

Mean-square field characteristics in conductivity of a two-component medium. Numerical modeling of a planar disordered lattice

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We investigate various mean-square characteristics of the electric fields that enter into the problem of conductivity in a two-component disordered square lattice. In particular, we compute the mean squared intensity of each electric field component; this allows us to find not only the effective conductivity but also its derivative with respect to one of the arguments. We also investigate more general bilinear combinations of electric fields, which can be used to tabulate two functions that enter into the expressions for the Hall coefficient and the magnetoresistance. We show that by studying these mean-square characteristics in the critical region, we can obtain detailed information about the consequences of the similarity hypotheses, information that allows us to verify its implications more completely than is normally possible.

1. INTRODUCTION

It is well known that the theoretical study of the various properties of randomly disordered media is fraught with difficulty. For this reason, numerical modeling of disordered lattices is a fundamental source of information about, e.g., the conductivity of such media. In these experiments, numerical simulation has been used to find the effective electrical conductivity $\sigma_e = \sigma_1 f(p, h)$ of two-component lattices (of various symmetries) as a function of the concentration p for various values of the parameter h (where $h = \sigma_2/\sigma_1$ is the ratio of conductivities of the components); see, among others, the review Ref. 1. By studying the function $f(p, h)$ in the neighborhood of the percolation threshold,² we can determine the critical indices of the conductivity²⁻⁴ and check the relations between them that follow from the hypothesis of similarity.^{3,4} To a certain extent, we may regard the numerical study of the electrical conductivity of disordered lattices as a solved problem, although quantitative refinement of the corresponding results is desirable (this is especially true with regard to the values of the critical indices). Therefore, if we remain within the framework of the standard formulation of this problem, it is reasonable to expect qualitatively new results only if we opt to broaden the range of characteristics of disordered systems that can be studied. For example, mean-square values of the electric field intensities in the medium belong to this class of characteristics.

As discussed in the paper by Dykhne,⁵ in a two-dimensional two-component randomly disordered system with critical composition ($p=1/2$) the mean-square electric field intensity grows without bound as $h \rightarrow 0$. This result of Ref. 5 implies critical behavior of this characteristic in the vicinity of the metal-insulator phase transition; however, the author did not associate it with the corresponding critical behavior of the electrical conductivity. Subsequently, general exact relations (valid for both two-dimensional and three-dimensional systems) were found in Ref. 6 between the mean-square values of the different field components and the functions f and f' , i.e., the derivative of f with respect to the

argument h . The existence of such relations makes it possible to obtain detailed information about the quantities f and f' (without difficult numerical differentiation) by computing the mean square of each field component. In particular, all of the critical indices can be found in the neighborhood of the metal-insulator phase transition and the validity of the similarity hypothesis can be verified in detail.

We note that there are reasons to address these questions that transcend the problem of electrical conductivity *per se*. A number of other problems involving the theory of transport phenomena in two-component media call for knowledge of the function f , its derivative f' , and the mean squares of the fields, e.g., the low-frequency dispersion of the conductivity,⁷ the thermoelectric power,⁸ and galvanomagnetic properties in a weak magnetic field \mathbf{H} .⁶ The effective Hall coefficient is completely specified once we have calculated a somewhat more general bilinear combination of the electric fields (see Refs. 6, 9). We also note that in the two-dimensional case the problem of galvanomagnetic properties of a two-component system has an exact solution,^{10,11} in which the components of the effective conductivity tensor can be expressed in terms of the galvanomagnetic characteristics of the components and the function f . On the one hand, once we have determined the Hall coefficients by numerical methods, this makes it possible to check the correctness of the computational methods that were used. On the other hand, once we have tabulated the functions f and f' , we can completely describe the galvanomagnetic properties of the corresponding two-dimensional two-component isotropic system (to second order in \mathbf{H}) over the entire range of the parameters entering into the problem.

In this paper, we investigate various mean-square characteristics of the electric fields in a two-component two-dimensional system within the framework of the problem of conductivity, for the example of a disordered square lattice (the bond problem). For a prespecified distribution (“realization”) of bonds with conductivities σ_1 and σ_2 , we find the potentials at all nodes of the lattice by numerical solution of the Kirchhoff equations. Using these potentials, we calculate

the mean-square intensity for each electric field component, thereby determining both the function f and its derivative f' . We then investigate the critical behavior of each of these quantities in the vicinity of the metal-insulator phase transition and find the corresponding critical indices. In parallel with the basic problem, we solve an analogous problem for the conductivity of the dual lattice (see, e.g., Ref. 12), which allows us to determine a function φ that enters into the expression for the effective Hall coefficient.^{6,9} In addition, we use the expressions obtained in Ref. 6 to tabulate one more function (χ) that enters into the expression for the magnetoresistance.

We note that there exist a number of exact relations and results for these characteristics (see, e.g., Refs. 5, 6, and 13), which we will use in this paper to monitor the accuracy of our calculations. As a rule, we calculated all quantities for ten realizations in order to improve the accuracy of our results. In the critical region, where calculations are most complex and where the results fluctuate appreciably as we pass from one realization to another, we increased the number of realizations to fourteen and doubled the linear dimensions of the lattice.

2. NUMERICAL MODELING

We set up the discrete (lattice) problem of conductivity in a nonuniform medium in the standard way, following the work of Kirkpatrick.¹ His numerical calculations were carried out on a square lattice with size $N \times N = 101 \times 101$ nodes, to each node $\mathbf{r} = (k, j)$ of which he attached a potential $V_{\mathbf{r}} = V_{k,j}$, where k identifies the row and j the column ($k = 1, \dots, N$ and $j = 1, \dots, N$). For all except the boundary nodes, these potentials satisfy the Kirchhoff equations

$$\sum_{\Delta} \sigma_{\mathbf{r}, \mathbf{r}+\Delta}^{-} (V_{\mathbf{r}} - V_{\mathbf{r}+\Delta}) = 0, \quad (1)$$

where the summation runs over the four vectors $\Delta = \pm \Delta_x = \pm(1, 0)$ and $\Delta = \pm \Delta_y = \pm(0, 1)$. In this "bond problem," as Kirkpatrick calls it, $\sigma_{\mathbf{r}, \mathbf{r}+\Delta}$ in Eq. (1) is the conductivity of the bond between nodes \mathbf{r} and $\mathbf{r}+\Delta$; it takes on the value $\sigma_1 = 1$ with probability p ("pure" bonds) and a value $\sigma_2 = h$ with probability $1-p$ ("defective" bonds). On the two opposing sides of the lattice (sample) that are perpendicular to the x axis, boundary values of the potential are specified at the nodes (0 and 1 respectively). In the direction of the y axis periodic boundary conditions are given, i.e., nodes $k=1$ and $k=N$ are treated as if they were the same node.

Numerical modeling was carried out as follows. For a certain fixed bond concentration p a "realization" is generated in which the remaining $1-p$ bonds per unit volume in the originally "pure" lattice are randomly replaced by "defective" bonds. Then the system of Eqs. (1) is solved for the resulting values of $\sigma_{\mathbf{r}, \mathbf{r}+\Delta}$ and the boundary conditions formulated above. In parallel with this problem, we solve the analogous problem of finding the potentials $\tilde{V}_{\mathbf{r}}$ at the nodes of the so-called dual lattice (see, e.g., Ref. 12). In this case, boundary values of the potentials 0 and 1 are assigned to the nodes at the top and bottom edges of the dual lattice, respectively (Fig. 1), and periodic boundary conditions are imposed

along the edges parallel to the x axis. As usual, we assume that for a bond problem with randomly distributed "defects," the macroscopic properties, i.e., the conductivity and other characteristics, coincide for the original (square) and dual lattices (see, e.g., Ref. 5). The calculations carried out in this work confirm this assertion within computational error. However, the real reason why we discuss the problem of conductivity of the dual lattice is that we can use the potentials $\tilde{V}_{\mathbf{r}}$ (along with $V_{\mathbf{r}}$) to compute the function φ , which enters into the expression for the effective Hall coefficient.

The specifics of the calculations make it convenient to rewrite the system of Eqs. (1) in the following matrix (quasi-one-dimensional) form:

$$\hat{A}\mathbf{U} = \mathbf{b}. \quad (2)$$

Here \hat{A} is an $M \times M$ matrix, where $M = (N-1)(N-2)$, having the so-called banded form. The vector \mathbf{b} in (2) is a column vector consisting of M elements, of which only $N-1$ are nonzero (note that the right side of Eq. (2) is nonzero because the system (1) does not apply to the nodes located at the left and right edges of the lattice). Finally, \mathbf{U} is a column vector of M elements consisting of the unknown (required) potentials $V_{k,j}$. The quantities $V_{k,j}$ are sorted in the column vector \mathbf{U} in the following way. The enumeration begins with $j=2$ fixed, letting k run from 1 to $N-1$. Then the potentials with $j=3$ fixed are listed, once more with k running from 1 to $N-1$, etc. The enumeration ends with $j=N-1$, again with k from 1 to $N-1$. As a result we obtain

$$\mathbf{U} = (V_{1,2}, V_{2,2}, \dots, V_{N-1,2}; V_{1,3}, \dots, V_{N-1,3}; \dots; V_{1,N-1}, \dots, V_{N-1,N-1}),$$

where, for convenience, \mathbf{U} is written here as a row vector. For the dual lattice, the numeration in the column $\tilde{\mathbf{U}}$ starts with fixed $k=2$ and runs from $j=1$ to $j=N-1$, etc. In this case the matrix \hat{A} and the vector $\tilde{\mathbf{b}}$ differ from \hat{A} and \mathbf{b} ; however, the equation for the dual lattice has the same form as (2).

System (2) is solved directly using the Chebyshev method of polynomial acceleration:¹⁴

$$\mathbf{U}^{(n+1)} = \rho \{ \gamma (\hat{G}\mathbf{U}^{(n)} + \mathbf{k}) + (1-\gamma)\mathbf{U}^{(n)} \} + (1-\rho)\mathbf{U}^{(n-1)}.$$

Here

$$\hat{G} = \hat{I} - \hat{D}^{-1}\hat{A}, \quad \mathbf{k} = \hat{D}^{-1}\mathbf{b},$$

where \hat{I} is the unit matrix, \hat{D} is the diagonal part of the matrix \hat{A} , $\mathbf{U}^{(n)}$ is the value of the vector \mathbf{U} at the n th iteration, and ρ and γ are the Chebyshev parameters.¹⁴ An analogous method of calculation is used for the dual lattice as well.

In order to monitor the calculations for correctness and assess their accuracy at every stage, the total current is calculated through each cross section of the sample (i.e., the total current flowing through those bonds located between columns j and $j+1$, where j is any of the intervals from 1 to $N-1$). The iteration process stops when the magnitude of the average scatter in the values of these currents does not exceed 0.1%. The values of the potentials $V_{\mathbf{r}}$ found as a result of this procedure (and also $\tilde{V}_{\mathbf{r}}$) are used to compute the con-

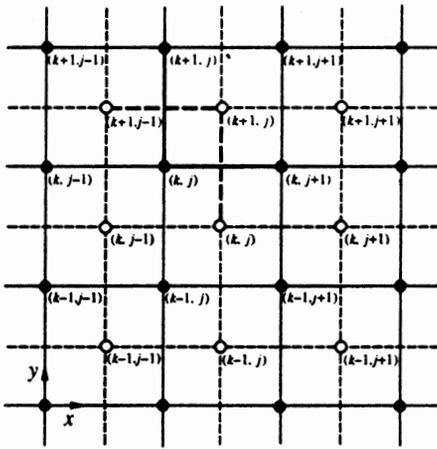


FIG. 1. Original lattice and its dual (dashed lines).

ductivity and other characteristics of the sample. In order to reduce the influence of the finite lattice sizes, all the calculations are repeated for several realizations, and the effective characteristics of the medium are determined by averaging over these realizations. The error in calculating the effective values is estimated by the mean-square deviation from this average.

Figures 2–10 show results for the effective values averaged over ten realizations (for $h=10^{-1}$, $h=10^{-2}$, and $h=10^{-3}$); the errors do not exceed 1%. Investigation of the critical behavior of the effective characteristics requires that we investigate samples with $h=10^{-4}$ and $h=10^{-5}$; for these values of h , the results begin to fluctuate strongly from one

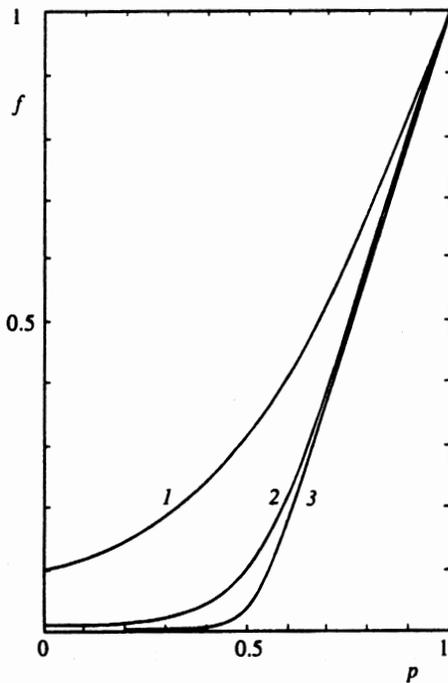


FIG. 2. Dimensionless effective conductivity $f=f(p, h)$ as a function of the concentration p for three values of the parameter h : 1— $h=10^{-1}$; 2— $h=10^{-2}$; 3— $h=10^{-3}$.

realization to the next. Therefore, we investigated the critical region on a lattice with dimensions 201×201 , using 14 realizations. However, even under these conditions the error in the effective values can be as high as 25%.

3. CONDUCTIVITY AND MEAN SQUARES OF THE FIELDS

Let the average electric field be directed along the x axis. Then the effective electrical conductivity σ_e of an isotropic medium (satisfying Ohm's law $\mathbf{j}=\sigma(\mathbf{r})\mathbf{E}$) is defined in the usual way:

$$\sigma_e = \langle j_x \rangle / \langle E_x \rangle. \quad (3)$$

Here j is the current density, \mathbf{E} is the electric field strength, and $\langle \dots \rangle$ denotes an average over the volume V (area in the two-dimensional case) of the sample:

$$\langle \dots \rangle = \frac{1}{V} \int_V (\dots) d\mathbf{r}, \quad (4)$$

where $V \rightarrow \infty$. The quantities $\langle j_x \rangle$ and $\langle E_x \rangle$ can be expressed in terms of the total current I and potential difference \mathcal{U} . In the two-dimensional case, it follows from (3) that for a sample in the shape of a square sheet

$$\sigma_e = I / \mathcal{U}. \quad (5)$$

For a two-component medium, the conductivity $\sigma(\mathbf{r})$ has constant values σ_1 and σ_2 for the first and second components, respectively. The effective conductivity $\sigma_e = \sigma_e(p; \sigma_1, \sigma_2)$ of such a system can be written in the form

$$\sigma_e = \sigma_1 f(p, h); \quad h = \sigma_2 / \sigma_1, \quad (6)$$

where p is the concentration (fraction of occupied volume) of the first component. The function f , i.e., the dimensionless effective conductivity, plays a fundamental role in all of the theory of transport phenomena in two-component media (see, e.g., Refs. 6–8, 10, 11) and is the fundamental object of study in standard numerical modeling.¹

Let us introduce the dimensionless electric field strength in the medium

$$\mathbf{e}(\mathbf{r}) = \mathbf{E}(\mathbf{r}) / \langle \mathbf{E} \rangle \quad (7)$$

and the mean-square quantities

$$\psi_i = \langle \mathbf{e}^2 \rangle^{(i)}, \quad (i=1, 2), \quad (8)$$

where $\langle \dots \rangle^{(i)}$ is an average over the volume of the i th component of V^i :

$$\langle \dots \rangle^{(i)} = \frac{1}{V^i} \int_{V^i} (\dots) d\mathbf{r}, \quad (9)$$

in our case, $\langle \dots \rangle^{(1)} + \langle \dots \rangle^{(2)} = \langle \dots \rangle$, with $\langle \dots \rangle$ defined in (4). According to Ref. 6, the quantities ψ_i defined in (8) can be expressed in terms of the function f :

$$\psi_1 = \langle \mathbf{e}^2 \rangle^{(1)} = f - hf', \quad (10)$$

$$\psi_2 = \langle \mathbf{e}^2 \rangle^{(2)} = f', \quad f' \equiv \frac{\partial f(p, h)}{\partial h}. \quad (11)$$

From (10) and (11) we can find an expression for the function f in terms of the quantities ψ_i :

$$f = \psi_1 + h\psi_2 = \langle e^2 \rangle^{(1)} + h \langle e^2 \rangle^{(2)}. \quad (12)$$

Expression (12) can also be obtained as a consequence of the well-known identity $\langle \mathbf{jE} \rangle = \langle \mathbf{j} \rangle \langle \mathbf{E} \rangle$ (see, e.g., Ref. 5).

Let us introduce a few more useful analytic results. For the linear field characteristics, according to Ref. 6 we have

$$\langle \mathbf{E} \rangle^{(1)} = \frac{f-h}{1-h} \langle \mathbf{E} \rangle, \quad \langle \mathbf{E} \rangle^{(2)} = \frac{1-f}{1-h} \langle \mathbf{E} \rangle. \quad (13)$$

For a two-component randomly nonuniform system, the simultaneous replacement $\sigma_1 \rightleftharpoons \sigma_2$ and $p \rightarrow 1-p$ does not change the macroscopic properties of the medium (see, e.g. Ref. 5), so that $\sigma_e(p; \sigma_1, \sigma_2) = \sigma_e(1-p; \sigma_2, \sigma_1)$. This implies that the function f defined as in (6) satisfies the relation

$$f(p, h) = hf(1-p, 1/h). \quad (14)$$

Note that results (13) and (14) (and also (19), (35), see below) are valid both for two-dimensional and three-dimensional systems.

In the two-dimensional case, the function f is found to satisfy the reciprocity relation⁵ (see also Refs. 7, 13):

$$f(p, h)f(p, 1/h) = 1. \quad (15)$$

For a randomly nonuniform system, relation (14) can be used to cast (15) in the form^{5,7,13}

$$f(p, h)f(1-p, h) = h. \quad (16)$$

At the critical concentration $p = p_c = 1/2$, the well-known result of Dykhne⁵ follows from (16):

$$f(1/2, h) = \sqrt{h}. \quad (17)$$

Furthermore, it is not difficult to use the methods of Refs. 5 and 13 to obtain a reciprocity relation for the function ψ_1 as well:

$$\psi_1(p, h)/f^2(p, h) = \psi_1(p, 1/h). \quad (18)$$

For a randomly nonuniform medium, we have by analogy with (14)

$$\psi_1(p, h) = \psi_2(1-p, 1/h), \quad \psi_2(p, h) = \psi_1(1-p, 1/h). \quad (19)$$

Taking into account the first Eq. (19), relation (18) takes the form

$$\psi_1(p, h)/f^2(p, h) = \psi_2(1-p, h). \quad (20)$$

By making the replacement $p \rightarrow 1-p$, we obtain from (20) and (16)

$$h^2 \psi_2(p, h)/f^2(p, h) = \psi_1(1-p, h). \quad (21)$$

Expression (18) can be verified directly by substituting Eqs. (10) and (11) into (18); taking into account relation (15), this converts (18) into an identity. Analogously, by using Eq. (16) we can verify Eqs. (19)–(21). We emphasize that Eqs. (15)–(18) and (20), (21) hold only for two-dimensional systems, and have no analog in the three-dimensional case.

In the lattice problem, we must define the quantity $E_x(\mathbf{r}) = E_x(k, j)$ to be the potential difference between neighboring nodes (along the x axis):

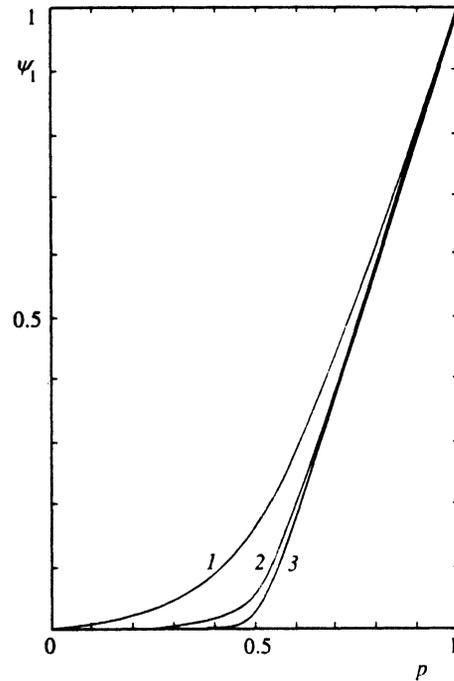


FIG. 3. The quantity $\psi_1 = \langle e^2 \rangle^{(1)} = f - hf'$ as a function of p for the same values of h .

$$E_x(k, j) = V_{k,j} - V_{k,j+1}. \quad (22)$$

Accordingly, we have for the total current

$$I = \sum_{k=1}^{N-1} \sigma(k, j; k, j+1) (V_{k,j} - V_{k,j+1}), \quad (23)$$

where j has any value on the interval from 1 to $N-1$. In the formulation of the problem given in the previous section ($\sigma_1 = 1, U = 1$), the function f coincides with the total current: $f = I$, with I defined in (23). For the quantities ψ_i , in the discrete case we likewise find that

$$\psi_i = \sum_{\{i\}} (V_{k,j} - V_{k,j+1})^2 + \sum_{\{i\}} (V_{k,j} - V_{k+1,j})^2, \quad (i=1,2), \quad (24)$$

where the summation runs over all the bonds with conductivity σ_i .

In this paper the function $f(p, h)$ is determined by numerical methods, using both Eq. (5) and Eq. (12). Both methods give the same result within the limits of computational error. In Fig. 2 we plot the quantity f as a function of the concentration p for three values of the second argument: $h = 10^{-1}$, $h = 10^{-2}$, and $h = 10^{-3}$. In Figs. 3 and 4 we also show the quantities ψ_1 and ψ_2 , plotted as functions of p for the same values of h . Although the functions f and ψ_1, ψ_2 are defined only for $h < 1$, their values for $h > 1$ can be found by using Eqs. (14) and (19). We note that Eqs. (13), (16), (20), and (21) were checked at every stage of the computations; their validity provided an additional way to monitor the correctness of the calculations. In addition, the values of the functions f and ψ_1, ψ_2 were checked at the reference point

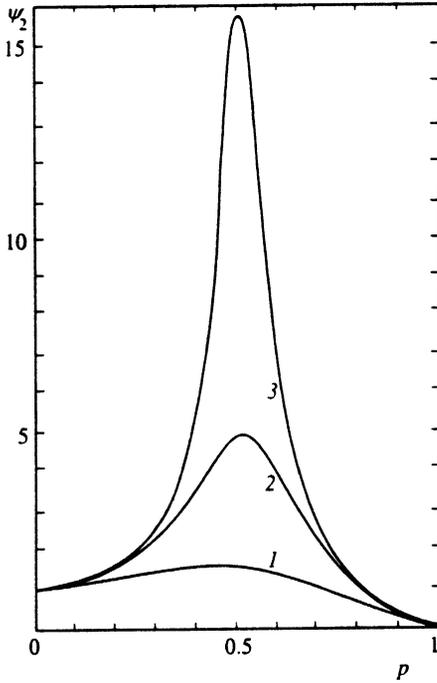


FIG. 4. The quantity $\psi_2 = (e^2)^{(2)} = f'$ as a function of p for the same values of h .

$p = 1/2$ using Eq. (17) (which is also valid in the discrete case for the problem under discussion here, i.e., bonds on a square lattice—see Ref. 5) and the expressions that follow from (10) and (11) after making the substitution (17).

4. THE FUNCTIONS f AND ψ_i IN THE CRITICAL REGION

For a system with a metal–insulator phase transition, the similarity hypothesis implies that in the critical region (i.e., $h \ll 1$, $|\tau| \ll 1$, where $\tau = (p - p_c)/p_c$ and p_c is the critical concentration) the function f has the expansion³ (see also, e.g., Refs. 6, 7)

$$\tau > 0, \Delta_0 \ll \tau \ll 1: f \approx \tau^t [A_0 + A_1(h/\tau^{s/t}) + A_2(h/\tau^{s/t})^2 + \dots], \quad (25a)$$

$$|\tau| \ll \Delta_0: f \approx h^s [a_0 + a_1(\tau/h^{s/t}) + a_2(\tau/h^{s/t})^2 + \dots], \quad (25b)$$

$$\tau < 0, \Delta_0 \ll |\tau| \ll 1: f \approx \frac{h}{(-\tau)^q} \left[B_1 + B_2 \frac{h}{(-\tau)^{t/s}} + \dots \right], \quad (25c)$$

$$q = \frac{t}{s} - t. \quad (26)$$

Here $\Delta_0 = h^{s/t}$ is the size of the smeared-out region,³ the critical indices t , s , and q are interrelated by equation (26). The numerical coefficients A_k , a_k , and B_k are of order unity; A_0 , a_0 , and B_1 are obviously positive. As noted in Ref. 7, $A_1 > 0$ and $B_2 < 0$. It is also not difficult to show that $a_1 > 0$.

For the problem of bonds on a square lattice, according to Ref. 5 we have $p_c = 1/2$ and $f(1/2, h) = \sqrt{h}$; see also Eq. (17). Therefore, in this case we have

$$s = 1/2, \quad q = t, \quad a_0 = 1, \quad (27)$$

where the second equation follows from (26) with $s = 1/2$. Note also that substituting (25) into Eq. (16) leads to a number of relations for the coefficients A_k , a_k , and B_k :

$$A_0 B_1 = 1, \quad A_0 B_2 + A_1 B_1 = 0, \dots, \quad a_2 = 1/2 a_1^2, \dots, \quad (28)$$

from which it follows, in particular, that $a_2 > 0$.

For the function ψ_1 , taking into account relation (26), we obtain from (10) and (25)

$$\tau > 0, \Delta_0 \ll \tau \ll 1: \psi_1 \approx \tau^t [A_0 - A_2(h/\tau^{s/t})^2 + \dots], \quad (29a)$$

$$|\tau| \ll \Delta_0: \psi_1 \approx h^s \left[(1-s)a_0 + \left(1-s + \frac{s}{t} \right) a_1 (\tau/h^{s/t}) + \dots \right], \quad (29b)$$

$$\tau < 0, \Delta_0 \ll |\tau| \ll 1: \psi_1 \approx -B_2 \frac{h^2}{(-\tau)^{2q+t}} + \dots \quad (29c)$$

Note that the correction in (29a) is quadratic in the small parameter $h/\tau^{s/t}$, in contrast to (25a). For $\tau < 0$ outside the smeared-out region, Eq. (29c) implies that the quantity ψ_1 is proportional to h^2 . The reason is the same as for the function φ , which enters into the expression for the effective Hall coefficient⁶ (see Eq. (48) from Sec. 6). The point is that when $p < p_c$ and $h \rightarrow 0$, the electric field is expelled from the high-conductivity (first) component, while the field $\mathbf{E}(\mathbf{r})$ goes to zero linearly with respect to the parameter h .

For the function ψ_2 , taking (26) into account, we have from (11) and (25) that

$$\tau > 0, \Delta_0 \ll \tau \ll 1: \psi_2 \approx \frac{1}{\tau^t} [A_1 + 2A_2(h/\tau^{s/t}) + \dots], \quad (30a)$$

$$|\tau| \ll \Delta_0: \psi_2 \approx \frac{1}{h^{1-s}} \left[s a_0 + s \frac{t-1}{t} a_1 (\tau/h^{s/t}) + \dots \right], \quad (30b)$$

$$\tau < 0, \Delta_0 \ll |\tau| \ll 1: \psi_2 \approx \frac{1}{(-\tau)^q} \times \left[B_1 + 2B_2 \frac{h}{(-\tau)^{t/s}} + \dots \right]. \quad (30c)$$

According to (30), the quantity ψ_2 is a sharply peaked function of the concentration near $p = p_c$ (see Fig. 4). As we mentioned above, the coefficient a_1 is positive, so that the dependence of ψ_2 on p exhibits a maximum for $p > p_c$ (see Fig. 4) that is shifted from the critical point p_c by a quantity of order $\sim h^{s/t}$.

The functions ψ_1 and ψ_2 are by definition positive, so that it follows from (10), (11) that

$$f > h f', \quad f' > 0. \quad (31)$$

Substituting Eq. (25b) into the first inequality (31) shows that $s < 1$. Furthermore, substituting (25a) and (25c) into (31) gives the inequalities stated above: $A_1 > 0$ and $B_2 < 0$. These inequalities were obtained in Ref. 7 from physical considerations.

As noted in Sec. 2, in the critical region we carried out our numerical modeling on a lattice with dimensions 201×201 for $h=10^{-4}$ and $h=10^{-5}$, using 14 realizations. In this case we began to observe critical behavior corresponding, e.g., to Eq. (25a), only when h had dropped to 10^{-5} , so that the accuracy to which the critical indices and the numerical coefficients were determined was rather small. To broaden the parameter range over which the system was critical, we needed to use still smaller values of h ($h=10^{-6}$, etc.). However, for $h=10^{-5}$ the finiteness of the lattice began to affect the results, a symptom of which was strong fluctuations (as $p \rightarrow p_c=1/2$) in the system conductivity from one realization to another. These difficulties can be overcome only by working with a larger lattice.

In processing the data from the numerical model with $p > p_c$ (i.e., outside the smeared-out region) it is convenient to define the index t not in terms of the function f itself but rather in terms of the quantity ψ_1 . This is because the correction to ψ_1 (due to finiteness of h) is smaller than the corresponding correction to f (see (25a) and (29a)). At the same time, along with the index t , we also determine the coefficient A_0 . Furthermore, by processing the data for ψ_2 using Eqs. (30a) and (30c), we can find both the index q and the coefficients A_1 and B_1 . As a result we obtain

$$\begin{aligned} t &= 1.3 \pm 0.3, \quad q = 1.3 \pm 0.3, \\ A_0 &= 1.7 \pm 1.1, \quad A_1 = 1.0 \pm 0.8, \\ B_1 &= 0.7 \pm 0.4, \quad B_2 \approx -1.5. \end{aligned} \quad (32)$$

In (32) we also give the value of the coefficient B_2 determined from the second relation (28). The results (32) show that the critical indices $q=t$ [see (27)] to within the limits of computational accuracy.

Thus, our combined investigation of the functions f , ψ_1 , and ψ_2 allows us to check more completely (than usual) the implications of the similarity hypothesis, and to find not only the coefficients A_0 and B_1 , but also A_1 and B_2 (which is quite difficult using the standard approaches¹). To complete the picture we should find, in some independent way, the index s as well. Unfortunately, due to the strong fluctuations mentioned above in the values of the functions f , ψ_1 , and ψ_2 , the quantity s cannot be reliably determined in the critical regime (i.e. in the present case when $h \leq 10^{-5}$ and $p = p_c = 1/2$). However, because the results of Dykhne¹⁷ hold for any h , even those portions of our data for f , ψ_1 , and ψ_2 outside the critical regime (from $h=10^{-1}$ to $h=10^{-4}$ and for $p=1/2$) can be processed to give results that are close to the exact ones (i.e., $s=1/2$, $a_0=1$): $s=0.50 \pm 0.02$, and $a_0=1.00 \pm 0.01$.

5. THE FUNCTIONS ψ_{1l} AND ψ_{2l}

Along with the quantities ψ_i , there is considerable interest in studying the functions

$$\psi_{il} = \langle \mathbf{e}_{\parallel}^2 \rangle^{(i)}, \quad \psi_{it} = \langle \mathbf{e}_{\perp}^2 \rangle^{(i)}, \quad (i=1,2), \quad (33)$$

where \mathbf{e}_{\parallel} and \mathbf{e}_{\perp} are the components of the vector \mathbf{e} defined in (7) parallel and perpendicular to the mean field (\mathbf{E}), respec-

tively; $\langle \dots \rangle^{(i)}$ is the same as in (9). The quantities (33) are related to ψ_i from (8) by the obvious expression:

$$\psi_i = \psi_{il} + \psi_{it}. \quad (34)$$

In the lattice problem (as formulated in Sec. 2), the function ψ_{il} is given by the first sum in Eq. (24), while ψ_{it} is given by the second. For the dual lattice (where the potential difference is applied along the y axis), $\bar{\psi}_{il}$ is conversely given by the second sum in (24), while $\bar{\psi}_{it}$ is given by the first; in this case $V_{k,j}$ is replaced by $\bar{V}_{k,j}$.

For a randomly nonuniform medium, we have by analogy with (19)

$$\psi_{1l}(p,h) = \psi_{2l}(1-p,1/h), \quad \psi_{1t}(p,h) = \psi_{2t}(1-p,1/h) \quad (35)$$

and two more equations that follow from (35) by replacement of the indices $1 \rightleftharpoons 2$. In the two-dimensional case, it is not difficult to obtain the following reciprocity relation from the methods of Refs. 5, 13, taking Eq. (35) into account:

$$\frac{\psi_{1l}(p,h)}{f(p,h)} = \psi_{2l}(1-p,h), \quad \frac{\psi_{1t}(p,h)}{f(p,h)} = \psi_{2t}(1-p,h). \quad (36)$$

By making the replacement $p \rightarrow 1-p$, we can obtain from (36) and (16) two more relations analogous to (21).

There are no known relations like (10) and (11) for the quantities ψ_{il} and ψ_{it} ; however, their fundamental properties can be established by starting from the definition (33) and Eqs. (34). The general form of ψ_{1l} (for $h < 1$) is clear from Fig. 5, where we plot it as a function of concentration p for three values of the argument h . (Note that the longitudinal function ψ_{1l} essentially mimics the behavior of ψ_1 , and is close to it quantitatively as well.) The transverse function ψ_{1t} is qualitatively reminiscent of ψ_{1l} and ψ_1 for $p \leq 0.6$; however, it differs from them markedly in the interval $0.6 \leq p \leq 1$, and it vanishes at $p=1$ (Fig. 6). The fact that ψ_{1t} goes to zero as $p \rightarrow 1$ is connected with the obvious fact that there are no transverse components to the electric field intensity in a uniform medium. Finally, in Figs. 7 and 8 we show the general form of the functions ψ_{2l} and ψ_{2t} , which qualitatively mimics that of ψ_2 .

For a system with a metal-insulator phase transition, the critical behavior of the function ψ_{1l} can be described by the following expressions, which are similar to (29) (here we give only the leading terms of the expansions):

$$\tau > 0, \quad \Delta_{1l} \ll \tau \ll 1: \quad \psi_{1l} \approx A_{0l}^{(1)} \tau^{t_{1l}}, \quad (37a)$$

$$|\tau| \ll \Delta_{1l}: \quad \psi_{1l} \approx a_{0l}^{(1)} h^{s_{1l}}, \quad (37b)$$

$$\tau < 0, \quad \Delta_{1l} \ll |\tau| \ll 1: \quad \psi_{1l} \approx B_{2l}^{(1)} \frac{h^2}{(-\tau)^{2q_{1l}+t_{1l}}}, \quad (37c)$$

$$q_{1l} = \frac{t_{1l}}{s_{1l}} - t_{1l}, \quad (38)$$

where $\Delta_{1l} = h^{s_{1l}/t_{1l}}$ is the size of the smeared-out region for the function ψ_{1l} . According to the similarity hypothesis,^{3,4} all the critical phenomena (in the absence of a magnetic field) are characterized by the same scale, so that Δ_{1l} should coincide in order of magnitude with Δ_0 from (25) (compare with

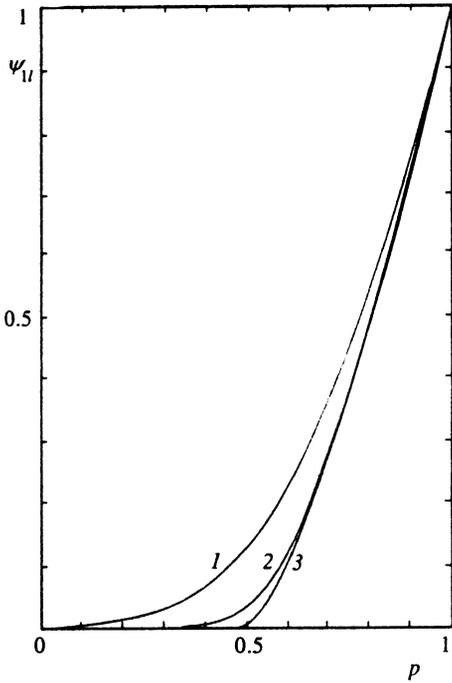


FIG. 5. The longitudinal function $\psi_{1l} = \langle e_{\parallel}^2 \rangle^{(1)}$.

the similar discussions in Ref. 6). From this we obtain a second relation between the critical indices we have introduced:

$$s_{1l}/t_{1l} = s/t. \quad (39)$$

Because ψ_{1l} and ψ_{1t} are positive, it follows from (34) that ψ_{1l} cannot decrease more slowly or increase more rapidly than ψ_1 . These conditions constrain the values of the corresponding indices: $t_{1l} \geq t$, $s_{1l} \geq s$, $2q_{1l} + t_{1l} \leq 2q + t$. In the two-dimensional case, where $s = 1/2$, we obtain $t_{1l} > t$, $s_{1l} \geq 1/2$ and $2q_{1l} + t_{1l} \leq 3t$. The critical behavior of the function ψ_{1t} is described in exactly the same way. For ψ_{1t} the

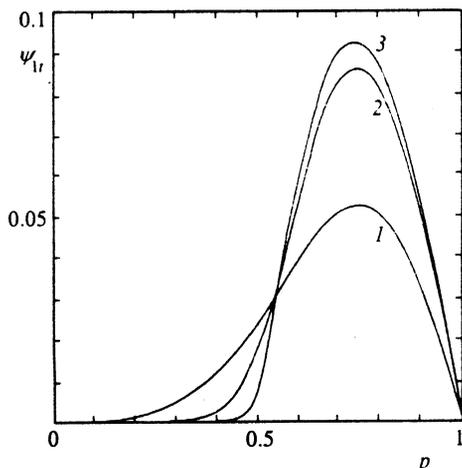


FIG. 6. The transverse function $\psi_{1t} = \langle e_{\perp}^2 \rangle^{(1)}$.

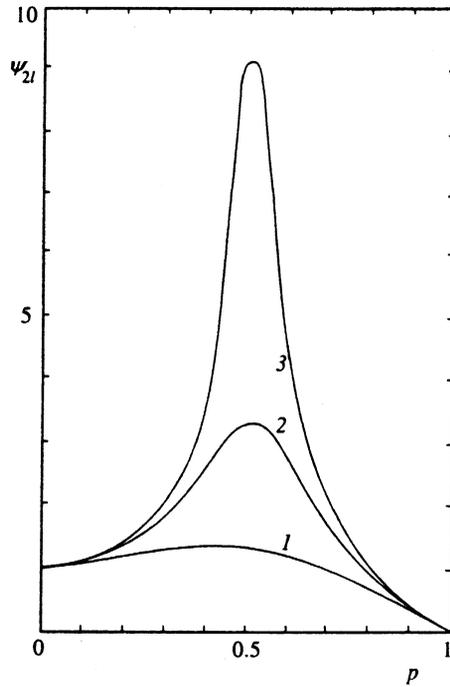


FIG. 7. The longitudinal function $\psi_{2l} = \langle e_{\parallel}^2 \rangle^{(2)}$.

same dependences and relations hold (with regard to form) as those for ψ_{1l} ; we obtain them by simply replacing the label l by t .

The behavior of the function ψ_{2l} in the critical region can be described in a way similar to (30) (here also we compute only the leading terms of the expansion):

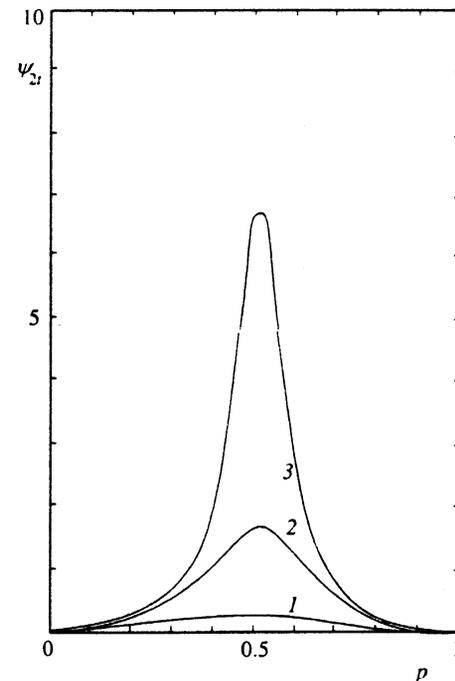


FIG. 8. The transverse function $\psi_{2t} = \langle e_{\perp}^2 \rangle^{(2)}$.

$$\tau > 0, \Delta_0 \ll \tau \ll 1: \quad \psi_{2l} \approx \frac{A_{1l}^{(2)}}{\tau^{q_{2l}}}, \quad (40a)$$

$$|\tau| \ll \Delta_0: \quad \psi_{2l} \approx \frac{a_{0l}^{(2)}}{h^{\lambda_{2l}}}, \quad (40b)$$

$$\tau < 0, \Delta_0 \ll |\tau| \ll 1: \quad \psi_{2l} \approx \frac{B_{1l}^{(2)}}{(-\tau)^{q_{2l}}}, \quad (40c)$$

$$\lambda_{2l}/q_{2l} = s/t. \quad (41)$$

Relation (41) follows from the condition that $\Delta_{2l} \sim \Delta_0$, where $\Delta_{2l} = h^{\lambda_{2l}/q_{2l}}$ is the size of the smeared-out region for the function ψ_{2l} . Because ψ_{2l} cannot be more singular than ψ_2 , we have $q_{2l} \leq q$ and $\lambda_{2l} \leq 1-s$, and in the two-dimensional case we find that $q_{2l} \leq t$ and $\lambda_{2l} \leq 1/2$. For the function ψ_{2l} in the critical region the same dependences and relations are valid as those for ψ_{2l} , which we find by replacing the label l by t .

Thus, the critical behavior of each of the functions ψ_{1l} , ψ_{1t} , ψ_{2l} , and ψ_{2t} is characterized by one new index; we choose these indices to be t_{1l} , t_{1t} , q_{2l} , and q_{2t} , respectively. The remaining indices can be expressed in terms of them as follows:

$$s_{1l} = (s/t)t_{1l}, \quad q_{1l} = (t/s) - t_{1l},$$

$$s_{1t} = (s/t)t_{1t}, \quad q_{1t} = (t/s) - t_{1t},$$

$$\lambda_{2l} = (s/t)q_{2l}, \quad \lambda_{2t} = (s/t)q_{2t}.$$

For a two-dimensional system, however, the quantities t_{1l} , t_{1t} , q_{2l} , and q_{2t} are further interrelated. Substituting Eqs. (37), (40), and (25) into Eq. (36) gives two more relations

$$q_{2l} = 2t - t_{1l}, \quad q_{2t} = 2t - t_{1t}. \quad (42)$$

Consequently, in the two-dimensional case the four functions ψ_{1l} , ψ_{1t} , ψ_{2l} , and ψ_{2t} are characterized by only two independent critical indices, for example, t_{1l} and t_{1t} , where $t_{1l} \geq t$ and $t_{1t} \geq t$. For the remaining indices we have

$$s_{1l} = (1/2)(t_{1l}/t), \quad q_{1l} = 2t - t_{1l},$$

$$s_{1t} = 1/2(t_{1t}/t), \quad q_{1t} = 2t - t_{1t},$$

$$\lambda_{2l} = 1/2(q_{2l}/t), \quad \lambda_{2t} = 1/2(q_{2t}/t)$$

along with the two Eqs. (42). In addition to (42), we can also derive a number of relations between the expansion coefficients from (36):

$$A_{0l}^{(1)} = (A_0)^2 B_{1l}^{(2)}, \quad a_{0l}^{(1)} = a_{0l}^{(2)}, \quad B_{2l}^{(1)} = (B_1)^2 A_{1l}^{(2)} \quad (43)$$

and three more relations of the form (43) by replacing the label l by t .

Processing of the numerical data for the functions ψ_{1l} , ψ_{1t} , ψ_{2l} , and ψ_{2t} gives

$$t_{1l} = 1.4 \pm 0.3, \quad t_{1t} = 1.2 \pm 0.3$$

$$q_{2l} = 1.3 \pm 0.3, \quad q_{2t} = 1.3 \pm 0.4. \quad (44)$$

From (44) and (32) it follows within the limits of computational error that we have equality of the indices:

$$t_{1l} \approx t_{1t} \approx q_{2l} \approx q_{2t} \approx t. \quad (45)$$

Study of the interval $|\tau| \ll \Delta_0$ is difficult for the same reasons as in the previous section. The corresponding critical indices can be determined from the relations found above. Within the approximation (45) we obtain the following estimates: $s_{1l} \approx s_{1t} \approx \lambda_{2l} \approx \lambda_{2t} \approx s = 1/2$. We also give here the values of several coefficients from the expansions (37) and (40):

$$A_{0l}^{(1)} = 1.2 \pm 0.8, \quad A_{0t}^{(1)} = 0.6 \pm 0.4,$$

$$A_{1l}^{(2)} = 0.6 \pm 0.4, \quad A_{1t}^{(2)} = 0.4 \pm 0.4.$$

The other coefficients can be found from relations like (43).

The main reason for the low accuracy of our results in the critical region is, as we have already noted, the finiteness of the sample. In order to bring to light the corresponding quantitative criterion, we will investigate the region $\tau > 0$, $\Delta_0 \ll \tau \ll 1$. Note that as $\tau \rightarrow 0$, the correlation radius increases according to $r_c \sim \tau^{-\nu}$ (see Ref. 2), reaching a maximum value of $(r_c)_{\max} \sim (\Delta_0)^{-\nu}$ at the boundary of the region $\tau \sim \Delta_0$. In order for the critical behavior of the conductivity to be unaffected by sample finiteness, the linear size L must be large compared to $(r_c)_{\max}$. Therefore, the criterion we want takes the form

$$L \gg L_c, \quad L_c = h^{-\nu s/t}.$$

From this there follows a bound on the parameter h for fixed L (see Ref. 3):

$$h \gg h_c, \quad h_c = L^{-t/\nu s}.$$

In the two-dimensional case $\nu \approx t$ (see Ref. 2), so that this criterion takes the form $h \gg L^{-2}$; for $L=100$ we have $h \gg 10^{-4}$. Thus, in order to increase the accuracy of the results in the critical region, it is necessary to use larger lattices (for example, $L=500$ or even $L=1000$).

6. HALL COEFFICIENT AND MAGNETORESISTANCE

A two-dimensional system in a transverse magnetic field \mathbf{H} is characterized by the conductivity tensor

$$\hat{\sigma} = \begin{pmatrix} \sigma_x & \sigma_a \\ -\sigma_a & \sigma_x \end{pmatrix}, \quad (46)$$

where our notation is the same as in Ref. 6. In a weak magnetic field ($\mathbf{H} \rightarrow 0$) the Hall component σ_a is linear in \mathbf{H} . In the same approximation, the Hall component of the effective conductivity tensor has the form⁶

$$\sigma_{ae} = \sigma_{a2} + (\sigma_{a1} - \sigma_{a2}) \varphi(p, h). \quad (47)$$

In expression (47), the galvanomagnetic characteristics of the components are shown explicitly; and the function $\varphi(p, h)$ is determined by the properties of the medium at $\mathbf{H}=0$. Equation (47) implies the following expression for the effective Hall coefficient $R_e = H^{-1} \sigma_{ae} / \sigma_e^2$:

$$R_e = \frac{h^2 R_2}{f^2} + (R_1 - h^2 R_2) \frac{\varphi}{f^2}, \quad (48)$$

where R_i is the Hall coefficient of the i th component and f is defined in (6).

Let $\mathbf{E}^{(\nu)}(\mathbf{r})$ be the electric field intensity in the medium, defined for a given $\langle \mathbf{E}^{(\nu)} \rangle$, where the index ν shows that the average field is directed along the ν -axis. According to Refs.

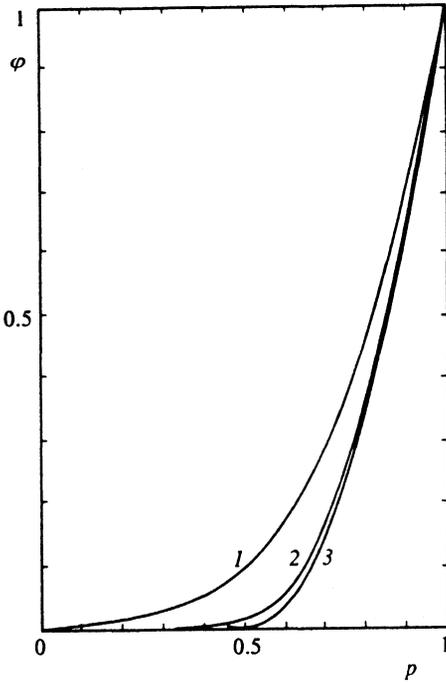


FIG. 9. The function φ defined according to expressions (49) and (50).

6, 9, the function $\varphi(p, h)$ from (47) can be expressed in terms of the electric fields defined within the framework of the conductivity problem (for $\mathbf{H}=0$) as follows:

$$\varphi(p, h) = \frac{\langle E_x^{(x)} E_y^{(y)} - E_y^{(x)} E_x^{(y)} \rangle^{(1)}}{\langle E_x^{(x)} \rangle \langle E_y^{(y)} \rangle}. \quad (49)$$

In the two-dimensional case, the following analytic expression for the function $\varphi(p, h)$ is valid:⁶

$$\varphi(p, h) = (f^2 - h^2) / (1 - h^2), \quad (50)$$

where f is the dimensionless effective conductivity defined by (6).

In this paper we have used Eq. (49), choosing for $E^{(x)}$ the field in the original lattice and for $E^{(y)}$ the field in the dual lattice. In this case the fields $E^{(x)}$ and $E^{(y)}$ can be expressed in terms of the potentials V_r and \bar{V}_r using equations like (22). The corresponding results of our numerical modeling are shown in Fig. 9, where $\varphi(p, h)$ is displayed as a function of the concentration p for three values of the argument h . Use of Eq. (50) gives the same values for the function $\varphi(p, h)$ as does direct computation using Eq. (49). For $h \ll 1$, we have from (50) that $\varphi \approx f^2$. The data from numerical modeling in the critical region confirm this dependence (to within the computational accuracy).

In a weak magnetic field ($H \rightarrow 0$), σ_x can be written in the form

$$\sigma_x = \sigma + \gamma, \quad (51)$$

where $\gamma \propto H^2$, and σ is the conductivity of the system for $\mathbf{H}=0$. According to Ref. 6, in the two-dimensional case the corresponding correction to the effective conductivity $\gamma_e = \sigma_{xe} - \sigma_e$ is found to be

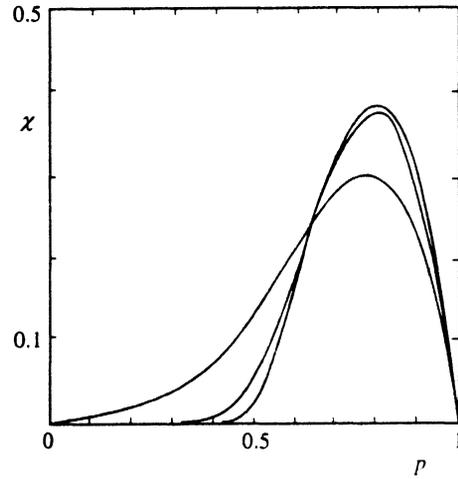


FIG. 10. The function χ defined according to expression (53).

$$\gamma_e = \gamma_1 \psi_1 + \gamma_2 \psi_2 + \frac{(\sigma_{a1} - \sigma_{a2})^2}{\sigma_1} \chi. \quad (52)$$

Here $\gamma_i = \sigma_{xi} - \sigma_i$ refers to the i th component, while the functions ψ_1 and ψ_2 are defined in (10), (11). The function χ is given by a more complicated expression in terms of the electric field in the medium (see Ref. 6), so that it is impossible to define it directly within the framework of this particular numerical model. However, in the two-dimensional case the problem of the galvanomagnetic properties has an exact solution for arbitrary \mathbf{H} ,^{10,11} so that the function χ can be explicitly written in terms of f (see Ref. 6):

$$\chi = (f - hf' - f\varphi) / (1 - h^2) \quad (53)$$

with φ from (50). By using Eq. (53) and our numerical results, we can find the dependence of the function χ on the concentration p for the three values of the argument h ; the results are shown in Fig. 10.

We note that $\chi \approx \psi_1$ over the entire critical region, so that the critical behavior of the function χ is, in fact, given by Eqs. (29).

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