows the Poisson law $\exp(-s)$. In the metallic regime, the large overlap of delocalized states induces correlations in the energy spectrum leading to level repulsion. In this case, if the system is invariant under rotational and under time-reversal symmetry, the normalized level spacing distribution closely follows the Wigner surmise of the Gaussian orthogonal ensemble of random matrix theory[9)]

$$P(s) = \frac{\pi}{2} s \exp\left(-\frac{\pi}{4} s^2\right).$$

The third system-size independent statistics directly at the MIT is usually called *critical statistics* and the corresponding wave functions are multifractal.

Our interest here is to use the *number variance* Σ_2 to characterize the MIT. The number variance is known to have the following general behavior as a function of the mean number of levels $\bar{n}$ in an energy interval, *i.e.*,

$$\Sigma_2 \sim \begin{cases} \log(\bar{n}) & \text{delocalized,} \\ \chi\bar{n} & \text{critical,} \\ \bar{n} & \text{localized.} \end{cases}$$

The number variance in the critical regime has been conjectured to be Poisson-like,[10)] *i.e.*, $\Sigma_2 \approx \chi\bar{n}$, where the level compressibility χ is another important parameter to characterize the MIT. Formally, the level compressibility is defined as

$$\chi \approx \lim_{\bar{n}\to\infty} \lim_{N\to\infty} \frac{d\Sigma_2(\bar{n})}{d\bar{n}}. \tag{1}$$

χ takes values $0 \leq \chi \leq 1$, being zero in the metallic state and unity in the insulating state; N is the system size, see P1 for details. Note that in order to perform any statistical calculations the eigenspectrum must be "unfolded"[11)] so that the average spacing between adjacent eigenvalues is one.

3. The Model Hamiltonian

We study the 3D AM of localization described by a Hamiltonian in the lattice site basis as

$$\mathcal{H} = \sum_i^N \varepsilon_i |i\rangle\langle i| + \sum_{\langle i,j\rangle} t_{ij} |i\rangle\langle j| \tag{2}$$

where $\langle i|j\rangle = \delta_{ij}$ and the t_{ij} are hopping integrals with $\langle i,j\rangle$ denoting nearest-neighbors on a regular cubic lattice with periodic boundary conditions. Our model includes anisotropy in the hopping integrals *i.e.*, *weakly coupled planes* defined by $t_x = t_y = 1$, $t_z = 0.1$, here t_x, t_y and t_z are hopping integrals in the three spatial directions. We emphasize that we have chosen strong anisotropy simply because this is the case with the most accurate data (with relative error range form 0.2 to 0.4%) from a previous study.[12)] In fact it has been shown that anisotropy has no effect on the universality class of the model[12,13)] except for changing non-universal properties such as the critical disorder W_c. The site energies ε_i are taken to be random numbers uniformly distributed in the interval $[-W/2, W/2]$.

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4. FSS and Results

To perform FSS with χ we fit Σ_2 data with a polynomial and then "extract" the linear coefficient χ_p which is an approximation to χ, see figures 1 and 2. In P1, we have shown that a polynomial fit is stable and reliable for the calculation of the critical exponent ν and the critical disorder W_c. The polynomial is of the form,

$$\chi_p \approx \frac{\Sigma_2(N,W,\bar{n})}{\bar{n}} - \sum_{k=1}^{m} \gamma_k(N,W)\bar{n}^k,$$

where m is the order of the fit and $\gamma_k(N,W)$ are assumed not to depend on $\bar{n}$. After performing FSS we are able to estimate the values of the critical exponent $\nu \approx 1.45\pm0.12$ and the critical disorder $W_c \approx 8.59\pm0.05$. These values are averages of the results of many fit parameters in the FSS procedure, see Table 3 of P1 for details. The above approach is only suited to giving the global behavior of χ in the neighborhood of the MIT. This implies that there is a *systematic* shift of χ_p toward higher values and as such this method exaggerates the value of the critical level compressibility χ_c at the MIT. For the calculation of the critical level compressibility χ_c, we fit Σ_2 data *via* an ansatz function that incorporates irrelevant scaling exponents y_k, *i.e.*,

$$\chi_c \approx \frac{\Sigma_2(N,W,\bar{n})}{\bar{n}} - \sum_{k=1}^{m} \Gamma_k(N,W)\bar{n}^{-y_k},$$

where $\Gamma_k(N,W)$ are assumed not to depend on $\bar{n}$. Note that this fit function works well for large system sizes and gives $\chi_c \approx 0.28\pm0.06$ as an average value, see Table 2 of P1 for details. This value is in good agreement with previous studies.[14)]

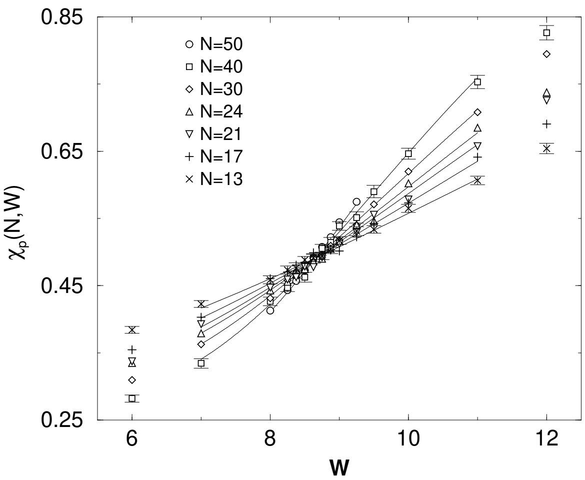

Fig. 1. $\chi_p(N,W)$ obtained from a polynomial fit (hence the subscript on χ) of degree $m = 3$. The N dependence is clearly evident. The solid lines are fit functions from FSS, see P1.

5. Summary

In summary, our results show that χ can be used to compute, with the help of FSS, estimates of W_c and of ν which are in good agreement with other spectral calculations. Secondly, we have established that a polynomial fit can be used to extract the universal content of the level compressibility in the vicinity of the MIT.

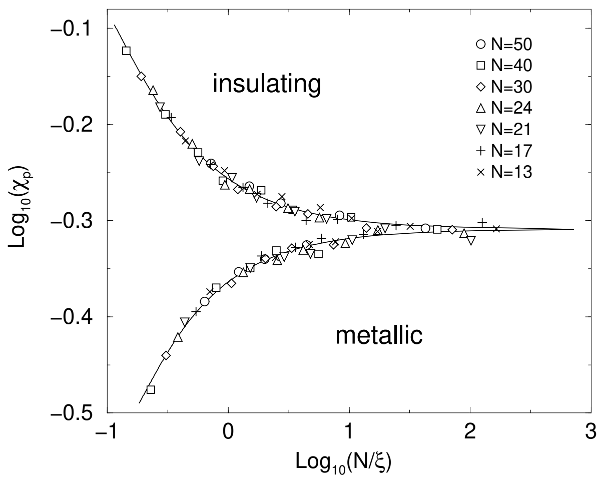

Fig. 2. One-parameter scaling dependence of χ_p on ξ for different system sizes N and disorders $W \in [6, 12]$.

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