Anderson Metal-Insulator Transitions with Classical Magnetic Impurities

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Abstract

We study the effects of classical magnetic impurities on the Anderson metal-insulator transition (AMIT) numerically. In particular we find that while a finite concentration of Ising impurities lowers the critical value of the site-diagonal disorder amplitude W_c, in the presence of Heisenberg impurities, W_c is first increased with increasing exchange coupling strength J due to time-reversal symmetry breaking. The resulting scaling with J is compared to analytical predictions by Wegner [1].

The results are obtained numerically, based on a finite-size scaling procedure for the typical density of states [2], which is the geometric average of the local density of states. The latter can efficiently be calculated using the kernel polynomial method [3]. Although still suffering from methodical shortcomings, our method proofs to deliver results close to established results for the orthogonal symmetry class [4]. We extend previous approaches [5] by combining the KPM with a finite-size scaling analysis.

We also discuss the relevance of our findings for systems like phosphor-doped silicon (Si:P), which are known to exhibit a quantum phase transition from metal to insulator driven by the interplay of both interaction and disorder, accompanied by the presence of a finite concentration of magnetic moments [6].

Models

→ Start from usual Anderson model Hamiltonian (3D simple-cubic lattice, $L \times L \times L$) [7],

$$\hat{H}_0 = t \sum_{\substack{i,j,\sigma \\ \text{(n.n.)}}} |j,\sigma\rangle\langle i,\sigma| + \sum_{i,\sigma} V_i\, |i,\sigma\rangle\langle i,\sigma| \qquad (1)$$

(i, j: lattice site index; σ: spin; t: constant hopping amplitude; V_i: random potential, box distribution of width W).

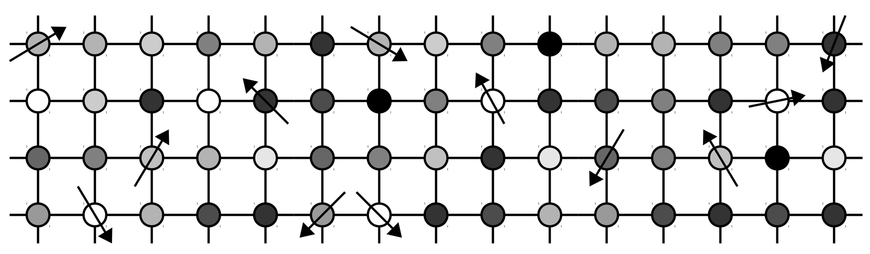
→ Add coupling to classical magnetic impurities,

$$\hat{H}_S = S \sum_i J_i \Bigg(\cos\theta_i \sum_{\sigma=\pm} \sigma\, |i,\sigma\rangle\langle i,\sigma| + \sin\theta_i \sum_{\sigma=\pm} \exp(i\sigma\varphi_i)\, |i,\sigma\rangle\langle i,-\sigma| \Bigg) \qquad (2)$$

(θ_i, φ_i: random angles; J_i: exchange coupling strength, non-zero at impurity sites, concentration n_M).

→ Total Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_S$ breaks time-reversal symmetry. ⇒ Unitary symmetry class.

→ Compare to Ising impurities (for $\theta_i \in \{0, \pi\}$). ⇒ Time-reversal symmetry remains intact, orthogonal symmetry class.



Ensemble averages

→ Arithmetic mean of the LDOS (ALDOS):

$$\rho_{av}(E) = \frac{1}{N_S} \sum_{\iota=1}^{N_S} \rho_\iota(E) \quad . \qquad (3)$$

⇒ Approaches *total density of states* for $N_S \to \infty$.

→ Geometric mean of the LDOS (GLDOS):

$$\rho_{typ}(E) = \exp\left(\frac{1}{N_S} \sum_{\iota=1}^{N_S} \log \rho_\iota(E) \right) \quad . \qquad (4)$$

⇒ *Typical density of states* [5].

→ In addition to different disorder realizations, the sample size N_S can also cover multiple lattice sites per disorder realization to save computational effort ($N_S \approx 10^4 \dots 10^6$).

Finite-size scaling and phase diagrams

→ Use simplistic fit model (empirical)

$$\rho_{typ}(L) = \frac{a}{L^p} \qquad (5)$$

(for fixed energy E and disorder parameters W, J, n_M).

→ Identify phase transition as the contour

$$p(E, W) = \alpha_0 - d \approx 1.048 \quad , \qquad (6)$$

with $\alpha_0 = 4.048(4.045, 4.050)$ [8].

→ 1σ-confidence level between the contours

$$p(E, W) \pm \sigma_p(E, W) = \alpha_0 - d \approx 1.048 \quad . \qquad (7)$$

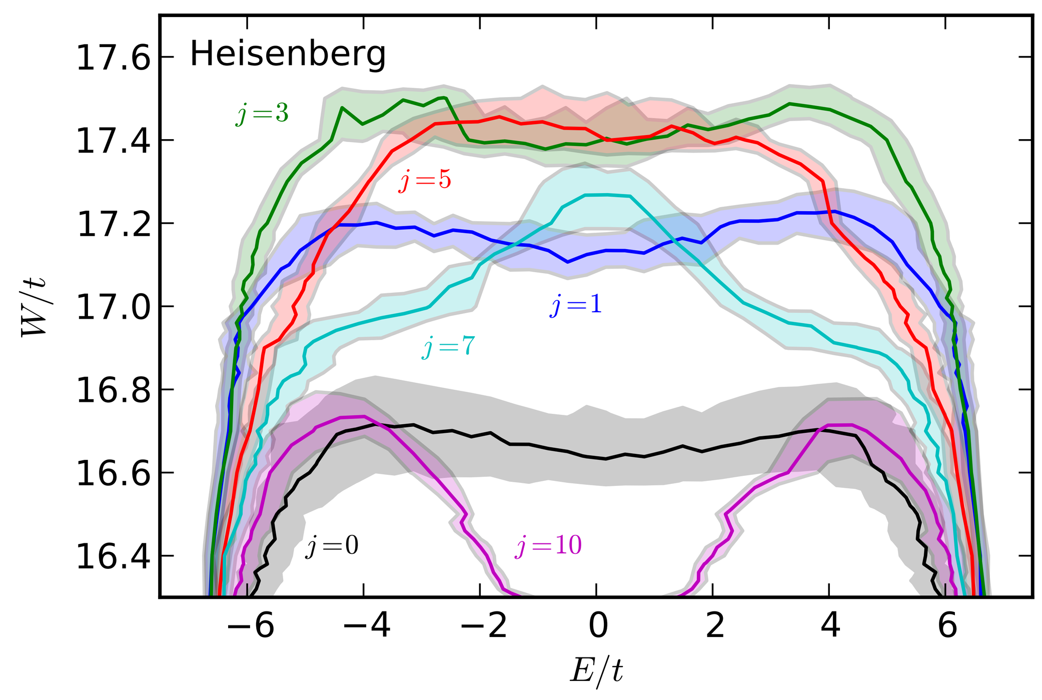


Figure 2: *Phase diagrams of the Anderson model including Heisenberg impurities ($j = J/t$, $n_M = 5\%$, $L = \{10, 15, 20, 25, 30\}$).*

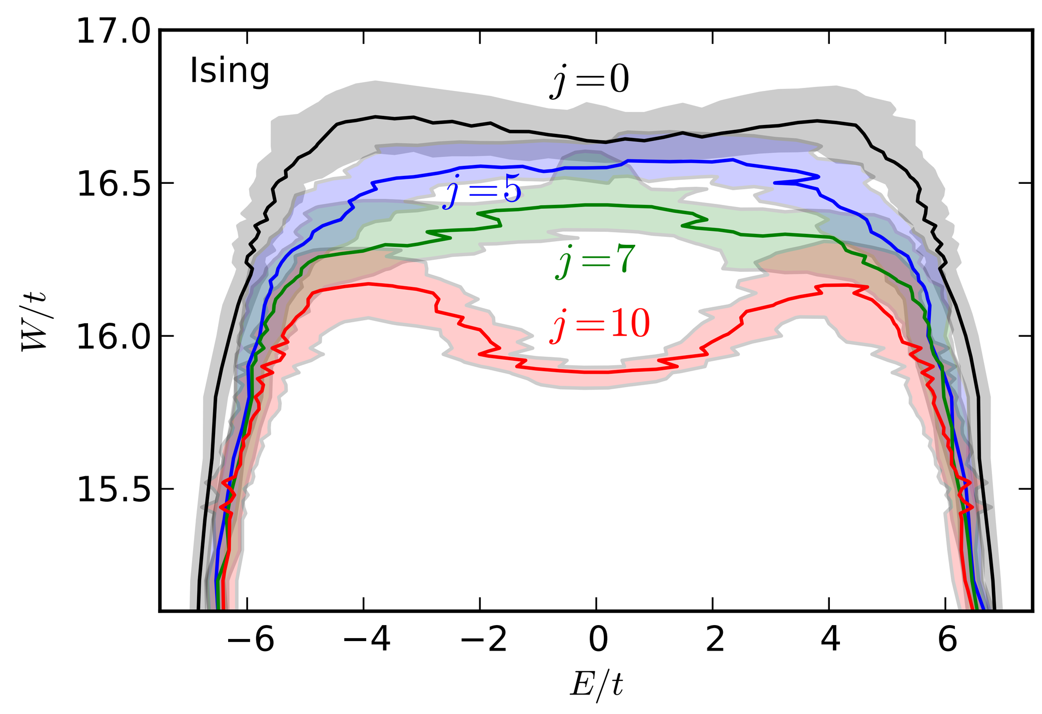


Figure 3: *Phase diagrams of the Anderson model including polarized Ising impurities ($\theta_i = 0$, $j = J/t$, $n_M = 5\%$, $L = \{10, 15, 20, 25, 30\}$).*

Shift of the metal-insulator transition

→ A finite concentration of magnetic moments can change the critical disorder W_c.

→ Analytic prediction [9]:

$$W_c = W_c^0 + W_c^0 \left(\frac{a_c^2}{D_e \tau_S^0} \right)^{\frac{1}{\varphi}} \quad , \qquad (8)$$

with $\varphi = 2\nu$ and $\nu = 1.590(1.579, 1.602)$ [8]. $1/\tau_S^0$ is the magnetic scattering range, $1/\tau_S^0 \sim J^2$. So the expected scaling with J (for small J) is

$$W_c(J) \sim J^\beta \quad , \qquad (9)$$

with $\beta = 2/\varphi$.

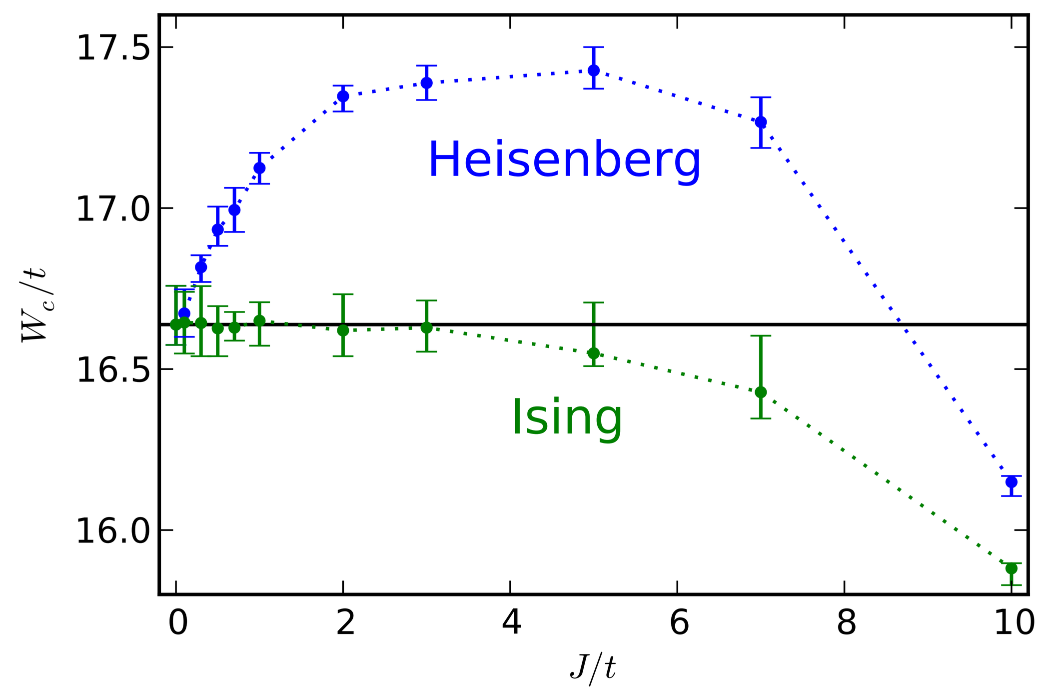


Figure 4: *Measured shift of the phase transition in dependence of J at the bandcenter ($E = 0$, $n_M = 5\%$, $L = \{10, 15, 20, 25, 30\}$).*

Table 1: *Expected values for β.*

method	expression	value	reference
	$2/2\nu$	0.63	[9, 10]
$2+\varepsilon$-expansion (for $\varepsilon = 1$)	$2/(2\nu+3)$	0.32	[1]

The kernel polynomial method

→ Polynomial series expansion

$$f(x) = \frac{1}{\pi\sqrt{1-x^2}} \left(\mu_0 + 2 \sum_{n=1}^{\infty} \mu_n T_n(x) \right) \qquad (10)$$

based on Chebychev polynomials

$$T_n(x) = \cos(n \arccos(x)) \quad . \qquad (11)$$

→ Efficient way to calculate (spin-resolved) LDOS of state $|i,\sigma\rangle$ using the coefficients (Chebychev moments) [3]

$$\mu_n^{|i,\sigma\rangle} = \int_{-1}^{1} f(x)\, T_n(x)\, dx = \langle i,\sigma|\, T_n(H)\, |i,\sigma\rangle \quad . \qquad (12)$$

→ Provides information about the whole energy spectrum at once. ⇒ Phase diagrams can be plottet.

→ Order-of-N method (given a $N \times N$ sparse matrix).

Conclusions

→ Use KPM [3] to calculate LDOS efficiently.

→ Utilize FSS behavior of the typical density of states to estimate phase transition.

→ Two types of magnetic impurities (Heisenberg and Ising) are shown to have different effect on W_c, in qualitative agreement with analytic Prediction [9].

Outlook

→ Consider isotropic distribution of the impurity spin directions (SO(3) symmetric).

→ Improve FSS procedure, obtain W_c, α_0 and ν as fitting parameters, no cutoff parameter neccessary.

→ Indications exist that for larger systems the critical disorder will be closer to known results ($W_c^0/t \approx 16.5$).

→ Analyse shift of the critical disorder with increasing exchange coupling quantitatively (see forthcoming paper).

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