Localization Phase Diagram for a Disordered Two-Dimensional System in a Magnetic Field

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The phase diagram for the Anderson transition of a two-dimensional disordered system with variable impurity concentration and a perpendicular magnetic field is investigated. A phase boundary is found, separating localized from extended states. It is calculated by means of a finite size scaling approach. The shape of the phase boundary and the change in the magnetoresistance are explained in terms of quantum interference effects, i.e., weak localization. A critical exponent for the correlation length and the onset of the delocalized phase are determined.

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In the zero temperature limit ($T = 0$) the electronic transport properties of a disordered system are mainly determined by the extent of the eigenstates over the system. Since the work of Anderson[1] it is well understood that localization due to disorder can lead to a metal–insulator (MI) transition (in the absence of a magnetic field). In two dimensions (2D) localization is predicted for any amount of disorder, whereas in 3D there is a critical value of disorder below which a mobility gap (region of extended states) exists. In this paper we show from a simple one-electron model for an impurity band that in the presence of an external perpendicular magnetic field a 2D system does exhibit two phase transitions above a critical impurity concentration as a function of the field strength. Moreover we demonstrate that the magnetoresistance is expected to change its sign at a critical magnetic field. In our model this behavior, usually discussed as the competing effect of a positive magnetoresistance due to electron-electron interactions with a negative contribution from localization[2–4], results solely from the partial suppression of quantum interference in the presence of the magnetic field.

We study the localization transition by calculating a correlation length based on a generalization of the concept of quantum connectivity.[5] We then employ a finite size scaling analysis[6–8] to determine the critical magnetic field as a function of the disorder and vice versa.[9] In the limit of a vanishing magnetic field ($B = 0$) we find complete localization as predicted by the 2D Anderson model and the scaling theories of localization.[10] Finally we give some arguments to interpret MI phase diagrams in terms of weak localization.

Our description of the model starts from the 2D Anderson tight-binding Hamiltonian

$$H = \sum_j |\phi_j\rangle \epsilon_j \langle\phi_j| + \sum_{j\neq k} |\phi_j\rangle\langle\phi_j|V|\phi_k\rangle\langle\phi_k| \,.$$

Disorder is introduced by one-electron atomic orbitals $\phi(\boldsymbol{r}_i)$ positioned at random in a 2D square box of side d. This model, known as topological disorder, has relevance to systems such as thin amorphous films or doped semiconductor layers at low temperatures. We introduce the magnetic field by gauge-invariant atomic orbitals[11]

$$\phi(\boldsymbol{r}, \boldsymbol{r}_i) = \phi(\boldsymbol{r} - \boldsymbol{r}_i) \exp\left[ie\, \boldsymbol{A}(\boldsymbol{r}_i) \cdot \boldsymbol{r}\,/\hbar c\right].$$

The symmetric gauge $\boldsymbol{A}(\boldsymbol{r}) = -\boldsymbol{r} \times \boldsymbol{B}/2$ is used throughout this paper. In strong magnetic fields (of order $B = 10\,\mathrm{T}$ in semiconductors) a significant shrinkage of the atomic orbitals adds to localization by reducing the overlap at the sites,[4] which is included using translated ground state solutions of the 2D harmonic oscillator of frequency ω_0 in the perpendicular magnetic field B as basis functions. This approach results in Gaussian type atomic orbitals with a radius that depends on the strength of the magnetic field,

$$\phi(r) = \left(\sqrt{\pi}a\right)^{-1} \exp -\left(r^2/2a^2\right),$$

where $a = (\hbar/m^*\Omega)^{1/2}$ is the effective oscillator radius, $\Omega = \left(\omega_0^2 + \omega_B^2\right)^{1/2}$ is an effective oscillator frequency, $\omega_B = eB/2m^*c$ is half the cyclotron frequency, and m^* is the electron effective mass. For small magnetic fields a is constant and we adjusted it to a typical doped semiconductor system[12] with a Bohr radius $a_B = \hbar^2\epsilon/e^2m^* \approx 100\,\text{Å}$. For $B = 0$ we identify $a_0 = a_B$ assuming a static dielectric constant $\epsilon = 20$, $m^* = 0.1\,m_e$. It is convenient to introduce a dimensionless length $L \equiv d/a_0$ and a dimensionless concentration of centers $c \equiv N/L^2$. The statistically distributed impurities act as attractive short-range scatterers which are considered by the potential

$$V(\boldsymbol{r}) = -V_0 \sum\nolimits_i \delta(\boldsymbol{r} - \boldsymbol{r}_i) \,.$$

We normalized $V_0 = \hbar\omega_0\pi a^2$. The eigenfunctions are calculated with the standard linear-combination-of-atomic-orbitals ansatz $|\psi\rangle = \sum_i c_i|\phi_i\rangle$, yielding the secular equation

$$\sum_j (H_{ij} - E_n S_{ij})\, c_{jn} = 0 \,,$$

which is solved numerically. For the expansion coefficients of the site states in the basis of the eigenstates

$|\phi_n\rangle = \sum_j a_{jn}|\Psi_j\rangle$ one obtains

$$a_{jn} = \sum_i c^*_{ij}\, S_{in}.$$

In order to determine the spatial extent of the eigenstates we introduce a correlation length for states within a finite energy range (ε). Considering the transition amplitude from an initial state ψ to a final state χ

$$A = \iint d^3x'\, d^3x\, \chi^*(\boldsymbol{x}', t')\, G(\boldsymbol{x}', t', \boldsymbol{x}, t)\, \psi(\boldsymbol{x}, t)$$

and using the retarded Green's function in the energy representation,

$$G(\boldsymbol{x}', \boldsymbol{x}, t' - t) = -i\Theta(t' - t) \sum_n \Psi_n(\boldsymbol{x}')\, \Psi^*_n(\boldsymbol{x}) \times \exp\left[-iE_n(t' - t)/\hbar\right],$$

the transition amplitude can be represented as a sum of alternatives $A = \sum_\varepsilon A_\varepsilon$. The alternatives are divided into the various energy ranges (ε) in which the transition can be made. The transition probability of a state $\psi(\boldsymbol{x}, t)$ into $\chi(\boldsymbol{x}', t')$ in the eigenstates of the energy range (ε) is

$$P_\varepsilon = \lim_{t' \to +\infty} |A_\varepsilon|^2 .$$

Expanding initial and final states into eigenfunctions at times t resp. t' we readily obtain

$$\begin{aligned} P_\varepsilon &= \lim_{\eta \to 0+} \eta \int_0^{+\infty} dt'\, |A_\varepsilon|^2 \exp\left(-\eta t'\right) \\ &= \sum_n |\langle\psi|n\rangle|^2 |\langle\chi|n\rangle|^2 + \sum_{\substack{n \neq m \\ E_n = E_m}} \langle\chi|n\rangle\langle n|\psi\rangle\langle\psi|m\rangle\langle m|\chi\rangle , \end{aligned}$$

where the sums are over states with an energy in the range (ε). If we identify initial and final states with our localized atomic orbitals at $\boldsymbol{r}_i$,$\boldsymbol{r}_j$ and neglect the contribution from degenerate states, the transition probabilities are

$$P^{ij}_\varepsilon = \sum_n |a_{in}|^2 |a_{jn}|^2 .$$

We then define an energy resolved quantum connectivity

$$\Delta^{ij}_\varepsilon = \frac{P^{ij}_\varepsilon}{(P_\varepsilon{}^{ii}\, P_\varepsilon{}^{jj})^{1/2}}$$

in analogy to Skinner's energy-independent connectivity.[5] The correlation (localization) length for eigenstates in the energy range (ε) is

$$(\xi^\varepsilon)^2 = \frac{\langle \sum_{ij} \Delta^{ij}_\varepsilon\, r^2_{ij} \rangle}{\langle \sum_{ij} \Delta^{ij}_\varepsilon \rangle} \qquad (1)$$

Here the angular brackets indicate a configurational average. The localization length and Hamilton matrices are generated with the minimum image convention to be consistent with our periodic boundary conditions.

If a correlation length is available the most simple finite size scaling analysis that can be done is the Nightingale (phenomenological) renormalization,[6]

$$T_L(K) = T_{L'}(K')$$

with the transformation function $T_L(K) = \xi_L(K)/L$. The fixed point of this renormalization-group transformation for two finite systems of sizes L and L' is an approximation for the critical threshold K_c in the infinite system. This relation is a direct consequence of the general finite size scaling hypothesis.[7,8] If we assume the singularity in the correlation length to be $\xi_\infty(K) \sim |K - K_c|^{-\nu}$, the critical exponent is obtained from a linearization around the fixed point,

$$\begin{aligned} \nu &= \ln(L'/L)/\ln|\lambda_{L'}/\lambda_L| , \\ \lambda_L &= \partial T_L/\partial K|_{K=K_c} . \end{aligned}$$

In our case the scaled variable K is the concentration c or the magnetic field B. To obtain the localization phase diagram in the c-B plane we assume a critical exponent $\nu_c(B)$ with $\xi_\infty(c, B) \sim |c - c_c(B)|^{-\nu_c(B)}$. Now the critical concentration depends parametrically on the magnetic field. Performing the renormalization-group transformation

$$T_L\Big(c(B)\Big) = T_{L'}\Big(c'(B)\Big) \qquad (2)$$

on c we can determine the critical values $c_c(B)$ for a series of values for B and hence determine the phase boundary. Similarly we can use $\xi_\infty(c, B) \sim |B - B_c(c)|^{-\nu_B(c)}$, and solve the fixed point equations

$$T_L\Big(B(c)\Big) = T_{L'}\Big(B'(c)\Big) \qquad (3)$$

for the critical magnetic field $B_c(c)$ for a series of concentrations c. It is important to note that in the latter case ξ_L is an even function of B. Thus we have to consider the second term in the expansion around $B_c(c)$ to find the approximate critical exponent $\nu_B(c)$.

The calculations were done for systems of sizes $L = 8, 10, 12, 13, 14, 16$ with the overlap matrix set to unity. Though there is no obvious justification for this orthogonality approximation it leads to a relatively small decrease in the critical concentrations as it has been noted by several authors.[5,13] The energy spectrum was divided into eight ranges with equal numbers of eigenstates. Our criterion for the MI transition is the first onset of a mobility gap, i.e., the finite-size scaling yields a fixed point in at least one of the energy ranges. Actually we found very narrow mobility gaps in the lower-energy band tails. We observed that averaging over larger (ε) (we also used five ranges) or over the full energy band can hide the onset of a narrow mobility gap in small systems, shifting c_c to slightly higher values. Smaller (ε) would require too many configurations to be handled in our calculation. All critical values obtained by (2) and (3) are compiled in the localization phase diagram Fig. 1. For increasing L, L' the critical values converged within the error bars

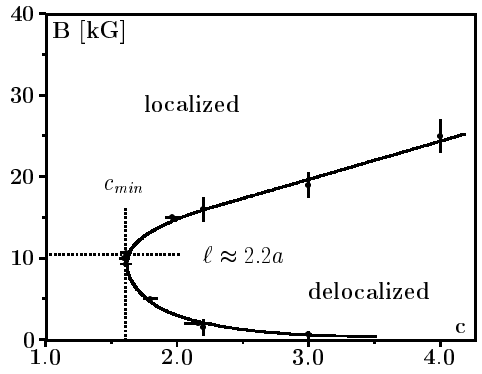

FIG. 1. Localization phase diagram in the c-B plane. The onset of a delocalized phase appears at $c_{min} = 1.6 \pm 0.05$, where the cyclotron radius is 2.2 times the Bohr radius.

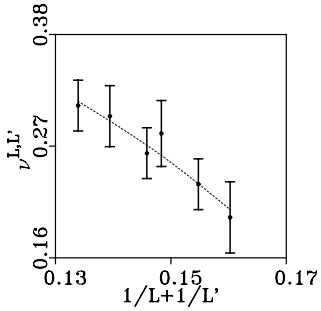

FIG. 2. Critical exponents $\nu^{L,L'}$ vs $1/L + 1/L'$ for all pairs $L, L' = 12, 13, 14, 16$. The dotted line results from the extrapolation (Ref. 7).

given in Fig. 1, according to the Nightingale extrapolation.[6,7] The error bars result from the averaging in (1); horizontal bars where obtained by (2), vertical ones by (3). For a fixed magnetic field $B = 10\,\mathrm{kG}$, corresponding to the onset of delocalization at minimal concentration (Fig.1), we calculated the critical exponent $\nu^{L,L'}$ for all pairs $L, L' = 12, 13, 14, 16$ averaging over 200 samples. The $\nu^{L,L'}$ clearly exhibit a scaling behavior, as shown in Fig. 2. We obtain an extrapolated value of $\nu_c = 0.85 \pm 0.35$. We did not achieve good enough statistics to obtain a sufficient estimate for the exponent $\nu_B(c)$, mainly because of the difficulty in determining the second derivatives at the fixed point with sufficient precision.

The most intriguing feature of the phase boundary is the existence of two critical fields for a fixed concentration $c > c_{min}$: When the magnetic field is increased the insulating system becomes metallic. At larger fields the mobility gap disappears and the system returns to the insulating state. This second transition occurs at a magnetic field strength 1 order of magnitude smaller than the field in which the shrinkage of our wave function becomes the dominant mechanism[4,12] of localization. The critical line has a constant slope in this region. In the limit $B = 0$ the localized regime penetrates the phase diagram. This is in agreement with the prediction of a complete 2D localization for any amount of disorder by Anderson and the scaling theories of localization.[10] The first onset of a delocalized phase, the tip of the nose (Fig.1), is observed at a critical value of the magnetic field satisfying $l = 2.2\,a$, where $l = (\hbar c/eB)^{1/2}$ is the cyclotron radius.

Finally, we give an estimate of this critical field strength discussing the essential influence of the magnetic field in terms of weak localization.[14] Weak localization considers the interference of electron wave packets on closed trajectories. A magnetic field destroys the coherence of amplitudes on time-reversed closed paths and thus decreases the localization. In the field the amplitudes acquire additional phase factors, $A \to A$ $\times \exp(\pm ie\phi/\hbar c)$, where $\phi = \boldsymbol{B} \cdot \boldsymbol{S}$ is the magnetic flux through a closed loop of the area $\boldsymbol{S}$. The phase shifts $\Delta\varphi(r) = 2e\phi/\hbar c = 2\pi r^2/l^2$ between time-reversed trajectories depend on the enclosed flux and thus on the mean radius r of the loops. An electron bound in a deep fluctuation in the random potential has the smallest possible mean radius for return to its starting point, given by the radius a of an atomic orbital. More delocalized electrons are scattered back to the starting point by paths of a larger mean radius $a + \Delta r$. We get maximal destructive interference between closed loops with radii between a and $a + \Delta r$ if all phase shifts between 0 and 2π appear: $2\pi = \Delta\varphi(a + \Delta r) - \Delta\varphi(a)$. The time dependence of the probability to find an electron at time t within a radius $\boldsymbol{r}$ around $\boldsymbol{r}_0$ is given by the classical diffusion law,

$$P(\boldsymbol{r}, t) = (4\pi D t)^{-1} \exp(-|\boldsymbol{r} - \boldsymbol{r}_0|^2/4Dt)\,.$$

This implies that after a time t the particle is found within a radius $\Delta r = 2\sqrt{D\,t}$ around $\boldsymbol{r}_0$ neglecting all probabilities less than $1/e$ of the maximum value. Here $D = \lambda\, v/2$ is the diffusion constant, λ is the mean free path, and v is the characteristic velocity of the particle. When there is already significant overlap between the orbitals ($c \approx 1$) the mean free path is $\lambda = a$ and the characteristic velocity is approximately $v = a\,\Omega$, i.e., the velocity of a particle bound in the Bohr orbital. Since there is only interference between closed paths that can be reached within diffusion times of the typical orbit times, we can set $\sqrt{\Omega\, t} \approx 1$ and arrive at the relation

$$l \approx 2.2\,a\,.$$

This criterion is in agreement with our numerical results and yields the critical magnetic field that results in a maximal destruction of weak localization. Suboptimal destruction for increasing fields gives the reason for the reentrant transition. Thus we find the onset of a delocalized phase on the line through the tip of the nose (Fig.1) and expect the sign of the magnetoresistance to change at a magnetic field satisfying the relation above. Such a switch was observed in recent experiments on δ-layer sys-

tems[12] at sufficiently low temperatures ($T < 4.2$ K).

Presently we are investigating possible corrections due to the orthogonality approximation. In a future work we would like to incorporate phonon coupling and Slater-type orbitals to investigate the temperature dependence and to consider the shrinkage of the atomic orbitals in a more realistic way.

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