Quadratic effective characteristics of transport in two-component materials. Computer simulation of a three-dimensional disordered lattice

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Averaged quadratic characteristics of electric transport in a disordered, two-component simple cubic lattice have been calculated in the context of the conductivity problem. Average squares of electric field strengths in each component have been found, thus we could derive not only the effective conductivity, but also its derivative with respect to one argument within the same accuracy. We have studied longitudinal and transverse quadratic characteristics as well as a more general bilinear form of electric field, which has allowed us to tabulate several functions of two parameters which determine the Hall coefficient and magnetoresistance in a weak magnetic field. We have demonstrated that calculations of average quadratic characteristics around the metal–dielectric transition yield detailed information about the critical behavior of kinetic parameters and permit a comprehensive verification of the similarity hypothesis.
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1. INTRODUCTION

The conductivity of disordered two-component lattices has been studied using computer simulations by many authors (see Refs. 1–4 and references therein). In standard computer simulations, only the effective conductivity $\sigma_e=\sigma_1 f(p,h)$ is usually calculated, where p is the concentration of the first component and $h=\sigma_2/\sigma_1$ is the ratio of the conductivities of the components. In this case, attention is usually focused on σ_e (or the function f, which is the same) around the metal–dielectric transition and the respective critical exponents. Nonetheless, not only the function f (throughout the domain of its arguments), but its derivative $f'=\partial f/\partial h$ is also important for studies of transport in two-component materials, namely for calculations of low-frequency dispersion of conductivity,[5] thermoelectric power,[6,7] and galvanomagnetic effects in low magnetic fields.[8] Other parameters, which are usually termed as effective quadratic characteristics,[8,9] must be also calculated.

The study of quadratic characteristics is interesting from several viewpoints. For example, calculations of the mean squares of electric field strength in each component yield not only the function f, but also its derivative f' within the same accuracy without labor-consuming numerical differentiation.[8] This allows one to obtain more information than usual about the behavior of the function f in the critical region and thus to verify the statements based on the similarity hypothesis more substantially. Furthermore, the longitudinal ψ_{il} and transverse ψ_{it} averaged quadratic functions (see Sec. 5) are needed for calculating magnetoresistance.[8] Finally, the effective Hall coefficient is derived from the more general quadratic characteristic, i.e., function φ (see Refs. 8 and 9, and Sec. 6). Note also that quadratic characteristics calculated in the critical region permit a comprehensive verification of the similarity hypothesis.

This has led us to a conclusion that even in studies of conductivity the set of calculated parameters must be enhanced to include quadratic characteristics in addition to σ_e. In the two-dimensional configuration, a generalized computer simulation was performed on a disordered quadratic lattice.[10] This simulation not only reproduced and improved the results by other authors, but also yielded new data. For example, not only the function f and its derivative f' were tabulated, but also the other functions included in the expressions for the Hall coefficient and magnetoresistance. The behavior of all these parameters was also studied in the critical region.

This paper describes a computer simulation on a three-dimensional, two-component lattice with randomly distributed bonds between lattice sites characterized by the conductivities σ_1 and σ_2. The simulation has been performed to comprehensively study the lattice's electric characteristics. Given a specific configuration of bonds of two sorts, a system of Kirchhoff's equations was solved on a computer, and potentials $V_{\mathbf{r}}$ were calculated at all lattice sites. They were used to calculate various linear and quadratic effective characteristics, specifically the function f and its derivative f'. Besides, we have calculated and tabulated (in a graphic form) the longitudinal and transverse functions ψ_{il} and ψ_{it} included in the expression for the magnetoresistance.[8] We solved concurrently a similar problem of the conductivity in an auxiliary lattice, which was a generalization of the two-dimensional dual lattice[10] to the three-dimensional case. This has allowed us to calculate the function φ in the expression for the effective Hall coefficient.[8,9] The behavior of each function has been studied around the metal–dielectric transition, and not only their critical exponents, but also the coefficients of the respective expansions have been determined.

The calculations have been performed on a Convex-C210 vector computer by simulating a $50\times50\times50$ lattice at six values of the parameter h, namely $h=10^{-m}$, where $m=1,\ldots,6$. The bond problem of the simple cubic lattice has been studied, in this case the critical concentration (percolation threshold) is $p_c\simeq0.247$.[2] The effective parameters were determined by averaging over twelve configurations. In the critical region, which is more difficult for calculation and

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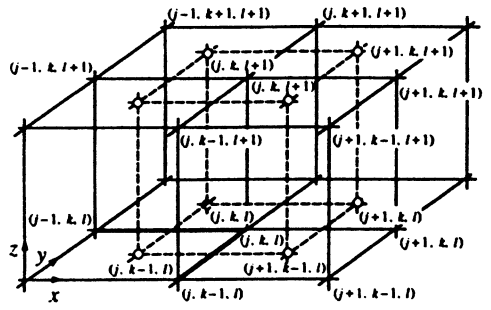

FIG. 1. Basic and auxiliary (dashed lines) lattices.

where the spread of parameters in different configurations is larger, the data were averaged over twenty configurations.

2. ORGANIZATION OF THE COMPUTER SIMULATION

The problem of the conductivity in an inhomogeneous lattice has been formulated in the conventional manner.[1,10] We have considered a simple cubic $N\times N\times N=51\times 51\times 51$ lattice (the number of links was $50\times 50\times 50$, accordingly). The potential at each lattice site $\mathbf{r}=(j,\ k,\ l)$ is denoted as $V_{\mathbf{r}}=V_{j,k,l}$, where $j=1,\ldots,N$, $k=1,\ldots,N$, and $l=1,\ldots,N$. At all the sites, except a fraction of them on the boundary, the potential is determined by the system of Kirchhoff's equations

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

where the sum is taken over the six vectors connecting nearest neighbors:

$$\Delta=\pm\Delta_x=\pm(1,0,0),\quad \Delta=\pm\Delta_y=\pm(0,1,0),$$

$$\Delta=\pm\Delta_z=\pm(0,0,1).$$

In Eq.(1) $\sigma_{\mathbf{r},\mathbf{r}+\Delta}$ is the conductivity between the sites with the coordinates $\mathbf{r}$ and $\mathbf{r}+\Delta$, which assumes the value $\sigma_1=1$ with a probability p ("pure" bonds) and $\sigma_2=h$ with the probability $1-p$ ("defect" bonds). The sites on the two opposite faces of the lattice perpendicular to the x-axis are under constant potentials equal to 0 and 1, respectively. In the directions of y- and z-axes the boundary conditions are periodic, i.e., the sites with $k=1$ and $k=N$ (just as with $l=1$ and $l=N$) are under identical conditions.

The calculations were performed as follows (compare to Ref. 10). At a fixed concentration p a specific configuration was generated, i.e., the fraction $1-p$ of the bonds selected at random were replaced with defect bonds, whose conductivity was $\sigma_2=h$. Then the equation system (1) was solved at given $\sigma_{\mathbf{r},\mathbf{r}+\Delta}$ with the boundary conditions defined above. Concurrently with the main problem, we solved a similar problem about the potentials $\tilde{V}_{\mathbf{r}}$ at sites of the auxiliary lattice that was generated by the transition to the dual lattice in the xy-plane and translation of vertical bonds (see Fig. 1, where the components of the auxiliary lattice are shown by dashed lines). In this case, the potentials on the opposite faces of the lattice perpendicular to the y-axis were defined as zero and unity, and periodic boundary conditions were imposed in the x and z directions. The potentials $\tilde{V}_{\mathbf{r}}$ were used in combinations with $V_{\mathbf{r}}$ to calculate the function φ, which determines the effective Hall coefficient (see Sec. 6).

In calculating parameters of a specific configuration, it is more convenient to present the equation system (1) in the following (quasi-one-dimensional) form:

$$\hat{A}\mathbf{v}=\mathbf{b}. \tag{2}$$

Here $\hat{A}$ is a banded square matrix with dimensions $M\times M$, where $M=(N-1)^2(N-2)$. The vector $\mathbf{b}$ on the right-hand side of Eq. (2) is a column of M elements, of which only $(N-1)^2$ are nonzero, and emerges because Eq. (2) cannot be applied to the sites on the opposite faces perpendicular to the x-axis. The vector $\mathbf{v}$ is a column of M elements composed of unknown potentials $V_{j,k,l}$. These parameters are ordered in the column as follows. The numeration starts at $j=2$, and k runs from 1 to $N-1$, whereas l also runs from 1 to $N-1$, and so on. The numeration ends at $j=N-1$, at which k also runs between 1 and $N-1$, whereas at each k l changes from 1 to $N-1$. As a result, we have the vector

$$\mathbf{v}=(V_{2,1,1},\ldots,V_{2,1,N-1};\quad V_{2,2,1},\ldots,V_{2,2,N-1};\ldots;$$

$$V_{2,N-1,1},\ldots,V_{2,N-1,N-1};\quad V_{3,1,1},\ldots,V_{3,1,N-1};$$

$$V_{3,2,1},\ldots,V_{3,2,N-1};\ldots;$$

$$V_{3,N-1,1},\ldots,V_{3,N-1,N-1};\ldots$$

$$V_{N-1,1,1},\ldots,V_{N-1,1,N-1};\quad V_{N-1,2,1},\ldots,$$

$$V_{N-1,2,N-1};\ldots;\quad V_{N-1,N-1,1},\ldots,V_{N-1,N-1,N-1}).$$

For convenience it is presented in the form of a row. In the auxiliary lattice, the numeration starts at the fixed $k=2$, whereas j runs from 1 to $N-1$ as l varies from 1 to $N-1$ at each j, and so on. In this case the matrix $\tilde{A}$ and vector $\mathbf{v}$ are different from $\hat{A}$ and $\mathbf{v}$, but the equation has the same form as Eq. (2).

The equation system (2) and the similar system for the auxiliary lattice were solved using Chebyshev's technique of polynomial acceleration of the basic iteration method.[11,10] For each configuration, the calculations were performed at six values of the parameter h: $h=10^{-m}$, where $m=1,\ldots,6$. The potentials calculated at a fixed m ($1\leqslant m\leqslant 5$) were used as initial values in the calculation at $m+1$.

In order to check the calculations and estimate their accuracy, we calculated at all stages the total current across each section of the lattice, i.e., the total current in the links perpendicular to the x-axis connecting the planes j and $j+1$, where j is a number ranging between 1 and $N-1$. The iteration process was interrupted when the spread of the integral current in the cross sections was within 0.1%. The resulting potentials $V_{\mathbf{r}}$ (and $\tilde{V}_{\mathbf{r}}$) were used to calculate linear and quadratic parameters of the lattice. In order to reduce the effect of fluctuations in the distribution of defect bonds owing to the finite lattice dimensions, we performed calculations for several random configurations and averaged the characteristics. The uncertainty in the effective parameters was estimated as the rms deviation from the average. The

calculations of the effective characteristics are given in Figs. 2–6,. Outside the critical region, the averaging was performed over twenty configurations, and the spread was within 1%. In studying the critical behavior of the parameters (around the percolation threshold at $p_c \simeq 0.247$), which takes place in the concentration range $0.2 \lesssim p \lesssim 0.3$, we detected large fluctuations of parameters calculated in different configurations (at $h=10^{-5}$, and especially at $h=10^{-6}$). Therefore, the number of configurations in the critical region was increased to twenty, but even under these conditions the spread of the effective parameters was up to 15–25%.

3. LINEAR AND QUADRATIC CHARACTERISTICS

1. Let the average electric field be directed along the x-axis. Then the effective conductivity σ_e of a material to which Ohm's law applies, $\mathbf{j}=\sigma(\mathbf{r})\mathbf{E}$, is defined conventionally:

$$\sigma_e=\langle j_x\rangle/\langle E_x\rangle. \tag{3}$$

Here $\mathbf{j}$ is the current density, $\mathbf{E}$ is the electric field strength, and $\langle \dots \rangle$ denotes averaging over the sample volume V:

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

In this definition $V\to\infty$. The parameters $\langle j_x\rangle$ and $\langle E_x\rangle$ can be expressed in terms of the total current I and potential difference U. As a result, for a cubic sample with an edge length L we have

$$\sigma_e=L^{-1}(I/U), \tag{5}$$

where $L=N-1$ if the bond length equals unity.

In a two-component lattice, the conductivity $\sigma(\mathbf{r})$ may have two constant values σ_1 and σ_2 in the first and second components, respectively. The effective conductivity $\sigma_e=\sigma_e(p;\sigma_1,\sigma_2)$ of this system can be expressed as

$$\sigma_e=\sigma_1 f(p,h), \quad h=\sigma_2/\sigma_1, \tag{6}$$

where p is the concentration (volume fraction) of the first component. The function f—the dimensionless effective conductivity—is a fundamental parameter in the theory of transport in two-component media,[5–8,10] and its calculation is the main goal of the computer simulation.

The parameter σ_e is a response function to an external field characterizing the medium as a whole. One may introduce "partial" response functions ξ_i $(i=1,\dots,n)$ for an n-component material $(n\geqslant 2)$:

$$\langle\mathbf{E}\rangle^{(i)}=\xi_i\langle\mathbf{E}\rangle, \tag{7}$$

where

$$\langle(\dots)\rangle^{(i)}=\frac{1}{V}\int_{V_i}(\dots)d\mathbf{r} \tag{8}$$

means averaging over the volume V_i of the i-th component. The parameters ξ_i are also effective characteristics of a medium when $V\to\infty$ and $V_i\to\infty$.

Since

$$\sum_i \langle\mathbf{E}\rangle^{(i)}=\langle\mathbf{E}\rangle, \tag{9}$$

the parameters ξ_i should obey the sum rule:

$$\sum_i \xi_i=1. \tag{10}$$

The average current density $\langle\mathbf{j}\rangle$ is expressed in terms of ξ_i as follows:

$$\langle\mathbf{j}\rangle=\sum_i \sigma_i\langle\mathbf{E}\rangle^{(i)}=\sum_i \sigma_i\xi_i\langle\mathbf{E}\rangle, \tag{11}$$

hence

$$\sigma_e=\sum_i \sigma_i\xi_i, \tag{12}$$

where σ_i is the conductivity of the i-th component. In the case of a two-component system $(i=1,\ 2)$, the parameters ξ_1 and ξ_2 can be expressed in terms of σ_e. We derive from Eqs. (10) and (12)

$$\xi_1=\frac{\sigma_e-\sigma_2}{\sigma_1-\sigma_2}, \quad \xi_2=\frac{\sigma_1-\sigma_e}{\sigma_1-\sigma_2}, \tag{13}$$

which are identical to the expressions given in Ref. 8. We define σ_e and ξ_i as linear effective characteristics.

2. Various quadratic effective characteristics are also specific response functions. They include the functions ψ_i which determine electric field strength squared averaged over the volume of the i-th component:

$$\langle\mathbf{E}^2\rangle^{(i)}=\psi_i(\langle\mathbf{E}\rangle)^2. \tag{14}$$

It is convenient to introduce the dimensionless electric field strength in the medium:

$$\mathbf{e}(\mathbf{r})=\frac{\mathbf{E}(\mathbf{r})}{|\langle\mathbf{E}\rangle|}. \tag{15}$$

Then the functions ψ_i are expressed in terms of $\mathbf{e}(\mathbf{r})$:

$$\psi_i=\langle\mathbf{e}^2\rangle^{(i)}. \tag{16}$$

In a two-component system, the functions ψ_i are expressed in terms of the dimensionless effective conductivity f[8]:

$$\psi_1=\langle\mathbf{e}^2\rangle^{(1)}=f-hf', \tag{17}$$

$$\psi_2=\langle\mathbf{e}^2\rangle^{(2)}=f', \quad f'\equiv\frac{\partial f(p,h)}{\partial h}. \tag{18}$$

According to Eq. (18), the derivative f' can be numerically calculated without differentiating f. The function f can be expressed in terms of the averaged parameters squared using Eqs. (17) and (18):

$$f=\psi_1+h\psi_2=\langle\mathbf{e}^2\rangle^{(1)}+h\langle\mathbf{e}^2\rangle^{(2)}. \tag{19}$$

Equation (19) also derives from the well-known identity $\langle\mathbf{jE}\rangle=\langle\mathbf{j}\rangle\langle\mathbf{E}\rangle$.

It is known that in a random inhomogeneous medium the simultaneous change of variables $\sigma_1\leftrightarrow\sigma_2$ and $p\to 1-p$ does not change the macroscopic properties of the material hence $\sigma_e(p;\sigma_1,\sigma_2)=\sigma_e(1-p;\sigma_2,\sigma_1)$ and the following relation applies to the function f defined by Eq. (6):

$$f(p,h)=hf(1-p,1/h). \tag{20}$$

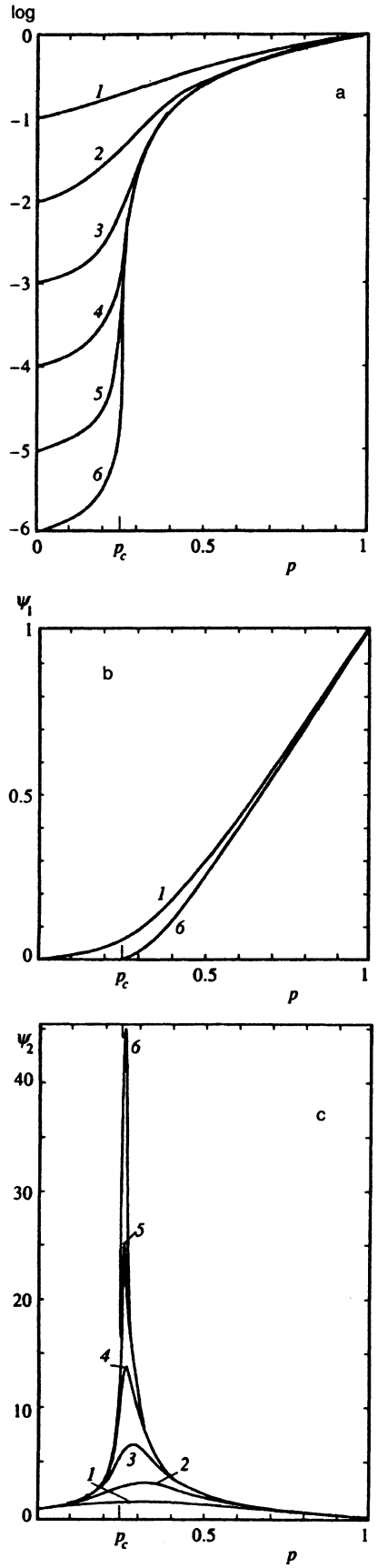

FIG. 2. (a) Common logarithm of the dimensionless effective conductivity, (b) $\psi_1=\langle e^2\rangle^{(1)}=f-hf'$, and (c) $\psi_2=\langle e^2\rangle^{(2)}=f'$ as functions of the concentration p at several values of the parameter h: (1) $h=10^{-1}$; (2) $h=10^{-2}$; (3) $h=10^{-3}$; (4) $h=10^{-4}$; (5) $h=10^{-5}$; (6) $h=10^{-6}$. The critical concentration $p_c=0.247$.

Similarly, we have the following relations for the functions ψ_i:

$$\psi_1(p,h)=\psi_2(1-p,1/h), \quad \psi_2(p,h)=\psi_1(1-p,1/h). \tag{21}$$

The validity of Eq. (21) is proved by substituting Eq. (20) into Eqs. (17) and (18).

In a calculation of lattice parameters, the electric field strength $E_x(\mathbf{r})=E_x(j,\ k,\ l,)$ is defined as a difference between potentials at neighboring sites (along the x-axis):

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

Therefore, we can express the total current as

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

where j is an arbitrary number ranging between 1 and $N-1$. In the problem statement given in the previous section ($\sigma_1=1$, $U=1$), the function f is expressed in terms of the total current as $f=I/(N-1)$, where I is defined by Eq. (23). In the case of a discrete lattice, the functions ψ_i are defined by the equation

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

where the sums are taken over all bonds with the conductivity σ_i and $L=N-1$.

In this work we calculate numerically the function $f(p,h)$ using both Eq. (5) and Eq. (19). The two results coincide within the calculation uncertainty. Figure 2a shows the common logarithm of the dimensionless effective conductivity versus concentration p at six values of the second argument h. Figure 2b shows the parameters ψ_1 and ψ_2 as functions of p at fixed h. Although the functions f, ψ_1 and ψ_2 have been calculated only at $h<1$, they can be easily extrapolated to $h>1$ using Eqs. (20) and (21). Note that at all stages of the calculations Eq. (13) was used as an additional criterion of correctness of results.

4. FUNCTIONS f AND ψ_i IN THE CRITICAL REGION

In a system undergoing the metal–dielectric phase transition, the function f can be expanded, according to the similarity hypothesis, in the critical region ($h\ll 1$, $|\tau|\ll 1$, where $\tau=(p-p_c)/p_c$, p_c is the critical concentration) as follows:[8,10]

$$f\simeq\tau^t\left[A_0+A_1\frac{h}{\tau^{t/s}}+A_2\left(\frac{h}{\tau^{t/s}}\right)^2+\ldots\right], \quad \tau>0,$$
$$\Delta_0\ll\tau\ll 1, \tag{25a}$$

$$f\simeq h^s\left[a_0+a_1\frac{\tau}{h^{s/t}}+a_2\left(\frac{\tau}{h^{s/t}}\right)^2+\ldots\right], \quad |\tau|\ll\Delta_0, \tag{25b}$$

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

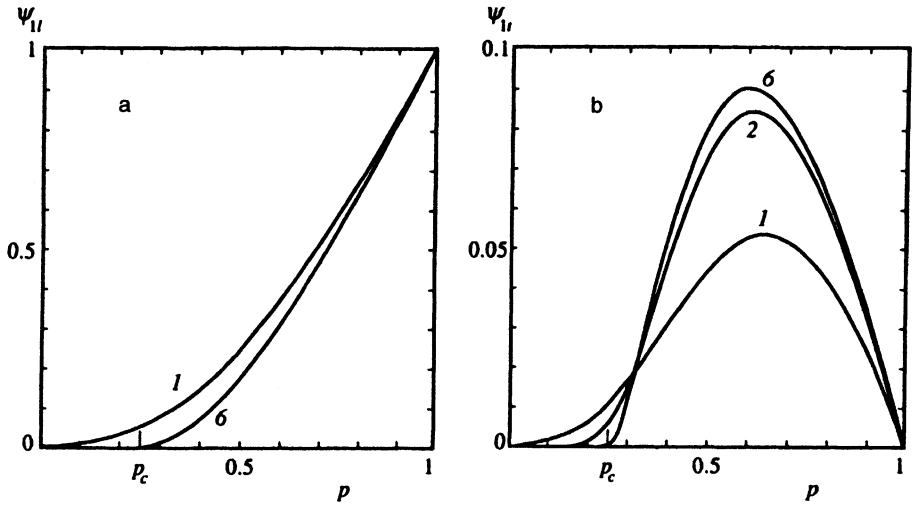

FIG. 3. (a) Longitudinal $\psi_{1l}=\langle e_{\parallel}^2\rangle^{(1)}$ and (b) transverse $\psi_{1l}=\langle e_{\perp}^2\rangle^{(1)}$ functions at several values of h (notations are given in the caption of Fig. 2).

$$q=\frac{t}{s}-t, \tag{26}$$

where

$$\Delta_0=h^{s/t} \tag{27}$$

is the transition width.[12] The critical exponents t, s, and q are related by Eq. (26). The numerical factors A_k, a_k, and B_k are equal to unity within one order of magnitude, and it is obvious that A_0, a_0, and B_1 are positive. As was proved in Ref. 5, $A_1>0$ and $B_2<0$. One can easily prove that $a_1>0$.

The following expansion of the function ψ_1 can be derived from Eqs. (17) and (25):

$$\psi_1\simeq\tau^t\left[A_0-A_2\left(\frac{h}{\tau^{t/s}}\right)^2+\ldots\right], \quad \tau>0, \quad \Delta_0\ll\tau\ll 1, \tag{28a}$$

$$\psi_1\simeq h^s\left[(1-s)a_0+\left(1-s+\frac{s}{t}\right)a_1\frac{\tau}{h^{s/t}}+\ldots\right], \quad |\tau|\ll\Delta_0, \tag{28b}$$

$$\psi_1\simeq -B_2\frac{h^2}{(-\tau)^{2q+t}}+\ldots, \quad \tau<0, \quad \Delta_0\ll|\tau|\ll 1. \tag{28c}$$

Note that, unlike Eq. (25a), the correction in Eq. (28a) is quadratic in the small parameter $h/\tau^{t/s}$. In deriving Eq. (28c) we have taken into account Eq. (26).

The expansion of the function ψ_2 is derived from Eqs. (18) and (25):

$$\psi_2\simeq\frac{1}{\tau^{q'}}\left[A_1+2A_2\frac{h}{\tau^{t/s}}+\ldots\right], \quad \tau>0, \quad \Delta_0\ll\tau\ll 1, \tag{29a}$$

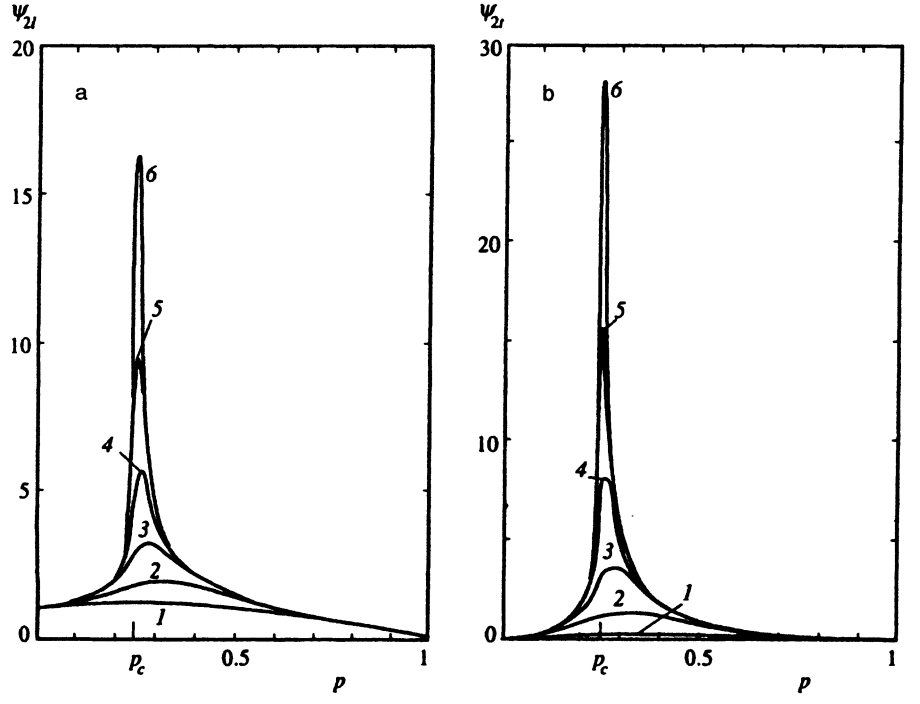

FIG. 4. (a) Longitudinal $\psi_{2l}=\langle e_{\parallel}^2\rangle^{(2)}$ and (b) transverse $\psi_{2l}=\langle e_{\perp}^2\rangle^{(2)}$ functions (notations are given in the caption of Fig. 2).

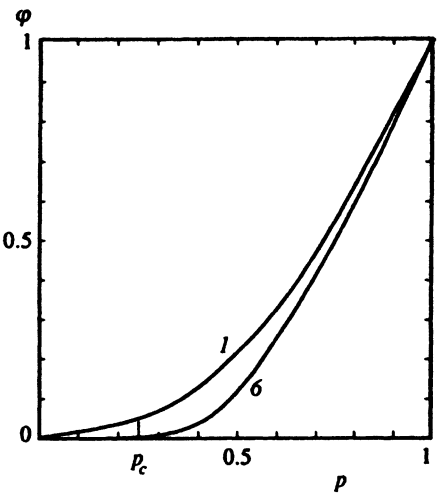

FIG. 5. Function φ calculated by Eq. (41).

$$\psi_2 \simeq \frac{1}{h^{1-s}}\left[sa_0 + s\frac{t-1}{t}a_1\frac{\tau}{h^{s/t}} + \ldots\right], \quad |\tau| \ll \Delta_0, \tag{29b}$$

$$\psi_2 \simeq \frac{1}{(-\tau)^q}\left[B_1 + 2B_2\frac{h}{(-\tau)^{t/s}} + \ldots\right],$$

$$\tau < 0, \quad \Delta_0 \ll |\tau| \ll 1, \tag{29c}$$

$$q' = \frac{t}{s} - t. \tag{30}$$

According to Eq. (29), ψ_2 as a function of the concentration has a sharp peak around $p = p_c$ if $h \ll 1$ (Fig. 2c). If Eqs. (26) and (30) are valid, $q' = q$, i.e., the critical exponents of ψ_2 at $\tau > 0$ and $\tau < 0$ coincide provided that the similarity hypothesis holds. As was noted above, the coefficient a_1 is positive, therefore the maximum of ψ_2 plotted against p is centered at $p > p_c$ (Fig. 2c) and is shifted with respect to the critical point p_c by the value $\sim h^{s/t}$.

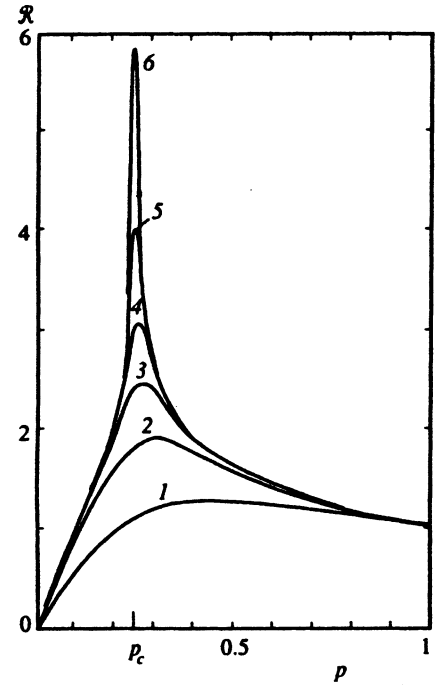

FIG. 6. Function $\mathscr{R}$ calculated by Eq. (43).

Since the functions ψ_1 and ψ_2 are positive by definition, it follows from Eqs. (17) and (18) that

$$f > hf', \quad f' > 0.$$

After substituting this into Eq. (25), we obtain the condition $s < 1$ and the inequalities $A_1 > 0$ and $B_2 < 0$ derived in Ref. 5 from physical considerations.

In processing the results of computer simulation at $p > p_c$ (outside the transition region), it is more convenient to derive the exponent t not from the function f, but ψ_1 because its correction is smaller than that of f owing to the smallness of h [compare Eq. (25a) with Eq. (28a)]. The factor A_0 was determined simultaneously with t. Then the exponent q, as well as the factors A_1 and B_1, can be derived by processing the calculations of ψ_2 using Eqs. (29a) and (29c) (the equality $q' = q$ can be also checked). Finally, the critical exponent s and the factor a_0 can be calculated by three methods, namely, from f, ψ_1, and ψ_2 as functions of h at $p = p_c$. The parameters of the critical region derived from computer simulations are listed in Table I.

5. LONGITUDINAL AND TRANSVERSE QUADRATIC CHARACTERISTICS

Beside the functions ψ_i, it is also interesting to investigate the functions

$$\psi_{il} = \langle \mathbf{e}_\parallel^2 \rangle^{(i)}, \quad \psi_{it} = \langle \mathbf{e}_\perp^2 \rangle^{(i)} \quad (i = 1, 2), \tag{31}$$

where $\mathbf{e}_\parallel$ and $\mathbf{e}_\perp$ are the components of the vector $\mathbf{e}$ defined by Eq. (15) and oriented parallel and perpendicular to the average electric field $\langle \mathbf{E} \rangle$, where $\langle \ldots \rangle^{(i)}$ has the same sense as in Eq. (8). The functions in Eq. (31) are related to ψ_i in Eq. (16) by an obvious equation

$$\psi_i = \psi_{il} + \psi_{it}. \tag{32}$$

In the case of a discrete lattice (problem statement in Sec. 2), the function ψ_{il} is defined by the first sum in Eq. (24), and ψ_{it} by the other two sums.

In the case of a random inhomogeneous medium, we have relations similar to Eq. (21) (see, for example, Sec. 7):

$$\psi_{1l}(p,h) = \psi_{2l}(1-p,1/h), \quad \psi_{1t}(p,h) = \psi_{2t}(1-p,1/h), \tag{33}$$

and two more relations derived from Eq. (33) by exchanging the indices $1 \rightleftarrows 2$. Equation (33) allows us to determine the functions $\psi_{il}(p,h)$ and $\psi_{it}(p,h)$ at $h > 1$ if their values at $h < 1$ are known.

No relations like Eqs. (17) and (18) are known for the functions ψ_{il} and ψ_{it}, but their basic properties can be derived from Eqs. (31) and (32). The shape of ψ_{1l} (for $h < 1$) can be seen in Fig. 3a, which shows ψ_{1l} as a function of concentration p at two values of the other argument, $h = 10^{-1}$ and $h = 10^{-6}$. Note that the shape of the longitudinal function ψ_{1l} is almost identical to that of ψ_1, as well as its amplitude. The shape of the transverse function ψ_{1t} (Fig. 3b) is similar to those of ψ_{1l} and ψ_1 at $p \lesssim 0.4$, but is very different in the interval $0.4 \lesssim p \lesssim 1$ and turns to zero at

TABLE I. Summary table of parameters in the critical region.

$p>p_c$		
ψ_1	ψ_{1l}	ψ_{1t}
$t=2.0\pm0.2$ $A_0=0.4\pm0.2$	$t_{1l}=2.1\pm0.2$ $A_{0l}^{(1)}=0.2\pm0.1$	$t_{1t}=1.9\pm0.2$ $A_{0t}^{(1)}=0.2\pm0.1$
ψ_2	ψ_{2l}	ψ_{2t}
$q=0.8\pm0.2$ $A_1=3.0\pm0.9$	$q_{2l}=0.7\pm0.1$ $A_{1l}^{(2)}=1.5\pm0.4$	$q_{2t}=0.8\pm0.3$ $A_{1t}^{(2)}=1.7\pm1.0$
	φ	$\mathscr{R}$
	$l=3.7\pm0.4$ $C=0.3\pm0.3$	$g=0.3\pm0.1$ $W=1.7\pm0.3$
$p=p_c$		
ψ_1	ψ_{1l}	ψ_{1t}
$s=0.7\pm0.1$ $(1-s)a_0=0.3\pm0.2$	$s_{1l}=0.8\pm0.1$ $a_{0l}^{(1)}=0.2\pm0.1$	$s_{1t}=0.7\pm0.1$ $a_{0t}^{(1)}=0.1\pm0.1$
ψ_2	ψ_{2l}	ψ_{2t}
$1-s=0.28\pm0.01$ $sa_0=0.8\pm0.1$	$\lambda_{2l}=0.23\pm0.04$ $a_{0l}^{(2)}=0.6\pm0.2$	$\lambda_{2t}=0.29\pm0.05$ $a_{0t}^{(2)}=0.4\pm0.2$
f	φ	$\mathscr{R}$
$s=0.71\pm0.03$ $a_0=1.1\pm0.2$	$u=1.3\pm0.1$ $c_0=1.4\pm0.7$	$k=0.10\pm0.06$ $w=1.2\pm0.6$
$p<p_c$		
ψ_1	ψ_{1l}	ψ_{1t}
$2q+t=3.6\pm1.1$ $B_2=-1.8\pm1.7$	$2q_{1l}+t_{1l}=3.6\pm1.1$ $B_{2l}^{(1)}=0.9\pm0.8$	$2q_{1t}+t_{1t}=3.6\pm1.1$ $B_{2t}^{(1)}=1.0\pm1.0$
ψ_2	ψ_{2l}	ψ_{2t}
$q=0.8\pm0.2$ $B_1=0.9\pm0.4$	$q_{2l}=0.6\pm0.2$ $B_{1l}^{(2)}=0.7\pm0.5$	$q_{2t}=0.8\pm0.2$ $B_{1t}^{(2)}=0.5\pm0.2$
	φ	$\mathscr{R}$
	$r=1.7\pm0.2$ $D=1.5\pm0.8$	$g=0.3\pm0.2$ $S=1.3\pm0.6$

Note. The first column lists parameters of f, ψ_1, and ψ_2; the second lists parameters of the longitudinal characteristics ψ_{1l} and ψ_{2l}, and the function φ; the third column shows parameters of ψ_{1t} and ψ_{2t}, and the function $\mathscr{R}$.

$p=1$. The drop of this function to zero at $p\to1$ is quite natural because in a homogeneous medium the transverse component of the electric field should be zero. Finally, the shapes of the functions ψ_{2l} and ψ_{2t}, which are similar to that of ψ_2, are shown in Fig. 4.

The critical behavior of the functions ψ_{1l} in system undergoing the metal–dielectric transition can be described similarly to Eq. (28) (only the expansion terms of the lowest order are given):

$$\psi_{1l}\simeq A_{0l}^{(1)}\tau^{t_{1l}},\quad \tau>0,\quad \Delta_{1l}\ll\tau\ll1, \tag{34a}$$

$$\psi_{1l}\simeq a_{0l}^{(1)}h^{s_{1l}},\quad |\tau|\ll\Delta_{1l}, \tag{34b}$$

$$\psi_{1l}\simeq B_{2l}^{(1)}\frac{h^2}{(-\tau)^{2q_{1l}+t_{1l}}},\quad \tau<0,\quad \Delta_{1l}\ll|\tau|\ll1, \tag{34c}$$

$$q_{1l}=\frac{t_{1l}}{s_{1l}}-t_{1l}. \tag{35}$$

Here $\Delta_{1l}=h^{s_{1l}/t_{1l}}$ is the peak width of the function ψ_{1l}. According to the similarity hypothesis,[12,13] all critical phenomena at zero magnetic field are characterized by one scale, therefore the value of Δ_{1l} should be comparable to Δ_0 in Eq. (27) (compare to the discussion in Ref. 8). Hence, follows the second relations among the introduced critical exponents:

$$s_{1l}/t_{1l}=s/t. \tag{36}$$

Since both ψ_{1l} and ψ_{1t} are positive, it follows from Eq. (32) that ψ_{1l} cannot decay more slowly or increase faster than ψ_1. From this condition we derive the limitations on the respective exponents:

$$t_{1l}\geqslant t,\quad s_{1l}\geqslant s,\quad 2q_{1l}+t_{1l}\leqslant 2q+t.$$

The critical behavior of the function ψ_{1t} is described identically. The same limitations and relations apply to ψ_{1t} as to ψ_{1l}, only the label l is substituted by t.

The behavior of the function ψ_{2l} in the critical region can be described similarly to Eq. (29) (here we also give only the expansion terms of the lowest order):

$$\psi_{2l}\simeq A_{1l}^{(2)}/\tau^{q_{2l}},\quad \tau>0,\quad \Delta_0\ll\tau\ll1, \tag{37a}$$

$$\psi_{2l}\simeq a_{0l}^{(2)}/h^{\lambda_{2l}},\quad |\tau|\ll\Delta_0 0, \tag{37b}$$

$$\psi_{2l}\simeq B_{1l}^{(2)}/(-\tau)^{q_{2l}},\quad \tau<0,\quad \Delta_0\ll|\tau|\ll1, \tag{37c}$$

$$\lambda_{2l}/q_{2l}=s/t. \tag{38}$$

Equation (38) derives from the condition $\Delta_{2l}\sim\Delta_0$, where $\Delta_{2l}=h^{\lambda_{2l}/q_{2l}}$ is the peak width of the function ψ_{2l}. Since the singularity of ψ_{2l} cannot be of a higher order than that of ψ_2, the following conditions should be satisfied:

$$q_{2l}\leqslant q,\quad \lambda_{2l}\leqslant 1-s.$$

In the critical region, the same relations and conditions apply to ψ_{2t} as to ψ_{2l}, only the label l is substituted by t.

Thus only one new critical exponent is needed to describe the critical behavior of the functions ψ_{1l}, ψ_{1t}, ψ_{2l}, and ψ_{2t}, and the complete set of critical exponents can be composed of t_{1l}, t_{1t}, q_{2l}, and q_{2t}. The rest of the critical exponents can be expressed as

$$s_{1l}=\frac{s}{t}t_{1l},\quad q_{1l}=\frac{t}{s}-t_{1l},$$

$$s_{1t}=\frac{s}{t}t_{1t},\quad q_{1t}=\frac{t}{s}-t_{1t},$$

$$\lambda_{2l}=\frac{s}{t}q_{2l},\quad \lambda_{2t}=\frac{s}{t}q_{2t}.$$

The parameters derived by processing computer simulations of the functions ψ_{il} and ψ_{it} in the critical region are listed in Table I.

6. HALL COEFFICIENT

The conductivity of an isotropic material in the magnetic field **H** is described by the tensor

$$\hat{\sigma}=\begin{pmatrix} \sigma_x & \sigma_a & 0 \\ -\sigma_a & \sigma_x & 0 \\ 0 & 0 & \sigma_z \end{pmatrix}, \tag{39}$$

in which we use the notations of Ref. 8. In a weak magnetic field ($H\to 0$) the Hall component σ_a is linear in H. In this approximation the Hall component of the effective conductivity tensor can be expressed as

$$\sigma_{ae}=\sigma_{a2}+(\sigma_{a1}-\sigma_{a2})\varphi(p,h), \tag{40}$$

where the galvanomagnetic parameters of the components are given in the explicit form. The function $\varphi(p,h)$ in Eq. (40) is determined by the medium properties at $\mathbf{H}=0$. In a randomly disordered system, the function φ satisfies the following condition (see the next section):

$$\varphi(p,h)+\varphi(1-p,1/h)=1,$$

hence the function $\varphi(p,h)$ can be determined at $h>1$ if it is known at $h<1$.

Let us denote the electric field in the medium determined in solving the conductivity problem at $\mathbf{H}=0$ for a given electric field $\langle\mathbf{E}^{(\nu)}\rangle$ as $\mathbf{E}^{(\nu)}(\mathbf{r})$, where the superscript ν denotes that the average field is aligned with the axis ν. The function $\varphi(p,h)$ can be expressed in terms of the electric field $\mathbf{E}^{(\nu)}(\mathbf{r})$ as follows:[8,9]

$$\varphi(p,h)=\frac{\langle E_x^{(x)}E_y^{(y)}-E_y^{(x)}E_x^{(y)}\rangle^{(1)}}{\langle E_x^{(x)}\rangle\langle E_y^{(y)}\rangle}. \tag{41}$$

In this paper $\mathbf{E}^{(x)}(\mathbf{r})$ in Eq. (41) is the field in the basic lattice, and $\mathbf{E}^{(y)}(\mathbf{r})$ is the field calculated in the auxiliary lattice (see Section 2). The field strength $\mathbf{E}^{(x)}(\mathbf{r})$ and $\mathbf{E}^{(y)}(\mathbf{r})$ are expressed in terms of the potentials $V_{\mathbf{r}}$ and $\tilde{\mathbf{V}}_{\mathbf{r}}$ by equations like Eq. (22). The result of the computer simulation is shown in Fig. 5, where $\varphi(p,h)$ is plotted against concentration p at two values of h.

The following expression for the effective Hall coefficient $R_e=H^{-1}\sigma_{ae}/\sigma_e^2$ has been derived from Eq. (40):[8,9]

$$R_e=\frac{h^2R_2}{f^2}+(R_1-h^2R_2)\mathscr{R}, \tag{42}$$

$$\mathscr{R}(p,h)=\varphi(p,h)/f^2(p,h), \tag{43}$$

where R_i is the Hall coefficient for the ith component ($i=1,\ 2$) and f is defined by Eq. (6). We should stress that in the approximation linear in **H** Eq. (42) is exact and its parameters are arbitrary. Figure 6 shows $\mathscr{R}$ as a function of concentration p at six values of h varying from 10^{-1} to 10^{-6}.

In a system undergoing the metal–dielectric transition, the functions φ and $\mathscr{R}$ in the critical region ($|\tau|\ll 1$, $h\ll 1$) are given by the following expressions derived from the similarity hypothesis[8,9]:

$$\varphi\simeq C\tau^{\,l},\quad \mathscr{R}\simeq W\tau^{-g},\quad \tau>0,\quad \Delta_0\ll\tau\ll 1, \tag{44a}$$

$$\varphi\simeq c_0h^u,\quad \mathscr{R}\simeq wh^{-k},\quad |\tau|\ll\Delta_0, \tag{44b}$$

$$\varphi\simeq D\frac{h^2}{(-\tau)^r},\quad \mathscr{R}\simeq S\frac{1}{(-\tau)^g},\quad \tau<0,\quad \Delta_0\ll|\tau|\ll 1. \tag{44c}$$

In order to characterize the function φ, we have introduced a new critical exponent labeled by l in addition to those of the function f. The other two exponents can be expressed in terms of l, t, and q[8,9]:

$$r=2(t+q)-l,\quad u=l/(t+q). \tag{45}$$

Hence, the exponents g and k are expressed as

$$g=2t-l=r-2q,\quad k=2s-u=gl/(t+q). \tag{46}$$

The equality of the critical exponents of the function $\mathscr{R}$ above ($\tau>0$, $\Delta_0\ll\tau\ll 1$) and below ($\tau<0$, $\Delta_0\ll|\tau|\ll 1$) the transition point derives from the first relation in Eq. (45). Equations (44) provide a comprehensive description (in the sense of the similarity hypothesis) of the critical behavior of the parameters σ_{ae} and R_e in the approximation linear in **H**. The parameters obtained by processing results of computer simulations of the functions φ and $\mathscr{R}$ in the critical region are listed in Table I.

7. MAGNETORESISTANCE

Under a weak magnetic field ($\mathbf{H}\to 0$), the corrections to the diagonal components of the conductivity tensor, σ_{xi} and σ_{zi}, are quadratic in **H**:

$$\sigma_{xi}=\sigma_i+\gamma_{xi},\quad \sigma_{zi}=\sigma_i+\gamma_{zi}(\gamma\propto H^2). \tag{47}$$

Here σ_i is the i-th component of conductivity at $\mathbf{H}=0$. Let us express the effective parameters σ_{xe} and σ_{ze} in the form similar to Eq. (47):

$$\sigma_{xe}=\sigma_e+\gamma_{xe},\quad \sigma_{ze}=\sigma_e+\gamma_{ze}, \tag{48}$$

where σ_e is the same as in Eq. (6). For a two-component system in the approximation quadratic in **H**, we have the following expressions for γ_{xe} and γ_{ze}:[8]

$$\gamma_{xe}=\gamma_{x1}\psi_x^{(1)}+\gamma_{z1}\psi_x^{(2)}+\gamma_{x2}\psi_x^{(3)}+\gamma_{z2}\psi_x^{(4)}+\frac{(\sigma_{a1}-\sigma_{a2})^2}{\sigma_1}\chi_x, \tag{49}$$

$$\gamma_{ze}=\gamma_{x1}\psi_z^{(1)}+\gamma_{z1}\psi_z^{(2)}+\gamma_{x2}\psi_z^{(3)}+\gamma_{z2}\psi_z^{(4)}+\frac{(\sigma_{a1}-\sigma_{a2})^2}{\sigma_1}\chi_z. \tag{50}$$

The factors $\psi_x^{(k)}$ $\psi_z^{(k)}$ χ_x, and χ_z are determined by the properties of the material at $\mathbf{H}=0$ and are the functions of the parameters p and h.

The factors $\psi_x^{(k)}$ and $\psi_z^{(k)}$ can be expressed in terms of the longitudinal and transverse functions introduced in Sec. 5:[8]

$$\psi_x^{(1)}=\psi_{1l}+\frac{1}{2}\psi_{1t},\quad \psi_x^{(2)}=\frac{1}{2}\psi_{1t},$$

$$\psi_x^{(3)}=\psi_{2l}+\frac{1}{2}\psi_{2t},\quad \psi_x^{(4)}=\frac{1}{2}\psi_{2t}, \tag{51}$$

$$\psi_z^{(1)}=\psi_{1t},\quad \psi_z^{(2)}=\psi_{1l},\quad \psi_z^{(3)}=\psi_{2t},\quad \psi_z^{(4)}=\psi_{2l}. \tag{52}$$

The properties of the functions ψ_{il} and ψ_{it} (in particular, their critical behavior) were discussed in detail in Sec. 5. The results of Sec. 5 can be directly applied to the functions $\psi_x^{(k)}$ and $\psi_z^{(k)}$, taking into account Eqs. (51) and (52).

The functions χ_x and χ_z are expressed in terms of the electric field strength at $\mathbf{H}=0$ in the medium in a more complex form,[8] therefore their determination may be a subject of a dedicated study. In this paper we only note that the shapes of the curves of χ_x and χ_z versus p (at fixed h) are similar to those of $\psi_{1t}(p)$ (compare to the results for the two-dimensional system).[8,10] Hence, their critical behavior can be described similarly to that of ψ_{1t}, although each new function demands a new critical exponent.

In a random inhomogeneous medium the simultaneous substitutions $p\to 1-p$ and $\hat{\sigma}_1 \rightleftarrows \hat{\sigma}_2$ do not change its macroscopic properties:

$$\hat{\sigma}_e(p;\hat{\sigma}_1,\hat{\sigma}_2)=\hat{\sigma}_e(1-p;\hat{\sigma}_2,\hat{\sigma}_1). \tag{53}$$

Hence, follow Eq. (20) in the approximation of zeroth order in $\mathbf{H}$, the expression for φ from the previous section in the linear approximation, and Eqs. (33) and the relations for χ_x and χ_z in the quadratic approximation with due account of Eqs. (47)–(52):

$$\chi_x(p,h)=\frac{1}{h}\chi_x\left(1-p,\frac{1}{h}\right),\quad \chi_z(p,h)=\frac{1}{h}\chi_z\left(1-p,\frac{1}{h}\right). \tag{54}$$

Using these relations, the functions $\chi_x(p,h)$ and $\chi_z(p,h)$ can be calculated at $h>1$ if they are known at $h<1$.

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