Impact of Local Magnetic Moments on the Anderson Metal-Insulator Transition

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Abstract

Doped semiconductors like phosphorus-doped silicon (Si:P) exhibit a quantum phase transition from metal to insulator, driven by both interaction and disorder (Mott-Anderson transition). Furthermore, local magnetic moments are formed by the singly-occupied, localized donor states, which interact with the itinerant electrons via an exchange coupling [1]. The formulation of an adequate theoretical description for such a transition is still pending.

We focus on the influence of the local magnetic moments, and approach the problem within an effective model for the impurity band electrons. It is based on the Anderson model [2], extended by a term describing an exchange coupling to classical magnetic impurities. The effects of Heisenberg impurities (H) are compared with those of Ising impurities (I). Heisenberg impurities are breaking time-reversal symmetry and hence cause a change of symmetry from orthogonal to unitary.

The results are obtained numerically, based on a finite-size scaling analysis of the typical density of states, which is the geometric average of the local density of states [3, 4]. The latter is calculated by means of the kernel polynomial method, which allows for an efficient estimation of spectral quantities [5].

The results show that the critical value W_c of the site-diagonal disorder amplitude is a monotonically decreasing function of the exchange coupling strength J in the case of Ising impurities. In the presence of Heisenberg impurities, W_c is first enhanced with increasing J, before it eventually decreases as well. The scaling of W_c with J is analyzed and compared to analytical predictions [6, 7].

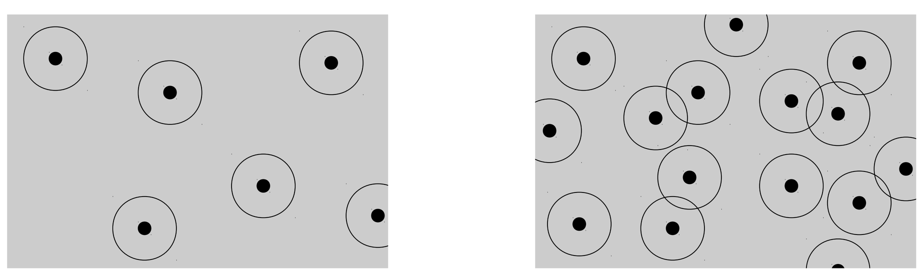
MIT in phosphorus-doped silicon

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

→ High concentration: Impurity band forms (half filled) [1].

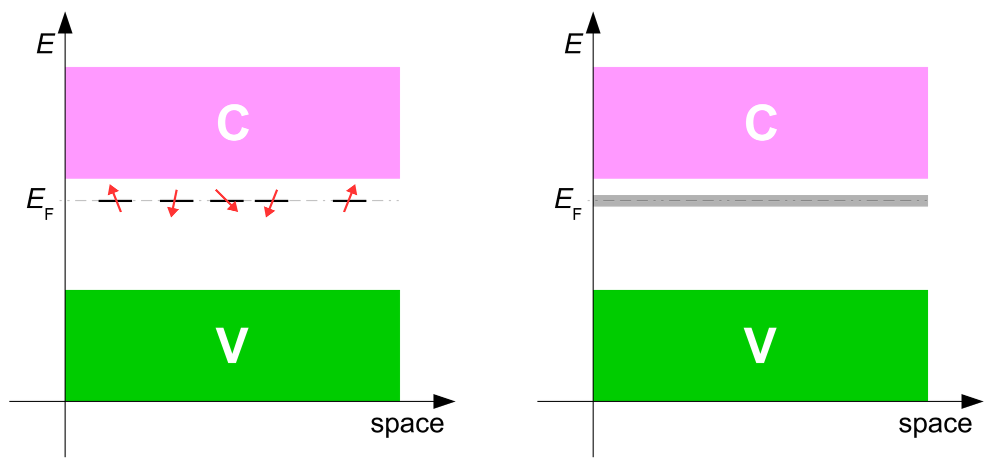
→ Impurity band contains localized and extended states, devided by mobility edges [1].

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



(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 MIT in Si:P?

The Anderson-Heisenberg model

→ Neglect random distribution of donor atoms and let disorder enter by a disorder potential, i.e. start from Anderson model [2]:

$$\hat{H}_0 = t \sum_{\langle i,j\rangle,\sigma} |j,\sigma\rangle\langle i,\sigma| + \sum_{i,\sigma} \varepsilon_i \, |i,\sigma\rangle\langle i,\sigma| \qquad (1)$$

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

→ Effective model for the impurity band electrons, donor atoms are placed on a hypercubic lattice

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

$$\hat{H}_s = \sum_{i=1}^{N} J_i \, \vec{S}_i \cdot \vec{\sigma}_i \qquad (2)$$

$\vec{S}$: Magnetic moment, random orientation (Ising: just ↑↓)
$\vec{\sigma}$: Pauli matrices

$$J_i = \begin{cases} J & \text{at impurity sites (concentration } n_M = 5\,\%) \\ 0 & \text{elsewhere} \end{cases}$$

J: Exchange coupling strength

The kernel polynomial method

→ Calculate spin-resolved LDOS of state $|i,\sigma\rangle$ efficiently using a polynomial series expansion based on Chebychev polynomials (exact for truncation limit $M \to \infty$) [5]:

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

Chebychev polynomials of first kind [5]:

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

Chebychev moments in case of the LDOS [5]:

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

→ Obtain information about the whole energy spectrum, without additional effort.

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

Finite-size scaling of the typical density of states

→ Calculate geometric average of the LDOS (GLDOS):

$$\rho_{\mathrm{typ}}^{(i)}(E) = \exp\langle \log \rho_i(E) \rangle_{\mathrm{dis.conf.}} \qquad (6)$$

⇒ *Typical density of states* [3].

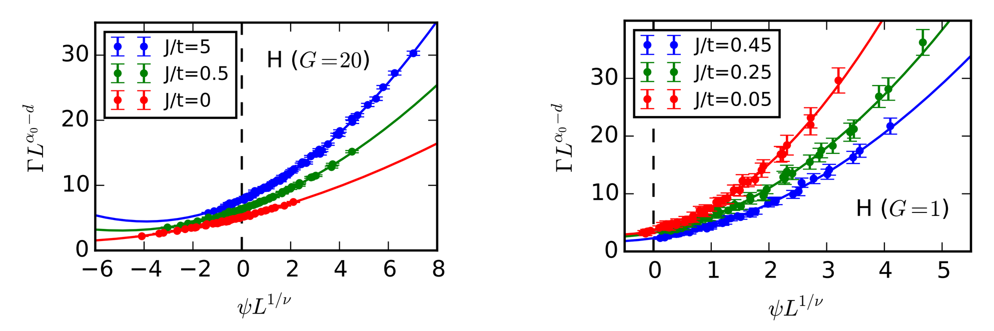
→ Finite-size scaling ansatz for fixed $\tilde{E} = 0$ and $G = L^d/M$ [8]:

$$\Gamma = L^{d-\alpha_0} \, F(\psi L^{1/\nu}) \qquad (7)$$

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

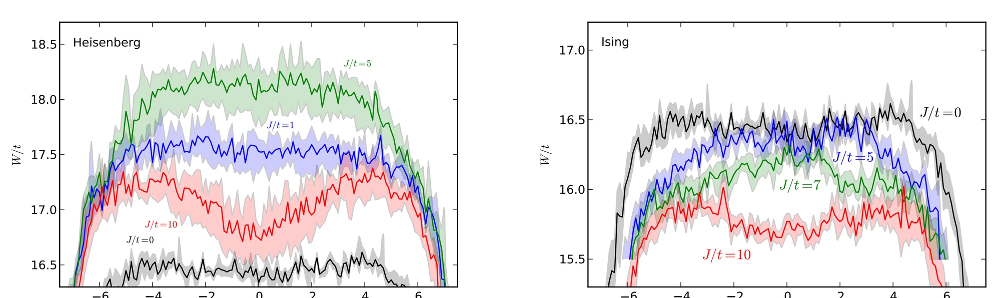
→ Expand unknown function $F(x)$ using a power series [8]:

$$F(x) = F_0 + F_1\,x + F_2\,x^2 + \mathcal{O}(x^3) \qquad (8)$$



(a) $G = 20$. (b) $G = 1$.

Figure 3: *Demonstration of the scaling ansatz (7) for the case of Heisenberg impurities and three parameter values J.*



(a) (b)

Figure 4: *Phase diagrams for (a) Heisenberg impurities and (b) Ising impurities, obtained using a simplified scaling ansatz $\rho_{\mathrm{typ}} \sim L^{-p}$ with cutoff $p_c = \alpha_0 - d$ [4] and $G = 20$.*

Shift of the metal-insulator transition

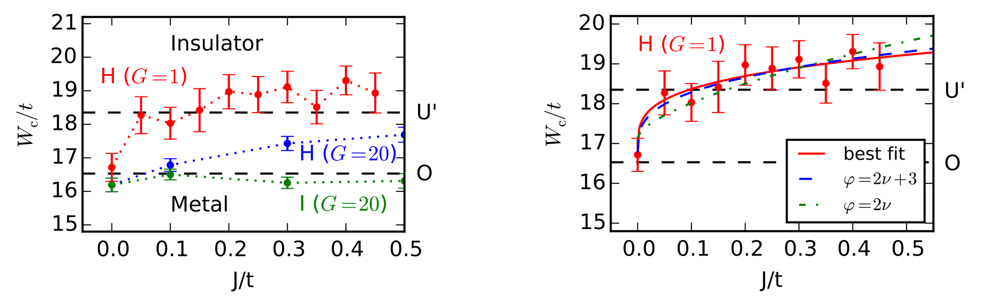
→ A finite concentration of magnetic moments can change the critical disorder W_c. Analytic prediction [9]:

$$W_c = W_c^0 + W_c^0 \left(\frac{a_c^2}{D_e \tau_s^0} \right)^{\frac{1}{\varphi}} \qquad (9)$$

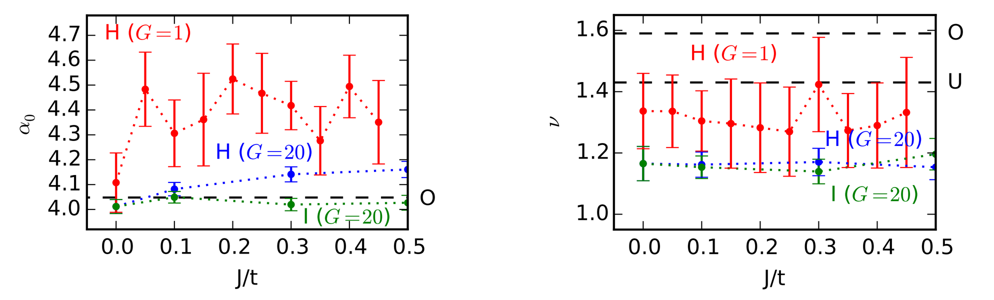
$1/\tau_s^0$: magnetic scattering range, $1/\tau_s^0 \sim J^2$.
⇒ Expected scaling with J (for small J):

$$W_c(J) \sim J^\beta \quad , \quad \beta = \frac{2}{\varphi} \qquad (10)$$

→ Predictions for φ: $\varphi = 2\nu$ [10], $\varphi = 2\nu + 3$ [6]



(a) Phase diagram in the W-J plane. (b) Fit $W_c(J)$ for $G = 1$. Result: $\beta = 0.26 \pm 0.10$.



(c) The parameter α_0 for increasing J. (d) The localization length exponent ν for increasing J.

Figure 5: *Fit results for fixed energy $E = 0$ and impurity concentration $n_M = 5\,\%$ in dependence of the exchange coupling parameter J. Dashed lines indicate established values [11, 12, 13].*

Conclusions

→ Use KPM [5] to calculate LDOS efficiently.

→ Analyse finite-size scaling of the typical density of states to estimate critical parameters [14].

→ Two types of magnetic impurities (Heisenberg and Ising) are shown to have different effect on the critical disorder. Heisenberg: Results support Wegner's prediction $\varphi = 2\nu + 3$ [6].

→ Choice of value $G = L^d/M$: Crucial in order to validate established values of the parameters W_c, α_0 and ν [14].

Outlook

→ Unitary values of α_0 and ν should be validated using alternative methods.

→ Obtain whole phase diagram ($E \neq 0$) using an extended fit model.

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References

[1] H von Löhneysen. *Advances in Solid State Physics* **40**, 143 (2000).
[2] P Anderson. *Physical Review* **109**, 1492 (1958).
[3] 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).
[4] D Jung, G Czycholl, S Kettemann. *International Journal of Modern Physics: Conference Series* **11**, 108 (2012).
[5] A Weiß e, G Wellein, A Alvermann, H Fehske. *Reviews of Modern Physics* **78**, 275 (2006).
[6] F Wegner. *Nuclear Physics B* **280**, 210 (1987).
[7] S Kettemann, M Raikh. *Physical Review Letters* **90**, 146601 (2003).
[8] Y Asada, K Slevin, T Ohtsuki. *unpublished* (2006).
[9] S Kettemann, E Mucciolo, I Varga, K Slevin. *Physical Review B* **85**, 115112 (2012).
[10] D Khmel'nitskii, A Larkin. *Solid State Communications* **39**, 1069 (1981).
[11] K Slevin, T Ohtsuki. *Physical Review Letters* **78**, 4083 (1997).
[12] T Dröse, M Batsch, I Zharekeshev, B Kramer. *Physical Review B* **57**, 37 (1998).
[13] A Rodriguez, L. J Vasquez, K Slevin, R Römer. *Physical Review B* **84**, 134209 (2011).
[14] D Jung, K Slevin, S Kettemann. *To be submitted* (2015).

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