

Theory of hopping magnetoresistance induced by Zeeman splitting

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We present a study of hopping conductivity for a system of sites that can be occupied by more than one electron. At a moderate on-site Coulomb repulsion, the coexistence of sites with occupation numbers 0, 1, and 2 results in an exponential dependence of the Mott conductivity upon Zeeman splitting $\mu_B H$. We show that the conductivity behaves as $\ln \sigma = (T/T_0)^{1/4} F(x)$, where F is a universal scaling function of $x = \mu_B H/T(T_0/T)^{1/4}$. We find $F(x)$ analytically at weak fields, $x \ll 1$, using a perturbative approach. Above some threshold x_{th} , the function $F(x)$ attains a constant value, which is also found analytically. The full shape of the scaling function is determined numerically, from a simulation of the corresponding "two-color" dimensionless percolation problem. In addition, we develop an approximate method which enables us to solve this percolation problem analytically at any magnetic field. This method gives a satisfactory extrapolation of the function $F(x)$ between its two limiting forms.

I. INTRODUCTION

Low-temperature conductivity in a disordered semiconductor is controlled by phonon-assisted electron hops between localized states. At sufficiently low temperatures, only those sites that have energy levels close to the Fermi level participate in the hopping transport. This defines the Mott variable range hopping (VRH) regime.¹ Mott conductivity depends exponentially on temperature, $\sigma(T) \propto \exp[-(T_0/T)^{1/(d+1)}]$, where $T_0 = \beta_d/ga^d$ is the characteristic Mott temperature, g is the density of localized states at the Fermi level, a is the localization radius for a single site, d is the dimensionality of the sample, and the numerical factor β_d is determined by percolation theory.² In the more standard case of lightly doped semiconductors, the strip of localized states in energy space is relatively narrow, and each site can accommodate at most one electron. Under these conditions, the spin degree of freedom of the hopping electrons has no effect upon the exponential factor of the hopping conductivity. The application of a magnetic field H results in the modification of this exponential factor due solely to the orbital effect of the field.²

Kamimura *et al.*³ recognized that the spin degree of freedom plays a significant role in the magnetoresistance if a certain fraction of the sites can accommodate more than one electron. Double occupancy is possible if the on-site Coulomb repulsion U between the electrons is smaller than the width of the distribution function of the energies of the localized sites. In this case, there are two types of sites that contribute to hopping transport. Sites of the first type, which we will call type A , have energies ϵ close

to μ . Sites of type B have one electron at a deep level with $\epsilon \sim \mu - U$, so that the energy for the second electron is close to μ . The sites that are neither type A nor type B have energy levels that are too far from the Fermi level to contribute to transport. At zero magnetic field, the probability for two electrons on two singly occupied sites to have opposite spins equals 1/2. Therefore, hops between A and B sites can occur. In the strong field limit, however, all spins are polarized, and $A \leftrightarrow B$ hops are completely suppressed,³ assuming that two electrons occupying the same site form a singlet state at all relevant magnetic fields.⁴ Thus, at sufficiently strong magnetic fields, the characteristic Mott temperature is determined by the larger of the two densities of states g_A and g_B rather than by the net density of states $g = g_A + g_B$. The increase in T_0 due to the field-induced suppression of $A \leftrightarrow B$ hops leads to a giant positive magnetoresistance.⁵

In this paper we present a detailed study of the hopping magnetoresistance induced by Zeeman splitting. We show that the criterion for the strong magnetic field limit described above corresponds to a *finite* threshold value H_{th} . Below this threshold value, the conventional Mott exponent, $(T_0/T)^{1/(d+1)}$, is modified by a factor $F(x)$,

$$\sigma \propto \exp \left\{ - \left(\frac{T_0}{T} \right)^{1/(d+1)} F(x) \right\}, \quad (1)$$

which is a *universal* function of a single scaling parameter

$$x = \frac{\mu_B H}{T(T_0/T)^{1/(d+1)}}. \quad (2)$$

The universality of the Zeeman splitting induced magne-

toresistance is a key result of this paper. Its significance is illuminated by noting that it reduces the calculation of the magnetoresistance to the determination of a universal function $F(x)$ of a single dimensionless parameter x , as opposed to previous solutions³ for which the magnetoresistance was calculated as a function of two variables, T and H .

Above a certain threshold $x \geq x_{\text{th}}$, the universal function $F(x)$ attains a constant value, which we determine analytically. In addition to the saturation value, we find the $x \ll 1$ asymptote of $F(x)$ analytically using a perturbative approach. In an attempt to obtain an analytically determined fitting curve for the universal scaling function $F(x)$, we extend the invariant technique² to the case of the "two-color" percolation problem. To determine the accuracy of these two analytical techniques, we find the scaling function $F(x)$ numerically by simulations of the corresponding two-color dimensionless percolation problem and compare it with the functions obtained analytically.

II. APPLICABILITY OF THE MODEL

Zeeman splitting can make the dominant contribution to the magnetoresistance in a number of important cases, which include those of undoped amorphous silicon^{3,6} and moderately disordered two-dimensional electron systems. In the latter case, the minima of the random potential may serve as sites accommodating several electrons. The orbital effect can be avoided altogether if the field H is applied parallel to the plane of the two-dimensional system. In amorphous silicon, electrons are localized at "dangling bonds."⁷ For the case of bulk α -Si, the orbital effects of the magnetic field cannot be eliminated, and Zeeman splitting makes the dominant contribution to the magnetoresistance only in a certain range of temperatures. To determine this range, we consider the tunneling of an electron a distance L through a barrier consisting of the superposition of an "intrinsic," V_0 , and a "magnetic," $m\omega_c^2 x^2/2$, barrier. ($\omega_c = eH/mc$ is the cyclotron frequency of the field H .) The action for the electron subbarrier motion is

$$\frac{S}{\hbar} = \frac{1}{\hbar} \int \sqrt{2m(V_0 + \frac{1}{2}m\omega_c^2 x^2)} dx \approx \frac{L}{a} + \frac{aL^3}{6\lambda^4}. \quad (3)$$

The localization radius of the electron in the absence of a magnetic field is related to the strength of the intrinsic barrier V_0 as $a = \hbar/\sqrt{2mV_0}$, and $\lambda = \sqrt{c\hbar/eH}$ is the magnetic length. The second term in Eq. (3) represents the correction to the subbarrier action due to the presence of a magnetic field. From Eq. (3), we see that the orbital effect of the magnetic field is negligible at

$$\frac{aL^3}{6\lambda^4} \ll 1. \quad (4)$$

The characteristic tunneling distance L in the VRH regime is, of course, determined by the temperature

$$L \approx a \left(\frac{T_0}{T} \right)^{1/(d+1)}. \quad (5)$$

Equations (4) and (5) determine the upper limit of the magnetic field. Requiring the Zeeman splitting to be strong limits the magnetic field from below:

$$T \ll \mu_B H \ll \frac{\sqrt{6}\hbar^2}{2ma^2} \left(\frac{T}{T_0} \right)^{3/2(d+1)}. \quad (6)$$

This relation places the restriction

$$T < T_0 \left(\frac{\hbar^2}{ma^2 T_0} \right)^{2(d+1)/(2d-1)} \quad (7)$$

upon the range of temperatures at which Zeeman splitting makes the dominant contribution to the magnetoresistance.

III. DERIVATION OF THE CONNECTIVITY CONDITIONS

Mott's arguments enable one to find the temperature dependence of the exponential factor in VRH conductivity. However, it is necessary to use percolation theory to determine the numerical factor β_d in the exponent.² Similarly, to study quantitatively the effect of Zeeman splitting upon the conductivity, one has to reformulate the problem in terms of percolation theory. Because two different site types are now involved, the percolation network that determines the hopping conductivity consists of three types of links: AA , BB , and AB . In order to find the VRH conductivity, we must first determine the conductances G_{AA} , G_{BB} , and G_{AB} of the three types of elementary links. To begin with, we introduce the probabilities P_i of having the site i occupied by zero (0), one (\uparrow or \downarrow), or two ($\uparrow\downarrow$) electrons:

$$P_i(0) = Z^{-1}, \quad (8)$$

$$P_i(\uparrow) = Z^{-1} \exp[-(\epsilon_i + \mu_B H)/T], \quad (9)$$

$$P_i(\downarrow) = Z^{-1} \exp[-(\epsilon_i - \mu_B H)/T], \quad (10)$$

$$P_i(\uparrow\downarrow) = Z^{-1} \exp[-(2\epsilon_i + U)/T]. \quad (11)$$

Here

$$Z = 1 + \exp[-(\epsilon_i + \mu_B H)] + \exp[-(\epsilon_i - \mu_B H)] + \exp[-(2\epsilon_i + U)/T]. \quad (12)$$

Neglecting the preexponential factors (which include, e.g., the deformation potential constant), we can express the three elementary link conductances as products of phonon and electron occupation numbers:

$$G_{AA} \propto [P_1(\uparrow) + P_1(\downarrow)]P_2(0)N(\epsilon_2 - \epsilon_1) \exp(-2R/a), \quad (13)$$

$$G_{BB} \propto P_1(\uparrow\downarrow)[P_2(\uparrow) + P_2(\downarrow)]N(\epsilon_2 - \epsilon_1) \exp(-2R/a), \quad (14)$$

$$G_{AB} \propto [P_1(\uparrow)P_2(\downarrow) + P_1(\downarrow)P_2(\uparrow)]N(\epsilon_2 + U - \epsilon_1) \times \exp(-2R/a). \quad (15)$$

Here R is the distance between two sites and N is the Bose distribution function.

The standard approach to the formulation of the percolation problem requires the exponential representation of the elementary link conductance, $G \propto e^{-\xi}$. In this colored percolation problem, there are three different exponents ξ_{AA} , ξ_{BB} , and ξ_{AB} , which are extracted from Eqs. (13)–(15). Assuming that the on-site Coulomb interaction is very strong $U \gg \mu_B H \gg T$, we find

$$\xi_{AA} = \frac{|\epsilon_2 - \epsilon_1| + |\epsilon_1 - \mu_B H| + |\epsilon_2 - \mu_B H|}{2T} + \frac{2R}{a}, \quad (16)$$

$$\xi_{BB} = \frac{|\epsilon_2 - \epsilon_1| + |\epsilon_1 + U + \mu_B H| + |\epsilon_2 + U + \mu_B H|}{2T} + \frac{2R}{a}, \quad (17)$$

$$\xi_{AB} = \frac{|\epsilon_2 + U - \epsilon_1| + |\epsilon_1 - \mu_B H| + |\epsilon_2 + U + \mu_B H|}{2T} + \frac{\mu_B H}{T} + \frac{2R}{a}. \quad (18)$$

The energies ϵ_1 and ϵ_2 in Eq. (18) correspond to the energy levels of sites of type A and B , respectively. The Fermi level depends upon magnetic field due to transitions from doubly to singly occupied sites, $\delta\mu = \mu_B H(g_B - g_A)/(g_A + g_B)$. However, this has no effect upon the resistance, provided that g_A and g_B are energy independent for energies on the order of $\mu_B H$. Unlike the case of semiconductors doped by shallow impurities,² in amorphous silicon the densities of states are independent of energy on this scale, since they vary with energies comparable to the on-site Coulomb interaction $U \approx 100$ meV.⁸ Therefore, we can safely make the assumption of constant densities of states in the vicinity of the Fermi level.

Instead of the energies ϵ_i , it is convenient to introduce a new set of variables ε_i , chosen in such a way that their values are close to zero for sites participating in electron transport:

$$\varepsilon = \epsilon - \mu_B H \text{ for } A \text{ sites}, \quad (19)$$

$$\varepsilon = \epsilon + U + \mu_B H \text{ for } B \text{ sites}.$$

We further define

$$\varepsilon_{12}(H) = \frac{|\varepsilon_2 - \varepsilon_1 - 2\mu_B H| + |\varepsilon_1| + |\varepsilon_2|}{2} + \mu_B H. \quad (20)$$

The new variables simplify the dimensionless exponents (16)–(18) to the forms

$$\xi_{AA} = \xi_{BB} = \frac{\varepsilon_{12}(0)}{T} + \frac{2R}{a}, \quad (21)$$

$$\xi_{AB} = \frac{\varepsilon_{12}(H)}{T} + \frac{2R}{a}. \quad (22)$$

In the absence of a magnetic field, $\xi_{AA} = \xi_{BB} = \xi_{AB}$, and we return to the standard percolation problem for VRH conductivity. At $H = 0$ only the net density of

states $g = g_A + g_B$ at the Fermi level is relevant, and the ratio of the densities of states g_A/g_B does not affect the conductivity.

IV. MAGNETORESISTANCE IN THE LIMITS OF WEAK AND STRONG FIELDS

A. Strong field limit

As follows from Eq. (22), the exponent ξ_{AB} cannot be smaller than $2\mu_B H/T$. Thus, at sufficiently strong magnetic fields the transitions between sites A and B cannot occur.³ In this limit, the conductivity is determined by two parallel percolation networks, one of which consists only of type A sites and the other of only type B sites. Therefore, the conductivity is independent of H and satisfies Mott's law with the density of states $\tilde{g} = \max\{g_A, g_B\}$. This picture is valid above a certain threshold for the magnetic field

$$H > H_{\text{th}} \equiv \frac{T}{2\mu_B} \tilde{\xi}_c, \quad (23)$$

when all possible ξ_{AB} exceed the critical exponent $\tilde{\xi}_c$ determined by the percolation theory solution of the VRH problem,²

$$\tilde{\xi}_c = \left[\frac{(g_A + g_B)T_0}{\tilde{g}T} \right]^{1/(d+1)}, \quad T_0 = \frac{\beta_d}{(g_A + g_B)a^d}. \quad (24)$$

B. Weak field limit

The opposite limit of weak fields also allows for analytical consideration by means of a perturbative approach applied to the percolation problem with the density of states $g = g_A + g_B$ and the percolation threshold $\xi_c^0 = (T_0/T)^{1/(d+1)}$. At $H \ll H_{\text{th}}$ possible field-induced variations of ξ_{AB} are small, $\Delta\xi_{AB} \ll \xi_c^0$. This enables us to use the perturbative approach proposed in Ref. 2. According to Ref. 2, one can find the small shift of the percolation threshold ξ_c as an average increment of ξ caused by the small perturbation, $\Delta\xi_c = \langle \Delta\xi \rangle$. To calculate the average $\langle \Delta\xi \rangle$ over the statistical ensemble of sites, one needs to find the correction $\Delta\xi$ to the exponent for each link due to a small magnetic field. Clearly, $\Delta\xi_{AA} = \Delta\xi_{BB} = 0$, whereas $\Delta\xi_{AB} = 2\mu_B H/T$ if $\varepsilon_1 > \varepsilon_2$, and $\Delta\xi_{AB} = 0$ otherwise, see Eqs. (21) and (22). Taking into account the fraction of AB links with $\varepsilon_1 > \varepsilon_2$ in the percolation cluster $g_A g_B / (g_A + g_B)^2$, we find

$$\Delta\xi_c = \langle \Delta\xi \rangle = \frac{2g_A g_B}{(g_A + g_B)^2} \frac{\mu_B H}{T}. \quad (25)$$

The dependence of the hopping conductivity upon the critical exponent ξ_c is $\sigma \sim e^{-\xi_c}$. Therefore, Eq. (25) enables us to find the dependence of the conductivity on the magnetic field:

$$\ln \frac{\sigma(T, H)}{\sigma(T, 0)} = - \frac{2g_A g_B}{(g_A + g_B)^2} \frac{\mu_B H}{T}. \quad (26)$$

This dependence is sensitive to the relative densities of A and B sites. As expected, there is no field dependence at $g_A = 0$ or $g_B = 0$.

The region of validity of (26) is determined by the applicability of the perturbative approach, i.e., by the requirement $\Delta\xi_{AB} \ll \xi_c^0$. In terms of the magnetic field strength, this condition reads $\mu_B H \ll \mu_B H_{\text{th}} \sim T\xi_c^0$. Since $\xi_c^0 \gg 1$, the latter condition does not contradict our initial assumption that $\mu_B H \gg T$. More precise limits of applicability of the perturbative calculation become apparent from the comparison of Eq. (26) with the results of numerical simulation, which we present later in this paper.

V. SCALING ANALYSIS

A. Scaling conjecture

It is worth noting that the dimensionless parameter of the perturbation theory is

$$x = \frac{\mu_B H}{T\xi_c^0} \equiv \frac{\mu_B H}{T(T_0/T)^{1/(d+1)}}. \quad (27)$$

The threshold field H_{th} corresponds to the universal (i.e., temperature independent) value of this parameter,

$$x_{\text{th}} = \frac{1}{2} \left(\frac{g_A + g_B}{\tilde{g}} \right)^{1/(d+1)}.$$

The existence of the dimensionless parameter x allowed us to make the conjecture (1), which corresponds to the following scaling behavior of the percolation threshold: $\xi_c(T, H) = \xi_c^0 F(x)$. This scaling function $F(x)$ determines the conductivity at finite magnetic fields

$$\sigma \propto \exp \left\{ - \left(\frac{T_0}{T} \right)^{1/(d+1)} F \left(\frac{\mu_B H}{T(T_0/T)^{1/(d+1)}} \right) \right\}. \quad (28)$$

From the cases of low and high fields discussed above, we already know the limiting behavior of the function $F(x)$. It has linear expansion at small x and reaches a constant value at large x :

$$F(x) = \begin{cases} 1 + \frac{2g_A g_B}{(g_A + g_B)^2} x & \text{at } x \ll 1 \\ \left(\frac{g_A + g_B}{\tilde{g}} \right)^{1/(d+1)} & \text{at } x \geq x_{\text{th}}. \end{cases} \quad (29)$$

B. Proof of the scaling conjecture

We will now prove our conjecture (1) and (2) by reducing the initial problem of hopping magnetoresistance to a dimensionless percolation problem.

We start from the conventional percolation approach to the hopping conductivity and introduce a positive variable ξ . At given ξ , all links are cut except for those with conductance $G > e^{-\xi}$. At small ξ , percolation does not occur, but at some particular value $\xi = \xi_c$ the network starts to percolate. This threshold value determines the

conductivity $\sigma \sim e^{-\xi_c}$. Our goal is to find the dependence of ξ_c on T and H . We generalize the approach of Ref. 2 and introduce a set of dimensionless variables Δ , ρ , and χ defined by the following relations:

$$\varepsilon = T\xi\Delta, \quad R = \frac{1}{2}a\xi\rho, \quad \mu_B H = T\xi\chi. \quad (30)$$

In these variables the connectivity condition for a link is

$$\begin{aligned} \Delta_{12}(0) + \rho &< 1 \quad \text{for } AA \text{ and } BB \text{ links,} \\ \Delta_{12}(\chi) + \rho &< 1 \quad \text{for } AB \text{ links,} \end{aligned} \quad (31)$$

where

$$\Delta_{12}(\chi) = \frac{|\Delta_1| + |\Delta_2| + |\Delta_1 - \Delta_2 - 2\chi|}{2} + \chi.$$

Clearly, only sites with the dimensionless energies $|\Delta| < 1$ can be connected. The dimensionless concentration of these sites in ρ space is

$$n = \frac{1}{2^{d-1}} (g_A + g_B) a^d T \xi^{d+1}. \quad (32)$$

We are now in a position to formulate the dimensionless percolation problem associated with the hopping magnetoresistance problem. Consider a random distribution of points with concentration n in a d -dimensional ρ space. Each point is characterized by its type (A or B), radius-vector ρ_i , and energy Δ_i . The latter is distributed uniformly over the interval $(-1, 1)$. Two points form a link if the condition (31) is satisfied. The problem is characterized by two dimensionless parameters: the ratio γ of concentrations of A and B points, and dimensionless magnetic field χ . At $\gamma = g_A/g_B$, this dimensionless problem is equivalent to the original percolation problem for the hopping magnetoresistance. To reach the percolation threshold, we increase the total dimensionless concentration n (holding γ constant) until the critical value $n_c(\chi)$ is reached. Once $n_c(\chi)$ is found, we can determine the threshold ξ_c for the original problem from the relation (32), which can be rewritten as

$$n_c(\chi)/n_c(0) = (\xi_c/\xi_c^0)^{d+1}. \quad (33)$$

Rewriting χ as defined by Eq. (30) in terms of the parameter x [see Eq. (27)] we find that ξ_c must be a solution of the following equation:

$$\frac{n_c(x\xi_c^0/\xi_c)}{n_c(0)} = \left(\frac{\xi_c}{\xi_c^0} \right)^{d+1}. \quad (34)$$

One can easily show that this equation has exactly one solution. Then it obviously has the form

$$\xi_c = \xi_c^0 F(x). \quad (35)$$

This proves our scaling conjecture (1) and (2).

VI. SIMULATION

As was previously mentioned, the accuracy of the perturbative approach used at small x , see Eq. (29), can only be determined by comparison with simulation data. In

addition, there is an intermediate range of field strengths within which $F(x)$ must be numerically determined, as the analytical theory does not extend to this range. To perform these tasks, we developed a code, which closely resembles that of Skal and Shklovskii.⁹ We will describe the method as applied in two dimensions. The simulation consists of the following: N sites are randomly thrown in an $l \times l$ box (which is large enough for the system to be well below the percolation threshold for the given value of N). Each of these sites is randomly assigned a site type, A or B , and an energy Δ . Two sites are connected if their parameters satisfy the condition (31). Percolation is said to occur when two strips (one at each end of the box), of width equal to the average distance between sites, are connected. We start with $l \gg l_c(\chi)$, and make l smaller until this connection occurs. This determines the percolation threshold $l_c(\chi)$. The critical site concentration is $n_c(\chi) = N/l_c^2(\chi)$.

We ran the simulation at $\gamma = 1$ and at $\gamma = 1/2$ on 3600 sites and averaged each point over 100 runs. One can see from the data shown in Fig. 1 that $F(x)$ is an increasing

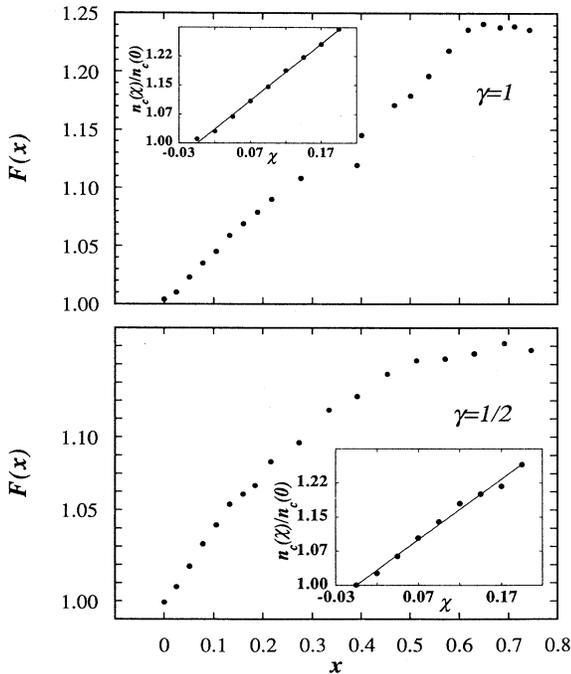


FIG. 1. The universal function, $F(x)$ for $d = 2$. The procedure for extracting $F(x)$ and x from the simulation data gives the standard errors 0.005 for $F(x)$ and less than 0.003 for x . Insets: normalized critical site concentration as a function of dimensionless magnetic field χ . The standard error of $n_c(\chi)/n_c(0)$ is 0.01 on average. (a) $\gamma = 1$; for $x \geq x_{th}$, there is a systematic suppression of $F(x)$ below its true value, $F(x_{th}) = 1.26$; inset: a linear fit to the data for $\chi \leq 0.20$ gave a slope of 1.47 ± 0.03 in good agreement with the theoretically predicted value, $3/2$. (b) $\gamma = 1/2$; for $x \geq x_{th}$, the function $F(x)$ attains its exact value, $F(x_{th}) = 1.14$; inset: a linear fit to the data taken at $\chi \leq 0.2$ yielded a slope of 1.33 ± 0.04 in good agreement with the value $4/3$ following from the perturbation approach.

monotonic function that attains a limiting value for $x \geq x_{th}$. At $\gamma = 1$, the limiting value of $F(x)$ is systematically suppressed below the exact result given by Eq. (29). This is an artifact of the simulation that occurs because $\gamma = 1$ corresponds to the same number of A and B sites. For $x \geq x_{th}$ at $\gamma = 1$, there are two parallel networks that can percolate. Thus, for $x \geq x_{th}$, the simulation is in effect being run twice, once on the A network and once on the B network, with the smaller value of the two resulting concentrations selected. Clearly, this finite size effect does not exist at any other value of γ . The simulation data of Fig. 1 used in conjunction with the scaling functional form (1) yields the magnetoresistance for $\gamma = 1$ and $\gamma = 1/2$ at arbitrary fields.

In order to determine the range of our small x asymptotic form, we replotted the data as critical site concentration n_c vs χ and found that $n_c(\chi)$ begins to deviate from being linear in χ for $\chi \gtrsim 0.20$. Weighted linear fits to the data yielded the zero field values $n_c(0) = 7.064 \pm 0.023$ at $\gamma = 1$ and $n_c(0) = 7.036 \pm 0.031$ at $\gamma = 1/2$ both of which are in good agreement with the accepted value of 6.9 ± 0.4 .⁹ To test the accuracy of our weak field perturbative approach, we performed a weighted linear fit to the data taken at and below $\chi = 0.20$. As one can see from the insets in Figs. 1(a) and 1(b), the fits to the simulation data yielded slopes and intercepts, which were in excellent agreement with those obtained perturbatively at both $\gamma = 1$ and $\gamma = 1/2$.

VII. APPROXIMATE INVARIANT FOR THE PERCOLATION PROBLEM

Ideally we would like to know the scaling function $F(x)$ for any value of γ . However, the simulations used to determine $F(x)$ for each value of γ require a large amount of computer time. Thus, we only found $F(x)$ for two values of gamma: $\gamma = 1$ and $\gamma = 1/2$. The development of an analytical method that yields an approximate form of the scaling function $F(x)$ is therefore highly desirable. The invariant method developed by Shklovskii and Efros² gives just such a simple approximate solution of the VRH problem. Unfortunately, this approach cannot be adapted to the case of the two-color percolation problem. In this paper we suggest an alternative invariant. This approach (i) gives a better estimate of the constant β_d for the standard percolation problem, and (ii) can be generalized to the two-color case. As it reduces the problem of determining the universal scaling function $F(x)$ to the solution of a simple integral equation, we have used it to obtain an analytically determined fitting curve for the universal scaling function $F(x)$. Recently the same invariant conjecture was independently proposed by Ioselevich.¹⁰

A. Invariant approach to the standard VRH problem

We will first formulate our invariant conjecture as applied to the standard (single color, $g_B = 0$) VRH prob-

lem. At the percolation threshold ($\xi = \xi_c$), the probability density of finding a defect state with energy ε_2 linked to one with energy ε_1 is

$$\begin{aligned} G_{AA}(\varepsilon_1, \varepsilon_2) &= \int \theta(\xi_c - \xi_{AA}(\varepsilon_1, \varepsilon_2, r)) d^d r \\ &= v_d g_A \left(\frac{a\xi_c}{2} \right)^d \left(1 - \frac{\varepsilon_{12}(0)}{T\xi_c} \right)^d \\ &\quad \times \theta \left(\xi_c - \frac{\varepsilon_{12}(0)}{T} \right). \end{aligned} \quad (36)$$

Here $v_d = 2\pi^{d/2}/\Gamma(d/2)d$ is the volume of a d -dimensional sphere of unit radius. For the VRH problem, the energies of the two sites are not fixed but rather are governed by distribution functions. Therefore, the normalized distribution of energies $f_1(\varepsilon_2)$ of sites, which can be connected to a site in the system, is

$$\begin{aligned} \Upsilon_1 f_1(\varepsilon_2) &= \int d\varepsilon_1 G_{AA}(\varepsilon_1, \varepsilon_2) f_0(\varepsilon_1) \\ &= g_A v_d \left(\frac{a\xi_c}{2} \right)^d \int \left(1 - \frac{\varepsilon_{12}(0)}{T\xi_c} \right)^d \\ &\quad \times \theta \left(1 - \frac{\varepsilon_{12}(0)}{T\xi_c} \right) f_0(\varepsilon_1) d\varepsilon_1. \end{aligned} \quad (37)$$

Here $f_0(\varepsilon_1)$ is the distribution of energies of the first site; the normalization coefficient Υ_1 is the average number of sites that can be directly linked to the first one (i.e., the average number of bonds per site). Repeating the procedure of Eq. (37) several times, we find that the distributions of site energies obtained in this manner converge rapidly to the eigenfunction of the dimensionless integral equation

$$\lambda_d f(\Delta_2) = \int [1 - \Delta_{12}(0)]^d \theta(1 - \Delta_{12}(0)) f(\Delta_1) d\Delta_1. \quad (38)$$

We conjecture that this eigenfunction is approximately equal to the distribution of energies for the sites in the infinite cluster. The largest eigenvalue λ_d is proportional to Υ , which would then be the average number of bonds per site in the infinite cluster,

$$\Upsilon = \lambda_d g_A v_d \left(\frac{a\xi_c}{2} \right)^d T\xi_c. \quad (39)$$

We further conjecture that Υ is an invariant of the percolation problem, and equals the average number of bonds per site B_c for the random sites (RS) problem.² With

$$\Upsilon \begin{pmatrix} h_A(\varepsilon_2) \\ h_B(\varepsilon_2) \end{pmatrix} = \int \begin{pmatrix} G_{AA}(\varepsilon_1, \varepsilon_2) & \gamma^{-1/2} G_{AB}(\varepsilon_1, \varepsilon_2) \\ \gamma^{-1/2} G_{AB}(\varepsilon_2, \varepsilon_1) & \gamma^{-1} G_{AA}(\varepsilon_1, \varepsilon_2) \end{pmatrix} \begin{pmatrix} h_A(\varepsilon_1) \\ h_B(\varepsilon_1) \end{pmatrix} d\varepsilon_1, \quad (43)$$

guaranteeing that all of its eigenvalues are real.

We now extend the method of invariants to the two-color percolation problem and conjecture that the maximal eigenvalue Υ is independent of the magnetic field.

this assumption, we obtain

$$\lambda_d = 2 \frac{n_c^{\text{RS}}}{n_c^{\text{VRH}}}, \quad (40)$$

where n_c^{RS} and n_c^{VRH} are the critical concentrations of the RS and VRH percolation problems.

A numerical solution of the integral equation (38) gives $\lambda_2 = 0.4301$, $\lambda_3 = 0.3154$, and $\lambda_4 = 0.2489$, in excellent agreement with the values given by Eq. (40), with n_c^{RS} and n_c^{VRH} obtained via simulations of the corresponding percolation problems $\lambda_2 = 0.410 \pm 0.004$, $\lambda_3 = 0.303 \pm 0.004$, and $\lambda_4 = 0.232 \pm 0.005$. The simulation procedures we used to find n_c^{RS} and n_c^{VRH} are nearly identical to the one described in Sec. VI and were run on $N = 8100$ sites and averaged over 50 runs for $d = 3$ and $d = 4$ and on $N = 6400$ and averaged over 100 runs for $d = 2$.

B. Generalization to the “colored” percolation problem

We shall now generalize the discussion of the previous section to the case of a two-color model, $g_B \neq 0$. The sites are now characterized by two parameters: a continuous variable ε and a discrete variable, A or B . Consequently, instead of a single equation (38), we now have a system of two integral equations:

$$\begin{aligned} \Upsilon \begin{pmatrix} f_A(\varepsilon_2) \\ f_B(\varepsilon_2) \end{pmatrix} &= \int \begin{pmatrix} G_{AA}(\varepsilon_1, \varepsilon_2) & G_{AB}(\varepsilon_1, \varepsilon_2) \\ \gamma^{-1} G_{AB}(\varepsilon_2, \varepsilon_1) & \gamma^{-1} G_{AA}(\varepsilon_1, \varepsilon_2) \end{pmatrix} \\ &\quad \times \begin{pmatrix} f_A(\varepsilon_1) \\ f_B(\varepsilon_1) \end{pmatrix} d\varepsilon_1. \end{aligned} \quad (41)$$

Here, $G_{AA}(\varepsilon_1, \varepsilon_2)$ is given by Eq. (36). The off-diagonal element $G_{AB}(\varepsilon_1, \varepsilon_2)$ is the probability density of finding a link between an A state with energy ε_1 and a B state with energy ε_2 . It can be obtained from the probability density G_{AA} given by Eq. (36) by making the replacement $\varepsilon_{12}(0) \rightarrow \varepsilon_{12}(H)$.

The kernel of this integral equation is not symmetric. However, it can be symmetrized by performing a linear transformation:

$$\begin{pmatrix} f_A \\ f_B \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & \gamma^{-1/2} \end{pmatrix} \begin{pmatrix} h_A \\ h_B \end{pmatrix}. \quad (42)$$

Clearly, this transformation preserves the eigenvalues. In the new basis, the integral equation (41) attains a symmetric form

Let us show that by assuming the invariance of Υ , we recover the results of the weak field perturbative approach described in Sec. IV B. First, we solve Eq. (43) at $H = 0$, for which $G_{AB}(\varepsilon_1, \varepsilon_2) = G_{AA}(\varepsilon_1, \varepsilon_2)$. One can easily see

that the normalized solution corresponding to the maximal eigenvalue has the form

$$|0\rangle \equiv \begin{pmatrix} h_A(\varepsilon_1) \\ h_B(\varepsilon_1) \end{pmatrix} = \frac{1}{\sqrt{1+\gamma}} \begin{pmatrix} \gamma^{1/2} \\ 1 \end{pmatrix} f(\varepsilon_1). \quad (44)$$

Here the function $f(\varepsilon)$ is defined as the normalized solution of the ‘‘monochromatic’’ integral equation

$$\Lambda_0 f(\varepsilon_2) = \int G_{AA}(\varepsilon_1, \varepsilon_2) f(\varepsilon_1) d\varepsilon_1, \quad (45)$$

corresponding to the maximal possible eigenvalue Λ_0 .

As we apply a small magnetic field H , the percolation threshold ξ_c shifts away from its zero field value, ξ_c^0 . However, according to our conjecture, the eigenvalue Υ remains constant. To first order in $\mu_B H$ and $\delta\xi_c$, the correction to Υ is simply $\delta\Upsilon = \langle 0|\delta G|0\rangle$, in complete analogy with first-order perturbation theory in quantum mechanics. Thus, the field-induced correction to Υ is given by the following relation:

$$\begin{aligned} \delta\Upsilon &= \frac{1}{1+\gamma} \int f(\varepsilon_2) (\gamma^{1/2}, 1) \\ &\times \begin{pmatrix} \delta G_{AA}(\varepsilon_1, \varepsilon_2) & \gamma^{-1/2} \delta G_{AB}(\varepsilon_1, \varepsilon_2) \\ \gamma^{-1/2} \delta G_{AB}(\varepsilon_2, \varepsilon_1) & \gamma^{-1} \delta G_{AA}(\varepsilon_1, \varepsilon_2) \end{pmatrix} \\ &\times \begin{pmatrix} \gamma^{1/2} \\ 1 \end{pmatrix} f(\varepsilon_1) d\varepsilon_1 d\varepsilon_2. \end{aligned} \quad (46)$$

The condition $\delta\Upsilon = 0$ may be rewritten in the form

$$\int f(\varepsilon_2) \{ (1+\gamma^2) \delta G_{AA}(\varepsilon_1, \varepsilon_2) + \gamma [\delta G_{AB}(\varepsilon_1, \varepsilon_2) + \delta G_{AB}(\varepsilon_2, \varepsilon_1)] \} f(\varepsilon_1) d\varepsilon_1 d\varepsilon_2 = 0. \quad (47)$$

This equation enables one to find the magnetic field-induced correction to ξ_c^0 , since

$$\lambda_d \begin{pmatrix} h_A(\Delta_2) \\ h_B(\Delta_2) \end{pmatrix} = \int \left(\begin{array}{l} [1 - \Delta_{12}(0)]^d \theta(1 - \Delta_{12}(0)) \\ \gamma^{-1/2} [1 - \Delta_{21}(\chi)]^d \theta(1 - \Delta_{21}(\chi)) \end{array} \right) \left(\begin{array}{l} \gamma^{-1/2} [1 - \Delta_{12}(\chi)]^d \theta(1 - \Delta_{12}(\chi)) \\ \gamma^{-1} [1 - \Delta_{21}(0)]^d \theta(1 - \Delta_{21}(0)) \end{array} \right) \begin{pmatrix} h_A(\Delta_1) \\ h_B(\Delta_1) \end{pmatrix} d\Delta_1. \quad (53)$$

Here, the eigenvalue λ_d is related to Υ by Eq. (39). For the two-color problem, $\lambda_d = \lambda_d(\chi, \gamma)$, and the invariance conjecture is equivalent to the assumption that the product $\lambda_d(\chi, \gamma) [\xi_c(\chi, \gamma)]^{d+1}$ is independent of both the magnetic field and the ratio γ of the two densities of states. Therefore, using Eq. (39), the universal scaling function $F(x) \equiv \xi_c(T, H)/\xi_c^0$ can be expressed in terms of the eigenvalue λ_d ,

$$F = \left[\frac{\lambda_d(0, 0)}{\lambda_d(\chi, \gamma)} \right]^{1/(d+1)}. \quad (54)$$

Formula (54) expresses F in terms of $\chi = \mu_B H/T\xi_c$, instead of $x = \mu_B H/T\xi_c^0$. Noting that $x/\chi = \xi_c/\xi_c^0 \equiv F$, we find

$$G_{AA}(\varepsilon_1, \varepsilon_2) = G \left(\xi_c - \frac{\varepsilon_{12}(0)}{T} \right), \quad (48)$$

$$G_{AB}(\varepsilon_1, \varepsilon_2) = G \left(\xi_c - \frac{\varepsilon_{12}(H)}{T} \right). \quad (49)$$

To first order in $\delta\xi_c$ and $\mu_B H$, the condition $\delta\Upsilon = 0$ (47) may be rewritten as

$$\int f(\varepsilon_2) f(\varepsilon_1) G' \left(\xi_c^0 - \frac{\varepsilon_{12}(0)}{T} \right) \left\{ \delta\xi_c (1+\gamma)^2 - \gamma \frac{H}{T} \frac{\partial(\varepsilon_{12} + \varepsilon_{21})}{\partial H} \Big|_{H=0} \right\} d\varepsilon_1 d\varepsilon_2 = 0. \quad (50)$$

From the definition (20) of $\varepsilon_{12}(H)$, one finds

$$\frac{\partial}{\partial H} [\varepsilon_{12}(H) + \varepsilon_{21}(H)] = 2\mu_B. \quad (51)$$

Using Eqs. (50) and (51), we recover the result of the perturbative approach:

$$\delta\xi_c = \frac{\gamma}{(1+\gamma)^2} \frac{2\mu_B H}{T}. \quad (52)$$

To consider the case of arbitrarily strong magnetic fields, we change to the dimensionless variables Δ_1 and Δ_2 and, in doing so, reduce the integral eigenvalue equation to a dimensionless form, which can then be solved numerically:

$$x = \chi \left[\frac{\lambda_d(0, 0)}{\lambda_d(\chi, \gamma)} \right]^{1/(d+1)} \quad (55)$$

Equations (54) and (55) determine $F(x)$ in parametric form.

In order to assess the validity of the invariant approach, we solved Eq. (53) numerically at the two values of γ used in Sec. VI, $\gamma = 1$ and $1/2$, over the entire relevant range of dimensionless magnetic fields. The resulting plots of $F(x)$ are shown in Figs. 2(a) and 2(b) together with the two plots obtained via simulations. Let us first examine the two curves obtained for $\gamma = 1/2$ [Fig. 2(a)]. It is clear that at weak fields the invariant method yields an accurate approximation of the universal scaling function $F(x)$ at $\gamma = 1/2$. In addition, we see that at $\gamma = 1/2$

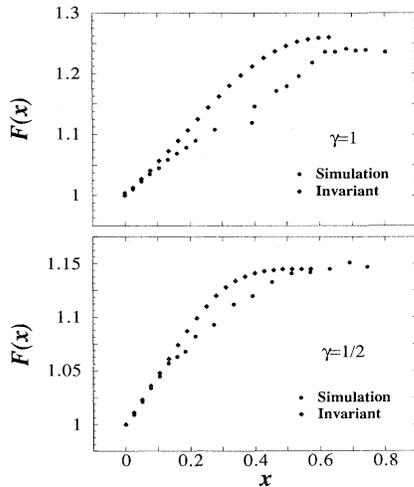


FIG. 2. The approximate scaling function $F(x)$ obtained via the invariant approach, for $d = 2$, shown with the corresponding curves extracted from simulations. (a) $\gamma = 1$; the analytically derived scaling function reproduces the simulation results only at very small values of x . The difference in the limiting values of the two curves can be attributed to the finite size effect, described earlier, which is present in simulations run at $\gamma = 1$. In addition, this finite size effect broadens the range of the scaling variable x , within which the two curves differ substantially. (b) $\gamma = 1/2$; for $x \ll x_{th}$ and $x \geq x_{th}$, the function $F(x)$ obtained via the invariant approach is in good agreement with the numerically determined function. Within a large range of intermediate values of the scaling variable x , however, the two functions differ by more than 0.005, the standard error of the numerically determined $F(x)$.

this approach gives the proper limiting value of $F(x)$. At intermediate fields, the function $F(x)$ obtained from the invariant method continues smoothly between its limiting forms, deviating from the corresponding values of $F(x)$ obtained from simulations by at most 2%.

Upon examination of the two curves in Fig. 2(b), it is equally clear that at $\gamma = 1$ the invariant method accurately reproduces the scaling function $F(x)$ at small fields. This method gives the proper limiting value of $F(x)$ at $\gamma = 1$ which, however, is higher than the corresponding simulation value by approximately 1.5%. This disagreement can be attributed to the systematic suppression of $F(x)$ at large x due to certain finite size effects in the simulations run at $\gamma = 1$ (see Sec. VI). The function $F(x)$ obtained from the invariant method smoothly continues between its limiting forms, differing from the corresponding values of $F(x)$ obtained from simulations by at most 6%. We believe that the magnitude of this discrepancy between the scaling functions, determined by simulations and the invariant method, at intermediate

fields is considerably enhanced by the above mentioned finite size effects in simulations run at $\gamma = 1$.

We should point out that for the values of $F(x)$ obtained from the simulations, the standard error in $F(x)$ is approximately 0.005. Thus, at $\gamma = 1/2$ there is a wide range of intermediate fields within which the difference between the numerically and analytically determined scaling functions is larger than the standard error. For $\gamma = 1$, the two curves differ by more than the standard error for $x \geq 0.05$. Thus, the invariant method does not suffice to accurately determine the universal scaling function $F(x)$. We see two possible reasons for this shortcoming: the first being that this procedure might not yield information about the infinite cluster and the second being the possibility that the average number of bonds per site, for sites belonging to the infinite cluster, is not an invariant of the dimensionless percolation problem. These questions are the subject of future work.

VIII. CONCLUSION

In this paper, we considered the problem of hopping magnetoresistance induced by Zeeman splitting. The problem has been reduced to the calculation of a universal function $F(x)$ of a single dimensionless parameter x (which depends upon magnetic field and temperature). To find $F(x)$, one has to solve a certain dimensionless two-color percolation problem. We found the limiting behavior of $F(x)$ analytically and obtained its full shape numerically for two values of the ratio $g_A/g_B = 1$ and $g_A/g_B = 1/2$. In addition, we developed an approximate method, which enables us to solve the two-color percolation problem analytically at any x . This approach gives a satisfactory extrapolation of the function $F(x)$ between its two limiting forms.

This theory can be applied to any system of localized electrons for which the width of the distribution function of the energies of the localized states is larger than the on-site Coulomb repulsion energy. Bulk amorphous silicon satisfies this condition.^{6,8} In the bulk ($d = 3$), there exists a range of temperatures (7) within which Zeeman splitting makes the dominant contribution to the magnetoresistance. As was proposed in Ref. 8, this theory can then be used to probe the relative concentration of singly and doubly occupied sites that contribute to transport.

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