Anderson Metal-Insulator Transitions With Classical Magnetic Impurities

D. Jung[1] **K. Slevin**[2] **S. Kettemann**[1]

[1] School of Engineering and Science, Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany
[2] Department of Physics, Graduate School of Science, Osaka University, 1-1 Machikaneyama, Toyonaka, Osaka 560-0043, Japan

d.jung@jacobs-university.de slevin@phys.sci.osaka-u.ac.jp s.kettemann@jacobs-university.de

Abstract

We study the effects of classical magnetic impurities on the Anderson metal-insulator transition numerically [1]. We find that a small concentration of Heisenberg impurities enhances the critical disorder amplitude W_c with increasing exchange coupling strength J due to time-reversal symmetry breaking. The resulting scaling with J is analyzed which supports an anomalous scaling prediction by Wegner due to the additional spin-rotational symmetry breaking. The results are obtained by a finite-size scaling analysis of the geometric average of the local density of states. The latter can efficiently be calculated by means of the kernel polynomial method. We discuss the relevance of our findings for systems like phosphor-doped silicon, which exhibit a metal-insulator transition driven by both interaction and disorder, accompanied by the presence of magnetic moments.

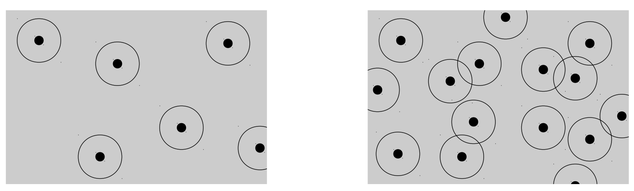
Metal-insulator transition in phosphorus-doped silicon

→ A rising concentration of phosphorus dopants increases the overlap between the hydrogen-like donor states (see figure 1), but also increases disorder [2], leading to regions of localized states in the DOS.

→ High concentration: Impurity band forms (half filled) [2].

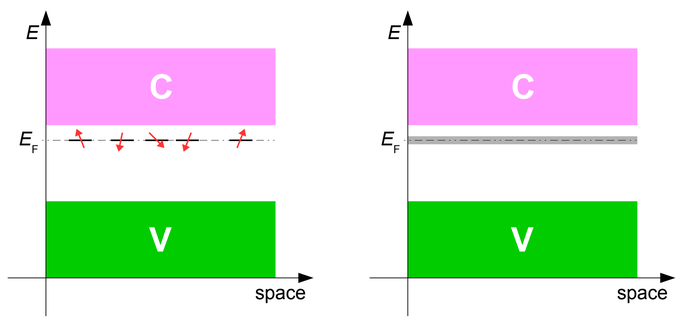
→ Impurity band contains localized and extended states, devided by mobility edges [2].

→ Coulomb repulsion favors single occupancy of the donor states, leading to the formation of spin-1/2 magnetic moments within the localized donor states [2].



(a) Low concentration. (b) High concentration.

Figure 1: *Sketch of the hydrogen-like orbitals of the phosphorus donors inside the silicon bulk (gray).*



(a) Insulating side. (b) Metallic side.

Figure 2: *Schematical band diagrams for phosphorus-doped silicon: (a) For low donor concentration, the singly-occupied donor states cause spin-1/2 moments. (b) For high donor concentration, an impurity band is forming. Far enough on the metallic side of the transition, the moments have vanished.*

How do the local magnetic moments affect the metal-insulator transition in phosphor-doped silicon?

References

[1] D Jung, K Slevin, S Kettemann. *Submitted to PRL, arxiv:1507.03374* (2015).

[2] H von Löhneysen. *Advances in Solid State Physics* **40**, 143 (2000).

[3] P Anderson. *Physical Review* **109**, 1492 (1958).

[4] A Weiße, G Wellein, A Alvermann, H Fehske. *Reviews of Modern Physics* **78**, 275 (2006).

[5] G Schubert, H Fehske. *Quantum and Semi-classical Percolation and Breakdown in Disordered Solids*, volume 762 of *Lecture Notes in Physics*. Springer Berlin Heidelberg, Berlin, Heidelberg (2009).

[6] Y Asada, K Slevin, T Ohtsuki. *unpublished* (2006).

[7] A Rodriguez, L. J Vasquez, K Slevin, R Römer. *Physical Review B* **84**, 134209 (2011).

[8] T Dröse, M Batsch, I Zharekeshev, B Kramer. *Physical Review B* **57**, 37 (1998).

[9] K Slevin, T Ohtsuki. *New Journal of Physics* **16**, 015012 (2014).

[10] L Ujfalusi, I Varga. *Physical Review B* **91**, 184206 (2015).

[11] S Kettemann, E Mucciolo, I Varga, K Slevin. *Physical Review B* **85**, 115112 (2012).

[12] D Khmel'nitskii, A Larkin. *Solid State Communications* **39**, 1069 (1981).

[13] F Wegner. *Nuclear Physics B* **280**, 210 (1987).

[14] D Jung, S Kettemann. Anderson metal-insulator transitions with classical magnetic impurities. In M Palassini, editor, *AIP Conference Proceedings*, volume 1610, pages 77–82, Melville, New York (2014). AIP Publishing.

[15] K Slevin, T Ohtsuki. *Physical Review Letters* **78**, 4083 (1997).

[16] Y Ueoka, K Slevin. *Journal of the Physical Society of Japan* **83**, 084711 (2014).

The Anderson-Heisenberg model

→ Effective model for the impurity band electrons in phosphor-doped silicon, donor atoms are placed on a three-dimensional lattice.

→ Neglect random distribution of donor atoms and instead let disorder enter by a random potential, i.e. start from the *Anderson model* [3]:

$$\hat{H}_0 = t \sum_{\langle i,j\rangle,\sigma} |j,\sigma\rangle\langle i,\sigma| + \sum_{i,\sigma} \varepsilon_i \, |i,\sigma\rangle\langle i,\sigma| \quad . \tag{1}$$

i,j: lattice site index σ: spin index
t: hopping amplitude
ε_i: random potential, box distribution of width W

→ Simulate the magnetic moments by adding an exchange coupling to classical magnetic impurities (*two-fluid model*):

$$\begin{aligned}\hat{H}_\mathrm{s} &= \sum_{i=1}^{N} J_i \, \vec{S}_i \cdot \vec{\sigma}_i \\ &= S \sum_i J_i \Bigg(\cos\theta_i \sum_{\sigma=\pm1} \sigma \, |i,\sigma\rangle\langle i,\sigma| \\ &\qquad + \sin\theta_i \sum_{\sigma=\pm1} \exp(i\sigma\varphi_i) \, |i,\sigma\rangle\langle i,-\sigma| \Bigg) \quad . \end{aligned} \tag{2}$$

$\vec{S}$: Magnetic moment, random orientation
$\vec{\sigma}$: Pauli matrices

$$J_i = \begin{cases} J & \text{at impurity sites (concentration } n_\mathrm{M} = 5\,\%) \\ 0 & \text{elsewhere.} \end{cases} \quad ,$$

J: Exchange coupling strength

→ Full hamiltonian of the "Anderson-Heisenberg model": $\hat{H} = \hat{H}_0 + \hat{H}_\mathrm{s}$.

→ Breaking *time-reversal* and *spin-rotational symmetry* for $J > 0$.
⇒ Entering *unitary regime*.

The kernel polynomial method

→ Calculate spin-resolved local density of states by a polynomial series expansion based on *Chebychev polynomials* (exact for $M \to \infty$) [4]:

$$\rho_{i,\sigma}(\tilde{E}) = \frac{1}{\pi\sqrt{1-\tilde{E}^2}} \left(\mu_0^{(i,\sigma)} + 2 \sum_{m=1}^{M} \mu_m^{(i,\sigma)} \, T_m(\tilde{E}) \right) \quad . \tag{3}$$

Chebychev polynomials (of first kind) [4]:

$$T_m(\tilde{E}) = \cos(m \, \arccos(\tilde{E})) \quad , \quad \tilde{E} \in [-1,1] \quad . \tag{4}$$

Chebychev moments in case of the LDOS [4]:

$$\mu_m^{(i,\sigma)} = \int_{-1}^{1} \rho_{i,\sigma}(\tilde{E}) \, T_m(\tilde{E}) \, \mathrm{d}\tilde{E} = \langle i,\sigma | \, T_m(\tilde{H}) \, |i,\sigma\rangle \quad . \tag{5}$$

→ Properties of the kernel polynomial method:
- Order-of-N method (given a $N \times N$ sparse matrix $\underline{\underline{H}}$).
- Recursive formulas to calculate the moments μ_n iteratively, allowing for efficient algorithms.
- Obtain information about the whole spectrum at once, without additional effort.
- Finite but well-defined spectral resolution $\tilde{\eta}$, depending on spectral position $\tilde{E}$ and number of moments M [5].

Finite-size scaling of the typical density of states

→ Calculate geometric average of the local density of states (GLDOS, also *typical density of states*) [5]:

$$\rho_\mathrm{typ}^{(i)}(E) = \exp\langle \log \rho_i(E) \rangle \quad . \tag{6}$$

(We average over 8000 disorder realizations and lattice sites.)

→ Finite-size scaling ansatz for fixed $\tilde{E} = 0$ and $L^d/M = 1$ [6]:

$$\Gamma(W,L) = L^{d-\alpha_0} \, \tilde{F}(\psi L^{1/\nu}) \quad . \tag{7}$$

with $\Gamma = \rho_\mathrm{typ}/\rho_\mathrm{av}$ and the *reduced disorder* $\psi = (W_\mathrm{c} - W)/W_\mathrm{c}$.

→ Expand unknown function $\tilde{F}(x)$ in a power series [6]:

$$\tilde{F}(x) = \sum_{n=0}^{n_\mathrm{F}} F_n \, x^n \quad . \tag{8}$$

→ Criterion for the selection of $n_\mathrm{F} \in \{2,3,4\}$: Minimize $|1/2 - Q|$, with the *goodness of fit probability* Q (GOF).

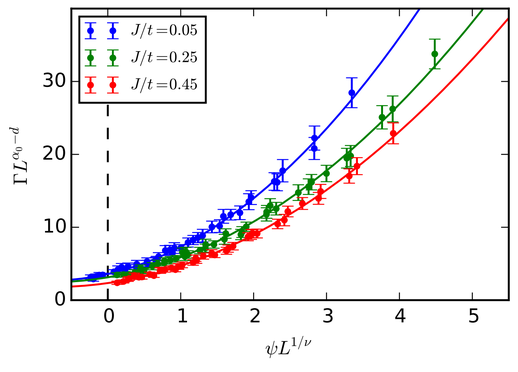


Figure 3: *Demonstration of the scaling ansatz* (7) *at half filling ($E = 0$) for $n_\mathrm{F} = 2$ and three different values J. The errorbars correspond to $95\,\%$ confidence.*

Shift of the metal-insulator transition

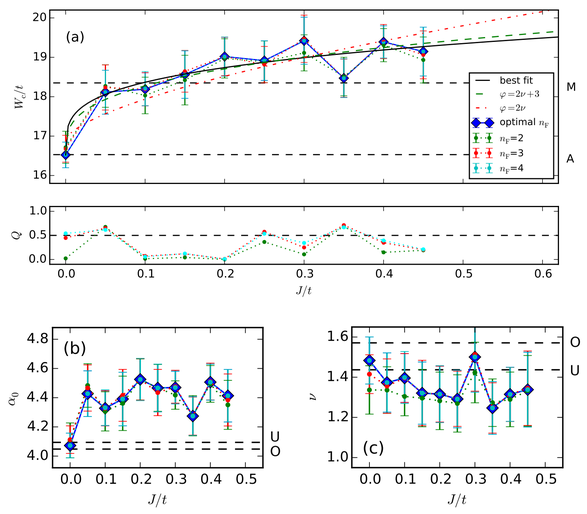


Figure 4: *Dependence of the fit parameters W_c (a), α_0 (b) and ν (c) on the exchange coupling J, using different series expansion orders n_F. The dashed horizontals mark established values for the pure Anderson model (A, realised by our model for $J = 0$) [7], a model considering an external magnetic field (M) [8], the 3D orthogonal (O) [9, 10] and the 3D unitary (U) universality class [10]. For $W_\mathrm{c}(J)$, the data with minimal $|1/2 - Q|$ (a) is fitted to* (10) *using $\nu = 1.571$ [9]. The errorbars correspond to $95\,\%$ confidence.*

→ A finite concentration of magnetic moments can change the critical disorder W_c. Analytic prediction [11]:

$$W_\mathrm{c} = W_\mathrm{c}^0 + W_\mathrm{c}^0 \left(\frac{a_\mathrm{c}^2}{L_\mathrm{s}^2} \right)^{\frac{1}{\varphi}} \quad . \tag{9}$$

$1/\tau_\mathrm{s}$: Magnetic scattering range, $1/\tau_\mathrm{s} \sim J^2$.
$L_\mathrm{s} = \sqrt{D_\mathrm{e}\tau_\mathrm{s}}$: Spin-relaxation length.

→ Expected scaling with J [11]:

$$W_\mathrm{c}(J) = aJ^\mu + b \quad \text{with} \quad \mu = \frac{2}{\varphi} \quad . \tag{10}$$

→ Analytical predictions for the exponent φ:

Simple scaling theory:	$\varphi = 2\nu$	[12]
2nd-order $2+\varepsilon$ expansion (for $\varepsilon = 1$) ...		
... for an external magnetic field:	$\varphi_\mathrm{a} = 2\nu$	[13]
... for local magnetic moments:	$\varphi_\mathrm{s} = 2\nu + 3$	[13]

Table 1: *Fit results for $W_\mathrm{c}(J)$. 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 [12, 13], using either $\nu = 1.571(1.563, 1.579)$ [9] or our own value $\bar{\nu} = 1.48 \pm 0.06$. The best fit result (smallest $|1/2 - Q|$) is marked.*

$\varphi = \ldots$	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	$4 \cdot 10^{-4}$
$2\bar{\nu} + 3$	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	$1 \cdot 10^{-4}$

→ Quality of fit probability Q is only within an acceptable range for the hypothesis $\varphi = 2\nu + 3$.

Conclusions

→ We observe a modification of the critical disorder W_c when adding magnetic impurities to the Anderson model that break both *time-reversal* and *spin-rotational symmetry*.

→ Results for the scaling exponent $\mu = 2/\varphi$ support Wegner's prediction $\varphi = 2\nu + 3$ [13] for the scaling of W_c with the coupling strength J.

→ We use the *kernel polynomial method* to efficiently calculate the local density of states [4, 5].

→ We analyse the *finite-size scaling* of the *geometrically-averaged local density of states* to obtain the critical parameters of the metal-insulator transition [6, 14, 1].

→ We estimate the critical parameters α_0 and ν for the 3D orthogonal ($J = 0$) and the 3D unitary ($J > 0$) universality class that mostly agree with other studies (with the exception of α_0^U) [15, 7, 9, 10].

Outlook

→ Use an even lower value of L^d/M within the kernel polynomial method to prevent mixing of critical with non-critical states.

→ Check higher-order $2+\varepsilon$ expansion results for φ using a refined Borel-Padé analysis [16].

→ Use data for the whole range of energies (provided by the kernel polynomial method for free) to obtain "phase diagrams" in the W-E plane.

Acknowledgements

→ We are grateful for discussions with Georges Bouzerar, Ki-Seok Kim, Hyun-Yong Lee and Eduardo Mucciolo.

→ Support: WCU program, NRF Korea, funded by KOSEF (R31-2008-000-10059-0), Division of AMS.

→ Computational resources: CLAMV Blackpearl cluster, Jacobs University Bremen, Germany.