Phase diagram of localization in a magnetic field

Thorsten Dröse\textsuperscript{1}, Markus Batsch\textsuperscript{1,2}, Isa Kh. Zharekeshev\textsuperscript{1}, and Bernhard Kramer\textsuperscript{1}
\textsuperscript{1} I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstrasse 9, D-20355 Hamburg, Germany
\textsuperscript{2} Physikalisch-Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig, Germany

(November 7, 2021)

The phase diagram of localization is numerically calculated for a three-dimensional disordered system in the presence of a magnetic field using the Peierls substitution. The mobility-edge trajectory shifts in the energy-disorder space when increasing the field. In the band center, localized states near the phase boundary become delocalized. The obtained field dependence of the critical disorder is in agreement with a power-law behavior expected from scaling theory. Close to the tail of the band the magnetic field causes localization of extended states.

Though being intensively investigated since the late 1950s\textsuperscript{17}, the problem of the disorder-induced metal-insulator transition (MIT) of non-interacting electrons in three dimensions (3D) can be considered as being still unsolved. There is a controversial discussion, whether the critical behavior at the Anderson transition (AT) can be classified with respect to the fundamental symmetry of the Hamiltonian as proposed within field theoretical descriptions.\textsuperscript{18} One would expect that critical properties governed by the exponent of the localization length $\nu$ were altered when the universality class was changed. For instance, by applying an external magnetic field to a system with spin rotation invariance, time reversal symmetry is broken and the universality class changes from orthogonal to unitary. On the basis of considerably reduced error bars recent numerical calculations\textsuperscript{19} seem to provide evidence that $\nu$ is sensitive to symmetry breaking in contrast to previous results.\textsuperscript{20} Therefore, it is particularly interesting to investigate the importance of the magnetic field for the localization mechanism that drives the MIT.

In this paper we report results on the influence of a homogeneous magnetic field on the phase diagram of localization of the disordered Anderson model (AM). Previous findings concerned the phase diagram without magnetic field, including both exact analytical solutions for the infinite Cayley tree (Bethe lattice)\textsuperscript{21} and numerical studies for a real 3D lattice.\textsuperscript{22} Based on numerical results obtained by the transfer-matrix approach some conclusions on the nature of the wave functions and localization properties have been drawn.\textsuperscript{23} In the band center, electrons are localized due to quantum interference, while outside the unperturbed band electrons become localized below a certain value of the density of states (DOS).\textsuperscript{24} Here, we consider the magnetic field as an additional continuous parameter which can induce the MIT.\textsuperscript{25} By using the transfer-matrix method we calculate a complete mobility-edge trajectory in the energy-disorder space for a finite magnetic field. We find two regimes with entirely different behavior with respect to the magnetic-field-driven MIT. In the band center, localized states near the zero-field phase boundary become extended when applying a magnetic field. In slightly disordered metallic systems for states close to the mobility-edge the field effect is opposite.

We use the AM with diagonal disorder\textsuperscript{26} and Peierls phase factors in the hopping matrix elements

$$H = \sum_r \epsilon_r |r\rangle\langle r| + \sum_{r,\Delta} t_{r,r+\Delta} |r\rangle\langle r+\Delta|.$$ (1)

Energies are measured in units of the modulus of the hopping matrix elements $t_{r,r+\Delta}$, lengths in units of the lattice constant $a = 1$. The states $|r\rangle$ are associated with the sites of a simple cubic lattice. The site energies $\epsilon_r$ are distributed uniformly at random between $-W/2$ and $W/2$. Only hopping between nearest neighbors $r$ and $r + \Delta$ is taken into account. The hopping matrix elements

$$t_{r,r+\Delta} = \begin{cases} e^{\pm 2\pi i \alpha z}, & \Delta \in \{\pm e_y\}, \\ 1, & \Delta \in \{\pm e_x, \pm e_z\}, \end{cases}$$ (2)

describe a system with a homogeneous magnetic field $B$ in the $x$ direction and the Peierls phase $\alpha = eB/hc$ is the number of flux quanta $\Phi_0 = hc/e$ per unit cell.\textsuperscript{28} Here, the Landau gauge with the vector potential $A = (0, -Bz, 0)$ is chosen. The Hamiltonian (1) is symmetric and periodic with respect to $\alpha$ with a period $\alpha = 1$ ($\Phi_0$ periodicity). For a quasi-1D, bar-shaped system of cross section $M \times M$ the Schrödinger equation $H|\Psi\rangle = E|\Psi\rangle$ with $|\Psi\rangle = \sum a_r |r\rangle$ can be written as a transfer matrix equation\textsuperscript{29}

$$u_z = T_z u_{z-1},$$

where the vector

$$u_z = (a_{1z+1}, \ldots, a_{Mz+1}; a_{1z}, \ldots, a_{Mz})^T$$ (3)

contains the coefficients of the planes $z$ and $z+1$ and

$$T_z = \begin{pmatrix} Z_z & -I \\ I & 0 \end{pmatrix}$$ (4)

is the $2M^2 \times 2M^2$ transfer matrix. Each matrix $Z_z$ is of the order $M^2 \times M^2$ and contains the elements of the Hamiltonian in the $z$ plane as presented in Ref.\textsuperscript{30}. The matrices $I$ connect successive $xy$ planes. The matrix $Z_z$ is
a function of the energy \( E \), the magnetic field parameter \( \alpha \), and the random site energies \( \epsilon_c \) on the slice \( z \).

In disordered quasi-1D systems all eigenstates are localized\(^4\). The wave function of a localized state decays exponentially with a localization length. The largest localization length \( \lambda_M \) can be identified as \( \gamma^{-1} \), the inverse of the smallest positive Lyapunov exponent (LE) \( \gamma = \min \{ \chi(u_0), \chi \geq 0 \} \) defined by

\[
\chi(u_0) = \lim_{L \to \infty} \frac{1}{L} \ln \| T_L \cdots T_1 u_0 \|, \tag{5}
\]

where \( u_0 \) is the initial vector for \( \lambda = 0 \).

By using the Benettin algorithm\(^{16}\), we extracted \( \gamma \) from the approximate spectrum of LEs\(^3\). The localization length \( \lambda_M \) is a function of the cross section \( M \) of the bar, the electronic energy \( E \), the number of flux quanta per unit cell \( \alpha \), and the disorder \( W \).

The critical behavior of \( \lambda_M \) near the MIT can be determined numerically by establishing the one-parameter scaling law\(^3\)

\[
\frac{\lambda_M(E, W, \alpha)}{M} = f \left( \frac{\lambda_\infty(E, W, \alpha)}{M} \right), \tag{6}
\]

where \( \lambda_\infty = \lim_{M \to \infty} \lambda_M \) is the localization length of the 3D system in the thermodynamic limit. The phase diagram of localization for a given \( \alpha \) describes the MIT in the \((E, W)\) plane. The mobility-edge trajectory \( E_c(W, \alpha) \) is determined by using the property that at the critical point the reduced localization length of a quasi-1D system \( \lambda_M/M \) is independent of the cross section \( M \),

\[
\frac{\lambda_M(E_c, W, \alpha)}{M} = \text{const.} \tag{7}
\]

As an example, Fig.\(^4\)\(a\) shows the inverse of the reduced localization length \( M/\lambda_M \) as a function of the disorder \( W \) at the band center \( E = 0 \). The Peierls phase was chosen to be \( \alpha = 0.25 \), at which the magnetic field has the strongest effect and the system belongs to the unitary universality class. The data were calculated for different \( M \) with a statistical accuracy of 0.25%.

The MIT is indicated by the common crossing point at \( W_c(E = 0, \alpha = 0.25) = 18.35 \pm 0.11 \). The sign of the size effect on \( \lambda_M \) changes when increasing the disorder from the metallic \((W < W_c)\) to the insulating regime \((W > W_c)\). In the same way we locate the critical disorders for energies up to \( E = 7 \). By expanding Eq. \((2)\) around the critical point at a given energy and fitting the numerical data to the linearized form

\[
\frac{\lambda_M}{M} = \Lambda_c + A(W - W_c)M^{1/\nu}, \tag{8}
\]

one can extract the critical exponent \( \nu \) and the disorder dependence of the localization length \( \lambda_\infty \), as has been performed in Refs.\(^4\) and\(^6\). We have found \( \Lambda_c = 0.568 \pm 0.076 \) for \( \alpha = 0 \) and \( \Lambda_c = 0.564 \pm 0.027 \) for \( \alpha = 0.25 \) consistent with data from Ref.\(^{12}\). For energies beyond the unperturbed band \( |E| > 6 \), it is convenient to determine the critical points from the energy dependence of the localization length \( \lambda_M \) at fixed \( W \). In Fig.\(^2\)(b), the localization length is shown as a function of the energy for various \( M \). The statistical accuracy is 1%. The intersect of the lines signalizes critical behavior and yields the position of the mobility edge. At \( W = 12 \), for example, \( E_c(\alpha = 0.25) = 7.22 \pm 0.14 \). Other critical points \( E_c(W, \alpha) \) were determined similarly.

Combining all the data obtained by the finite-size scaling analysis as described above, one can construct the entire phase diagram of the AM in the parameter space spanned by \( E \) and \( W \). Figure\(^2\) shows the mobility-edge trajectory with and without a magnetic field. For zero field the states in region I are extended whereas the states in II are localized. The regimes I (metallic) and II (insulating) are separated by the mobility-edge trajectory (solid line). The latter is modified when a magnetic field is applied. For \( \alpha = 0.25 \) states in region III become extended and the phase boundary shifts to higher values of critical disorder. It is known from the theory of weak localization\(^4\) that in the presence of a magnetic field coherent time-reversed paths are eliminated and hence backscattering is suppressed. Without a magnetic field, states in III are localized by quantum interference effects. In this case a weak magnetic field leads to a delocalization\(^4\). As a consequence, a stronger disorder is required in order to localize these states (see Fig. 2).

Thus, insulating systems with \( W \) slightly larger than the critical disorder at zero field \([W > W_c(\alpha = 0)]\) undergo a transition to a metal when the magnetic field is applied. This behavior is consistent with the mechanism of the field-induced MIT proposed by Shapiro\(^{19}\).

The increase of the critical disorder \( W_c \) with the magnetic field \( \alpha \) at \( E = 0 \) is shown in the inset of Fig.\(^2\). For small \( \alpha \) the field dependence can be described by the following relation:

\[
W_c(\alpha) - W_c(0) = (E_c(\alpha) - E_c(0)) \frac{dW_c}{dE} \bigg|_{E=E_c(0)} \propto \alpha^{1/\nu}, \tag{9}
\]

which was obtained previously using the scaling approach\(^3\). Our data for \( W_c(\alpha) \) are in agreement with this power law where the critical exponent \( \nu \approx 1.4 \) is taken from Refs.\(^4\) and\(^6\).

In region IV, the trajectory moves into the metallic phase in contrast to region III. Here, states that are extended for \( \alpha = 0 \) become localized for \( \alpha = 0.25 \). This cannot be explained by the interference mechanism discussed above. A qualitative understanding can be achieved by considering the motion of the trajectory of slightly disordered systems when applying a magnetic field. In the limit \( W \to 0 \) the mobility edge merges with the band edge of an ordered system. The zero-field value of the band edge is \( E_b(\alpha = 0) = 6 \). In a magnetic field, the band edge as a function of \( \alpha \) can be calculated numerically by using Hofstadter’s algorithm\(^4\), generalized to
3D. The band shrinks if a magnetic field is applied and varies with a period of one flux quantum per unit cell, \( \alpha = 1 \) (\( \Phi_0 \) periodicity). For example, for \( \alpha = 0.25 \) the unperturbed band edge shifts to \( E_b(W, \alpha) \approx 1.8 \) (Fig. 2). In slightly disordered systems this behavior persists. The band edge of such a system moves to a lower value \( E_b(W, \alpha) < E_b(W, 0) \), indicating that the DOS for energies near the zero-field mobility edge decreases dramatically with increasing \( \alpha \). Below a certain value of the DOS an MIT is induced. In region IV, this causes a shift of the mobility edge to lower energies \( E_c(W, \alpha) < E_c(W, 0) \) when applying a magnetic field (Fig. 2).

In fact, the shift of the phase boundary is due to the combination of both types of field effect mentioned above which compete with each other. Close to the band center (III), where the DOS changes negligibly with \( E \), the interference effect dominates. On the other hand, in region IV, close to the band tails, the DOS effect is much stronger than the interference effect. Here, the behavior of \( E_c(\alpha) \) is determined mainly by the energy and field dependence of the DOS. For example, for \( \alpha = 0.25 \) we find an intersect of the two phase trajectories at \( W^* \approx 14.5 \) and \( E^* \approx 7.8 \), where the two effects are of the same order of magnitude. We believe that a similar field dependence of the phase diagram is also valid for a Gaussian distribution of on-site energies \( \epsilon_r \).

We now again concentrate on the band center \( E = 0 \) in order to investigate the field dependence of the critical parameters. Figure 3 shows the localization length \( \lambda_M \) of quasi-1D systems as a function of magnetic field for various \( W \) corresponding to the delocalized, critical, and localized regime in zero field, respectively. The data were calculated with a precision of 0.25%. For \( \alpha \) different from half integers, \( \lambda_M(E = 0) \) is larger than without a magnetic field. This field-induced enhancement of the localization length is directly related to the shift of the phase boundary in region III. One sees in Fig. 3 that for \( E = 0, W \geq 16.5, and \ M = 4 \) the localization lengths \( \lambda_M \) coincide for both \( \alpha = 0 \) and \( \alpha = 0.5 \) within the statistical uncertainties. They vary with a period of half a flux quantum per unit cell (\( \Phi_0/2 \) periodicity). This was also checked for other widths of \( M = 5, \ldots, 12 \) by comparing \( \lambda_M(E = 0, \alpha = 0) \) with \( \lambda_M(E = 0, \alpha = 0.5) \). In the insulating region our results are consistent with a periodically varying transition amplitude of strongly localized electrons as derived analytically with a directed path method by Lin and Nori. However, we find that the \( \Phi_0/2 \) periodicity does not persist for \( E \neq 0 \) as shown in Fig. 3. Thus the former seems to be an intrinsic property of the band center, around which the on-site energies \( \epsilon_r \) are distributed symmetrically. Furthermore, for the investigated systems of width \( M = 4, \ldots, 12 \) we observe that \( \lambda_M(\alpha = 0.5) < \lambda_M(\alpha = 0) \), though for both values of \( \alpha \) the Hamiltonian belongs to the orthogonal universality class. Assuming that \( \Lambda_c \) does not change in this case, one obtains that for \( \alpha = 0.5 \) and \( E \neq 0 \) the MIT should unexpectedly occur at a lower disorder than in the zero field case, \( W_c(\alpha = 0.5) < W_c(\alpha = 0) \).

The maximum-entropy ansatz predicts the increase of the localization length in quasi-1D systems by a universal factor of 2, when breaking the time reversal symmetry. Since in the present calculations the parameters are beyond the range of validity of this universal relation, it would be desirable to extend the investigations to this regime for checking the prediction. Another interesting problem is to study the disappearance of this relation, as was argued in Ref. 2, for \( d \geq 2 \), when extrapolating to 3D systems by scaling the cross section \( M \) of the quasi-1D bar.

In conclusion, we have numerically calculated the phase diagram of localization in 3D disordered systems in the presence of a magnetic field. Comparing the obtained diagram with the zero-field result, we identify two regimes with different magnetic field dependence of the phase boundary. In the band center, the phase boundary is shifted towards higher values of critical disorder, so that the metallic phase is broadened. This is mainly due to the suppression of the interference of time-reversed paths by a magnetic field, leading to the delocalization of electron states. On the other hand, close to the band tails the location of the MIT in slightly disordered systems \( (W \rightarrow 0) \) is dominated by the field dependence of the DOS. Here, the mobility edge shifts towards smaller energies, thus diminishing the metallic phase. Our numerical findings for small fields show that the behavior of the critical disorder is consistent with predictions by scaling theory. Thus, we have shown that the phase diagram of localization is influenced by an external perturbation which breaks the time reversal invariance.

Discussions with D. Belitz are gratefully acknowledged. This work was supported by DFG-Projekt No. Kr627/8-1, the Graduiertenkolleg “Physik nanostukturierter Festkörper”, University of Hamburg, and NATO Grant No. CRG 941250.

1. P. W. Anderson, Phys. Rev. 109, 1492 (1958).
2. F. Wegner, Nucl. Phys. B 36, 663 (1989).
3. S. Hikami, Prog. Theor. Phys. Suppl. 107, 213 (1992).
4. K. Slevin and T. Ohtsuki, Phys. Rev. Lett. 78, 4083 (1997).
5. See for review B. Kramer and A. MacKinnon, Rep. Prog. Phys. 56, 1469 (1993) and references therein.
6. M. Henneke, B. Kramer, and T. Ohtsuki, Europhys. Lett. 27, 389 (1994).
7. R. Abou-Chacra and D. J. Thouless, J. Phys. C 7 65 (1974).
8. T. Kawarabayashi, J. Phys.: Condens. Matter 6, L65 (1993).
9. B. Bulka, B. Kramer, and A. MacKinnon, Z. Phys. B 60, 13 (1985); B. Bulka, M. Schreiber and B. Kramer, Z. Phys. B 66 21 (1987).
10. J. Kroha, T. Kopp, and P. Wölfle, Phys. Rev. B 41, 888 (1990); J. Kroha, Physica A 167, 231 (1990).
11 H. Grussbach, M. Scheriber, Phys. Rev. B 51, 663 (1995).
12 B. Shapiro, Phil. Mag. B 50, 241 (1984).
13 P. A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys 57, 287 (1985).
14 R. Peierls, Z. Physik 80, 763 (1933); J. M. Luttinger, Phys. Rev. 84, 814 (1951).
15 J. Pichard and G. Sarma, J. Phys. C 14, L 127 and L 617 (1981).
16 V. I. Oseledec, Trans. Moscow Math. Soc. 19, 197 (1968); G. Benettin, L. Galgani, A. Giorgilli, and Strelcyn, J.-M., Meccanica 15,9 (1980).
17 A. MacKinnon and B. Kramer, Phys. Rev. Lett. 47, 1546 (1981); Z. Phys. B 53, 1 (1983).
18 D. Khmel’nikskii and A. I. Larkin, Solid State Comm. 39, 1069 (1981).
19 D. R. Hofstadter, Phys. Rev. B 14, 2239 (1976).
20 Y.-L. Lin and F. Nori, Phys. Rev. Lett. 76, 4580 (1996).
21 D. A. Browne, J. P. Carini, K. A. Muttalib, S. R. Nagel, Phys. Rev. B 30, 6798 (1984); J. P. Carini, K. A. Muttalib, and S. R. Nagel, Phys. Rev. Lett. 53, 102 (1984).
22 A. D. Stone, P. A. Mello, K. A. Muttalib and J.-L. Pichard in Mesoscopic Phenomena in Solids edited by B. L. Altshuler, P. A. Lee and R. A. Webb (North-Holland, Amsterdam 1991), p. 369
23 I. V. Lerner and Y. Imry, Europhys. Lett., 29, 49 (1995)

FIG. 1. Disorder and energy dependence of the reduced localization length $\lambda_M/M$ of quasi-1D disordered systems for various cross sections $M$ in a magnetic field $\alpha = 0.25$. a) $M/\lambda_M$ vs. disorder $W$ at the band center $E = 0$. b) $\ln(\lambda_M/M)$ vs. energy $E$ at $W = 12$ outside the unperturbed band. Lines are polynomial interpolations.

FIG. 2. The phase diagram of the Anderson model of localization. Full dots show the critical points $\{E_c, W_c\}$ for a magnetic field $\alpha = 0$. The error bars indicate the statistical uncertainties due to the finite length of the quasi-1D systems. The open circles show numerical results for $\alpha = 0$ taken from Ref. 9. The full and the dotted line represent the mobility edge trajectory for $\alpha = 0$ and $\alpha = 0.25$ respectively. Inset: critical disorder $W_c$ vs. magnetic field $\alpha$ in the band center $E = 0$. The curve shows the power-law behavior from scaling arguments.

FIG. 3. Localization length $\lambda_M$ of a quasi-1D disordered system with a cross section $M = 4$ for various disorders $W$ corresponding to different regimes (extended states, critical region and localized states) as a function of the number of flux quanta per unit cell $\alpha$ for $E = 0$ (full dots) and $E = 4$ (open circles). The continuous lines are fits by $\Phi_0/2$-periodic functions.
fig. 1, "Phase diagram of localization in a magnetic field", Dröse et al.
fig. 2, "Phase diagram of localization in a magnetic field", Dröse et al.
fig. 3, "Phase diagram of localization in a magnetic field", Dröse et al.