

Anderson metal-insulator transitions with classical magnetic impurities

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We study numerically the effects of classical magnetic impurities on the Anderson metal-insulator transition. We find that a small concentration of Heisenberg impurities enhances the critical disorder amplitude W_c with increasing exchange coupling strength J . The resulting scaling with J is analyzed which supports an anomalous scaling prediction by Wegner due to the combined breaking of time-reversal and spin-rotational symmetry. Moreover, we find that the presence of magnetic impurities lowers the critical correlation length exponent ν and enhances the multifractality parameter α_0 . The new value of ν improves the agreement with the value measured in experiments on the metal-insulator transition (MIT) in doped semiconductors like phosphor-doped silicon, where a finite density of magnetic moments is known to exist in the vicinity of the MIT. The results are obtained by a finite-size scaling analysis of the geometric mean of the local density of states which is calculated by means of the kernel polynomial method. We establish this combination of numerical techniques as a method to obtain critical properties of disordered systems quantitatively.

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Experimental studies of uncompensated doped semiconductors like $\text{Si}_{1-x}\text{P}_x$ (Si:P) show a metal-insulator transition (MIT) as function of dopant density x . This is one of the most extensively studied cases of a quantum phase transition [1–3]. The doping increases the carrier density and thereby the conductivity but also creates the onsite disorder potential. The random positioning of the dopants results in random hopping amplitudes between the dopant sites. Moreover, the electron-electron interaction causes spin and charge correlations. Therefore, the MIT can neither be described completely by an Anderson MIT (AMIT) [4,5], driven solely by disorder, nor by a correlation-driven MIT, the Mott transition [6]. Taking into account both correlations and disorder remains an open problem of condensed matter theory [7,8].

Thermodynamic measurements prove the presence of localized magnetic moments in the metallic regime in the excess specific heat and a low-temperature divergence of the magnetic susceptibility [1,2,9,10]. Indications of magnetic moments can also be seen in transport measurements, such as the thermoelectrical Seebeck coefficient [1,2]. These experiments have been interpreted by assuming that up to 10% of all P atoms contribute localized paramagnetic moments at the MIT [11–14], which originate from the localized states in the tails of the impurity band. Thus, it is an essential step in understanding the MIT in doped semiconductors to understand the influence of magnetic impurities on the AMIT.

Since the work of Hikami *et al.* [15] it is known that weak localization is suppressed in the presence of a finite concentration of localized magnetic moments because the exchange interaction with the spins of the conduction electrons breaks time-reversal invariance. The breaking of time-reversal

symmetry (TRS) is known to weaken Anderson localization, so the localization length ξ is enhanced. In quasi-one-dimensional (quasi-1D) disordered wires this leads to an enhancement $\xi = s\beta\xi_0$, with $\beta = 1$ ($\beta = 2$) when TRS is unbroken (broken) and $s = 1$ ($s = 2$) when spin-rotational symmetry (SRS) is unbroken (broken) [16,17]. Here, $\xi_0 = M_t l_e$, where M_t is the number of transverse channels and l_e is the elastic mean-free path [16]. With SRS intact, there are independent channels for the localization of up and down spins. Otherwise the spin-up and spin-down channels are mixed, and the electrons have effectively twice as many channels, which enhances ξ accordingly.

Three-dimensional disordered systems are known to bear an AMIT. It can be expected that the breaking of TRS and SRS shifts the critical disorder W_c towards stronger disorder amplitudes W , which is a measure of the width of the distribution of the disorder potential. Likewise, the critical electron density n_c in doped semiconductors is decreased [18,19]. The symmetry class of the transition is thereby changing from *orthogonal* to *unitary* [18,19]. In the presence of an external magnetic field, this change of symmetry class of the conduction electrons is governed by the parameter $X_B = \xi^2/l_B^2$, where l_B is the magnetic length. Therefore, in analogy, the spin scattering rate due to magnetic impurities τ_s^{-1} is expected to enter through the symmetry parameter $X_s = \xi^2/L_s^2$, where $L_s = \sqrt{D_e\tau_s}$ is the spin relaxation length, D_e is the diffusion coefficient, and ξ is the correlation (localization) length on the metallic (insulating) side of the AMIT [15]. When $X_s \geq 1$, the electron spin relaxes before it can cover the area limited by ξ and the system is in the *unitary regime*.

The crossover at the mobility edge can be studied through a scaling ansatz for the conductivity σ on the metallic side, as done in Ref. [18] for the case of an external magnetic field. Following this approach, using the spin scattering rate τ_s^{-1} yields $\sigma(\tau_s^{-1}) = e^2 f(X_s)/(h\xi)$. As a function of the energy difference $\Delta E = E - E_M$ to the mobility edge E_M one then

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obtains [19]

$$\sigma(\tau_s^{-1}) = \Delta E^{(d-2)\nu} \tilde{f}(\tau_s^{-1} \Delta E^\nu). \quad (1)$$

Simple scaling theory yields $\varphi = 2\nu$ [18], with ν being the critical exponent describing the divergence of ξ at the mobility edge [in the three-dimensional (3D) orthogonal universality class]. Wegner argues that, while an external magnetic field yields $\varphi_a = 2\nu$, the additional SRS breaking by magnetic impurities rather yields

$$\varphi_s = 2\nu + 3 \quad (2)$$

in a second-order $d = 2 + \varepsilon$ expansion [19,20]. Thus, a numerical analysis of φ in the presence of magnetic moments is called for. The value of φ_a in a magnetic field has been studied in Ref. [21], and they find good agreement with $\varphi_a = 2\nu$ within their numerical accuracy for W_c . A random magnetic field should yield the same value. On the other hand, if a finite concentration of classical magnetic impurities n_M with spin S is present, the spin relaxation rate is finite, resulting in a shift of the critical disorder amplitude W_c that can be obtained from the scaling ansatz for the conductivity (1). For classical spins with a Heisenberg exchange coupling of strength J , it follows that [22]

$$W_c = W_c^0 + W_c^0 \left(\frac{a_c^2}{D_e \tau_s} \right)^{\frac{1}{\varphi}}, \quad (3)$$

where W_c^0 is the critical disorder strength without magnetic impurities, $D_e = v_F^2 \tau / d$, v_F is the Fermi velocity, and τ^{-1} is the total elastic scattering rate. a_c is a constant representing the smallest length scale, which is identical to the lattice spacing here.

We start from the *Anderson model* Hamiltonian [23],

$$\hat{H}_0 = t \sum_{(i,j),\sigma} |j,\sigma\rangle \langle i,\sigma| + \sum_{i,\sigma} V_i |i,\sigma\rangle \langle i,\sigma|, \quad (4)$$

where $|i,\sigma\rangle$ denotes an electron state with spin σ located at site i of a 3D cubic lattice with $N = L^3$ sites and periodic boundary conditions. For the local potential V_i , random values are drawn from a box distribution of width W , $V_i \in [-W/2, W/2]$, while the hopping amplitude t between neighboring lattice sites remains constant.

We add another term to the Hamiltonian, describing a local coupling of the conduction electron spin σ_i to a classical spin \mathbf{S}_i (two-fluid model) [10,11,24] with $\mathbf{S}_i^2 = S^2 = 1$ and random orientation (Heisenberg like), given by the (polar and azimuth) angles θ_i and φ_i . The angles are drawn uniformly from the intervals $\cos \theta_i \in [-1, 1]$ and $\varphi_i \in [0, 2\pi]$. σ_i are the Pauli matrices, so the general form of the coupling term, $\sum_i J_i \sigma_i \cdot \mathbf{S}_i$, can be written as

$$\begin{aligned} \hat{H}_s = S \sum_i J_i \left(\cos \theta_i \sum_{\sigma=\pm 1} \sigma |i,\sigma\rangle \langle i,\sigma| \right. \\ \left. + \sin \theta_i \sum_{\sigma=\pm 1} \exp(i\sigma \varphi_i) |i,\sigma\rangle \langle i,-\sigma| \right). \quad (5) \end{aligned}$$

We fix the concentration of sites carrying a magnetic moment to $n_M = 5\%$. Note that this is a realistic value for real materials like Si:P [11–14]. J_i is drawn from a binary probability

distribution, $J_i \in \{J, 0\}$, taking a nonzero value with probability n_M , for which it conforms to the exchange coupling strength J . Equation (4) by itself leads to a nonmagnetic scattering rate $\tau_0^{-1} = 2\pi W^2 \rho(\varepsilon_F) / (6\hbar)$. The scattering from the magnetic impurities enhances the total scattering rate to $\tau^{-1} = \tau_0^{-1} + \tau_s^{-1}$.

The spin-resolved *local density of states* (LDOS) is given by $\rho_{i,\sigma}(E) = \sum_{k=1}^{2N} |\langle i,\sigma | k \rangle|^2 \delta(E - E_k)$, where $|k\rangle$ denotes the eigenstate with eigenenergy E_k of the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_s$. We use the *kernel polynomial method* (KPM) [25–27] in combination with the *Jackson kernel* which is known to yield optimal results for the calculation of the LDOS, as it smooths *Gibb's oscillations* most efficiently [25]. The KPM expands the target function in a series of *Chebyshev polynomials* that are only defined on the interval $[-1, 1]$, so a rescaling of the original spectrum of \hat{H} is necessary, which we achieve by applying a factor $a = 24t$ to all energies, $E = a\tilde{E}$. The Jackson kernel comes with an energy broadening of $\tilde{\eta} = \pi/M$ at the center of the considered interval ($E = 0$), which is rescaled by the same factor, $\eta = a\tilde{\eta}$ [28].

We consider two ensemble averages: The arithmetically averaged local density of states (ALDOS),

$$\rho_{av}(E) = \frac{1}{N_S} \sum_{n=1}^{N_S} \rho_n(E), \quad (6)$$

which corresponds to the average density of states (ADOS) in the thermodynamic limit (large number of samples N_S) [29], and the geometrically averaged local density of states (GLDOS),

$$\rho_{typ}(E) = \exp \left(\frac{1}{N_S} \sum_{n=1}^{N_S} \ln \rho_n(E) \right), \quad (7)$$

which is also known as the *typical density of states* [30]. Here, the index n takes into account both site index i and spin σ of the conduction electrons. N_S denotes the total number of considered local densities $\rho_n(E)$ (in this work, $N_S = 8000$). Although the LDOS is known to be spatially correlated, to save some computation time, we take into account $p = 32$ random lattice sites from each disorder realization in the geometric mean.

In contrast to the ALDOS, the GLDOS is sensitive to the localization character of quantum states. It is reduced by both increasing disorder and increasing system size within the whole energy spectrum [26]. In the thermodynamic limit ($L \rightarrow \infty$), the GLDOS approaches zero in energy regions of localized states, and a positive value in the case of extended states [30]. For finite system sizes the GLDOS stays positive, even for perfectly localized states. In Ref. [30], localized states are detected by defining a threshold value for the GLDOS, which is adjusted to previously known values for the critical disorder W_c . For a quantitative analysis of the critical parameters (including W_c), it is necessary to perform a finite-size scaling (FSS) analysis of the GLDOS. To this end, we use the scaling ansatz [31]

$$\Gamma(W, L) = L^{d-\alpha_0} F(\psi L^{1/\nu}, \eta \rho_{av} L^d) \quad (8)$$

for the GLDOS at half filling ($E = 0$), where $\Gamma(E) = \rho_{typ}(E) / \rho_{av}(E)$, $d = 3$, $\psi = (W_c - W) / W_c$ is the *reduced*

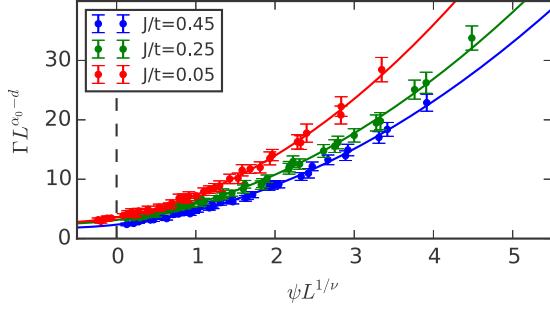


FIG. 1. Demonstration of the scaling ansatz (8) at half filling ($E = 0$) for three different values J and $n_F = 2$. The error bars correspond to 95% confidence.

disorder, ν is the correlation or localization length exponent [5], and α_0 is a multifractality parameter [5,32,33]. We neglect the disorder dependence of $\rho_{av}(E)$. By fixing the ratio $G = L^d/M = 1$, the function $F(x, y)$ (8) only depends on the first argument, $x = \psi L^{1/\nu}$. We expand the function $\tilde{F}(x) \equiv F(x, \rho_{av}\pi G)$ to order n_F in x by using the power series $\tilde{F} = \sum_{n=0}^{n_F} \tilde{F}_n x^n$ so our fit model (8) possesses $N_P = n_F + 4$ parameters, $(W_c, \alpha_0, \nu, \tilde{F}_0, \tilde{F}_1, \dots, \tilde{F}_{n_F})$. The scaling (8) is demonstrated in Fig. 1 for $n_F = 2$.

Table I summarizes the fit results. Considering five system sizes $L \in \{10, 20, \dots, 50\}$ and eight disorder strengths $W/t \in \{15, 15.5, \dots, 18.5\}$, each fit has access to $N_D = 40$ data points [34]. To assess the quality of the fit, the χ^2 statistic and the goodness of fit (GOF) probability Q are computed [28]. For every J , we select an optimal series expansion order $n_F \in \{2, 3, 4\}$ so that $|Q - 1/2|$ is minimized, as $Q = 0.5$ indicates an optimal fit [35].

Figure 2 shows how the fit parameters W_c , α_0 , and ν depend on the coupling strength J by using different series expansion orders n_F . Our result for W_c at $J = 0$ (corresponding to the original Anderson model) is $W_c^A/t = 16.52 \pm 0.17$, which agrees with established, more precisely measured values [32,33,36] like $W_c^A/t = 16.530(16.524, 16.536)$ [32]. As the coupling strength J is increased, the critical disorder W_c approaches a higher value of $W_c^U/t \approx 19.4$. This tendency is expected, as the symmetry class is changing from orthogonal

TABLE I. Fit parameters W_c , α_0 , and ν for different exchange coupling strengths J with their standard errors, found by expanding the function $\tilde{F}(x)$ to order n_F . To assess the quality of the fit, we provide the χ^2 statistic and the goodness of fit probability Q [28].

J/t	n_F	W_c/t	α_0	ν	χ^2	Q
0.00	4	16.52 ± 0.17	4.07 ± 0.04	1.48 ± 0.06	30.5	0.54
0.05	4	18.12 ± 0.28	4.43 ± 0.08	1.37 ± 0.08	29.0	0.62
0.10	3	18.19 ± 0.21	4.33 ± 0.06	1.40 ± 0.06	45.5	0.07
0.15	4	18.56 ± 0.31	4.39 ± 0.09	1.32 ± 0.08	41.4	0.12
0.20	3	19.02 ± 0.25	4.53 ± 0.07	1.32 ± 0.07	54.1	0.01
0.25	4	18.92 ± 0.26	4.47 ± 0.08	1.29 ± 0.07	30.6	0.54
0.30	4	19.42 ± 0.31	4.47 ± 0.06	1.50 ± 0.09	34.6	0.34
0.35	4	18.47 ± 0.25	4.27 ± 0.07	1.25 ± 0.07	28.0	0.67
0.40	4	19.39 ± 0.21	4.51 ± 0.06	1.31 ± 0.07	33.5	0.39
0.45	4	19.15 ± 0.32	4.41 ± 0.09	1.34 ± 0.10	38.1	0.21

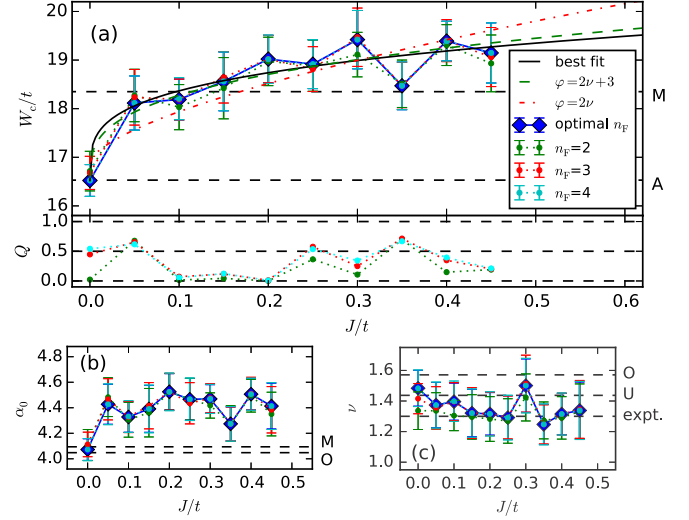


FIG. 2. Dependence of the fit parameters (a) W_c , (b) α_0 , and (c) ν on the exchange coupling J , using different series expansion orders n_F . The dashed horizontal marks established values for the pure Anderson model (A, realized by our model for $J = 0$) [32], a model considering an external magnetic field (M) [21], the 3D orthogonal (O) [33,37], and the 3D unitary (U) universality class [33], and the experimental value (expt.) [1]. For $W_c(J)$, the data with minimal $|Q - 1/2|$ (d) is fit to Eq. (9) by using $\nu = 1.571$ [37] (see also Table II). The error bars correspond to 95% confidence.

to unitary. Another study considering an external magnetic field has found a value of $W_c^M/t \approx 18.35$ [21]. We conclude that the additional SRS breaking of the magnetic impurities causes a further increment. This can qualitatively be expected, since the mixing of the spin-up and spin-down channels by the SRS breaking enhances the number of available spin channels and thereby weakens the localization [16,17].

As can be seen in Fig. 2(b), the value of α_0 undergoes a gradual transition to a larger value by tuning up the coupling strength J . Remarkably, this value is larger than that of a recent study using multifractal analysis of the 3D Anderson model in a magnetic field, $\alpha_0^M = 4.094(4.087 \dots 4.101)$ [33]. This suggests that the additional spin-symmetry breaking enhances α_0 beyond the unitary value as obtained when only TRS is broken. For $J = 0$, our value is in agreement with other studies, for example $\alpha_0^O = 4.048(4.045, 4.050)$ [32].

Our result for the localization length exponent ν in the orthogonal regime ($J = 0$) agrees within the achieved accuracy with established values [32,33,36,37] like $\nu^O = 1.571(1.563, 1.579)$ [37]. However, the error obtained within our method is about eight times larger than that obtained within the well-established transfer matrix method [37]. During preliminary calculations we observed that ν is increasing when lowering the ratio $G = L^d/M$ [28]. This is expected since G is proportional to the ratio between the KPM broadening and the average level spacing. For $G = 0.1$ the broadening should be of the order of the mean level spacing, while our calculations for $G = 1$ could still mix critical and noncritical states [28]. Since the computational effort scales inversely linear with G , we are forced to make a trade-off between the largest considered system size $N = L^3$, the chosen value of G , and the resulting computation time, so we have decided

TABLE II. Fit results for $W_c(J)$. In the top row, μ is a free fit parameter. Otherwise, $\mu = 2/\varphi$ is fixed to values (shown in bold) according to the given analytic formulas for φ [22,38], using either $\nu = 1.571(1.563, 1.579)$ [37] or our own value for $J = 0$, $\bar{\nu} = 1.48 \pm 0.06$.

$\varphi = \dots$	a	μ	b	χ^2	Q
Free fit	3.40 ± 0.46	0.27 ± 0.09	16.52 ± 0.21	11.3	0.13
$2\nu + 3$	3.61 ± 0.34	0.33	16.57 ± 0.19	12.0	0.15
2ν	4.52 ± 0.70	0.64	16.89 ± 0.26	28.4	$4e - 04$
$2\bar{\nu} + 3$	3.64 ± 0.35	0.34	16.58 ± 0.19	12.2	0.14
$2\bar{\nu}$	4.62 ± 0.75	0.67	16.93 ± 0.27	30.9	$1e - 04$

to choose $G = 1$ for this analysis. Note that experimental investigations have always yielded values of ν considerably smaller than theoretical predictions, partly because they face a similar problem of low energy resolution [1], just like our numerical method does.

For disordered systems in a magnetic field (3D unitary universality class), values ν smaller than that of the 3D orthogonal universality class have been reported [33,36], like $\nu^M = 1.437(1.426, 1.448)$ [33] [marked in Fig. 2(c)]. Note that within the achieved accuracy, our results for ν with magnetic impurities ($J > 0$) are of similar or smaller magnitude and in good agreement with the experimental value $\nu^{\text{expt.}} \approx 1.3$ [1] of real materials in which magnetic impurities are known to exist at the MIT.

The scaling of W_c with J has been analyzed in Fig. 2(a). Equation (3) suggests a scaling $W_c(J) \sim J^{2/\varphi}$. Hence, we use

$$W_c(J) = aJ^\mu + b \quad (9)$$

for the fit, with $\mu = 2/\varphi$. The fit results are summarized in Table II. The best fit (smallest $|Q - 1/2|$) is found for Wegner's scaling (2) with $\epsilon = 1$ [19]. Also, the free fit of the parameter μ shows good agreement with this analytic prediction. Our results clearly do not support the relation $\varphi = 2\nu$ [18,22], which results in GOF probabilities that are orders of magnitude away from an acceptable range (e.g., $Q \in [0.1, 0.9]$). This interpretation remains intact even when using our own value for the localization length exponent $\bar{\nu} = 1.48 \pm 0.06$ (for $J = 0$) instead of the value $\nu = 1.571(1.563, 1.579)$ [37].

To conclude, we have shown numerically how local magnetic moments which break TRS and SRS affect the metal-insulator transition in the 3D Anderson model. We found that the critical exponent ν decreases for increasing coupling strength J and determined its value as $\nu^S \approx 1.3 \pm 0.1$ for 5% magnetic impurities. Within the obtained accuracy, this value agrees with experimental results obtained from conductivity scaling at the MIT in phosphor-doped silicon [1]. We also find the multifractality parameter $\alpha_0^S \approx 4.4 \pm 0.1$ when both TRS and SRS are broken, a value larger than the unitary value when only TRS is broken [33]. We considered the scaling of the critical disorder amplitude $W_c(J)$ and confirm an analytical prediction by Wegner [19]. Thus, the present investigation may relate the systematically lower values for the critical exponent ν found in experiments to the presence of a finite density of localized magnetic moments. We note that magnetic moments are known to form due to the local interaction in localized states [3,14]. Recently, it has been shown that the interplay between the Kondo screening of magnetic moments and Anderson localization may result in a novel quantum phase transition [22,39,40]. It remains to combine this effect with long-range Coulomb interaction in disordered electron systems [41,42] in order to achieve a complete understanding of the experimental results [1]. Furthermore, we established a method to obtain critical properties of disordered electron systems by a finite-size scaling ansatz for the geometric mean of the local density of states, which enables us to make use of the kernel polynomial method to efficiently calculate the LDOS. This method should be further developed in order to reach an accuracy comparable to more established methods like the transfer matrix method [43].

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result for $\varepsilon = 1$. Second-order [19], fourth-order [38], and fifth-order [44] results have so far shown poor agreement with numerical values [32,37,33] for the localization length exponent ν . However, a new Borel–Padé analysis has recently been suggested [45] that greatly improves agreement between the fifth-order $2 + \varepsilon$ expansion [44] and numerical values for ν . Thus, it should be checked if this new Borel–Padé analysis could lead to refined predictions of φ_a and φ_s as well.

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