MAGNETOCONDUCTANCE IN QUANTUM PERCOLATION*

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Quantum percolation problem on 3D simple cubic lattice under influence of external magnetic field is discussed. Results of numerical simulations of magnetoconductance and its dependence on both the system size (temperature) and the concentration of metallic component p are presented. Qualitative agreement with theory for metals is obtained for large p, when the system is delocalized. For small p, when the system is localized, the agreement with weak localization theory predictions is successfully verified as well.

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1. Introduction

Electron motion may occur without diffusion, first time suggested by Anderson [1], which takes place under some circumstances causing localization of electron waves which in turn manifests itself in vanishing electrical conductivity at temperature $T = 0$ K. Nevertheless the electron transport is still possible in localized systems and is experimentally often observed in weak localization region [2], in which localization length is large enough as compared with relevant length scales. According to one parameter scaling theory of localization [3] electron in noninteracting disordered systems of one and two dimensions (1D and 2D) is always localized for every strength of the disorder. In three dimensional system (3D) there exists a transition point, which separates localized states region from delocalized one. In the latter the electron waves can spread out over the whole system resulting in metallic behavior (large conductivity) and thus this transition is called metal–insulator or

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Anderson transition. Both the energy and disorder can drive the transition around critical point.

At sufficiently low temperatures electron can travel coherently over long distance. This may lead to constructive interference which manifests in backscattering effect. It is observed experimentally as negative temperature correction to the conductivity. External magnetic field B destroys the latter contributing in that way to positive magnetoconductivity $\Delta\sigma(B)$. The formula for $\Delta\sigma(B)$ in 3D originally given by Kawabata [4,5] predicts for weak magnetic field the behavior $\Delta\sigma(B) \propto B^2$ and $\Delta\sigma(B) \propto B^{1/2}$ for strong magnetic field. It is often used to fit experimental data in low temperatures and weak magnetic field to extract relevant time scales of the system being considered. In general, scattering processes that concern spin, spin–orbit and e–e interactions obscure weak localization. In contrast to weak localization, magnetoconductivity in metallic systems is negative and for small B follows Kohler's rule [6], $\Delta\sigma(B) \propto -B^2$.

The aim of this paper is to present new results concerning the influence of the magnetic field on the quantum conductance in 3D percolation model. The motivation for this work is twofold. First, we seek a model with quantum effects which could explain experimentally observed very small magnetoconductance in real metal–insulator nanocomposities like RuO_2-glass thick films [7]. Second, is a desire to report on studies, being the result of systematic development, our earlier works concerning electrical properties of disordered systems near the metal–insulator transition in the framework of quantum percolation. We present here the influence of temperature and magnetic field on quantum conductance in percolation model in both weak localization (small p) and metallic (p close to 1) regimes. This opens an interesting question about the role of volume fraction of metallic component in metal–insulator nanocomposities with respect to temperature behavior of magnetoconductance.

The paper is organized as follows. Model and description of numerical procedure are described in the following section. Then results obtained from numerical simulations are presented in Section 3. Finally Section 4 includes conclusions.

2. Model and numerical approach

We consider 3D site-percolation problem on a simple cubic lattice described by tight-binding one-electron Hamiltonian with diagonal disorder of the form

$$\boldsymbol{H} = \boldsymbol{H}_0 + \boldsymbol{V} = \sum_{\boldsymbol{n}} |\boldsymbol{n}\rangle \varepsilon_{\boldsymbol{n}} \langle \boldsymbol{n}| + \sum_{\boldsymbol{n},\boldsymbol{m}} |\boldsymbol{n}\rangle V_{\boldsymbol{nm}} \langle \boldsymbol{m}| . \tag{1}$$

The transfer energy $V_{\boldsymbol{nm}}$ vanishes unless $\boldsymbol{n}$, $\boldsymbol{m}$ are nearest neighbors. In quantum percolation model the onsite energy has a binary probability distribution

$$P(\varepsilon_{\boldsymbol{n}}) = p\delta(\varepsilon_{\boldsymbol{n}} - \varepsilon_A) + (1-p)\,\delta(\varepsilon_{\boldsymbol{n}} - \varepsilon_B)$$

where $\varepsilon_A = 0$ and $\varepsilon_B = \infty$ and p $(1-p)$ is the concentration of metallic (insulating) component.

The homogeneous magnetic field B applied in the direction z is introduced into the Hamiltonian by modification of the hopping elements which acquire phase factors [8]. Namely,

$$V_{\boldsymbol{nm}} = t\,\exp\left(-\frac{2\pi i}{\phi_0}\int\limits_{\boldsymbol{n}}^{\boldsymbol{m}} \boldsymbol{A}\cdot d\boldsymbol{l}\right),$$

where t is taken to be unit of energy, $\boldsymbol{A}$ is vector potential in Landau gauge, $A = (0, Bx, 0)$, x is the direction of current flow $\boldsymbol{l}$ is the path between sites $\boldsymbol{m}$ and $\boldsymbol{n}$ on which the electron is exposed to the magnetic field, and ϕ_0 is the quantum flux. Recalling that $V_{\boldsymbol{nm}} \neq 0$ only for $\boldsymbol{m}$ and $\boldsymbol{n}$ being nearest neighbors, one arrives at $V_{\boldsymbol{nm}} = t\exp(\pm 2\pi i\alpha x)$, where $\alpha = Ba^2/\phi_0$ is the fraction of quantum flux per unit cell, and $a \equiv 1$ is lattice spacing.

In order to calculate dimensionless conductance g we attach two perfect leads to the opposite sides of the sample. g is then evaluated using multichannel Büttiker–Landauer formula [9]

$$g \equiv \frac{G}{e^2/h} = 4\left(\sum_{i=1}^{N_0} T_i\right)\left(\sum_{i=1}^{N_0} v_i^{-1}\right)\left(\sum_{i=1}^{N_0}(1+R_i-T_i)\,v_i^{-1}\right)^{-1}, \qquad (2)$$

where summations are over all N_0 propagating quantum-mechanical channels in the leads. This number is determined as the number of real solutions of the dispersion relation in the leads, $E = 2t\sum\limits_{j=x,y,z}\cos(k_j a)$, where k_j is the component of wave vector $\boldsymbol{k}$ in j direction. At a given channel i, the velocity v_i is calculated as $v_i \equiv \frac{\partial E}{\partial k_x}\Big|_{k_x = k_x(i)} = -2t\sin(k_x(i)\,a)$, where $k_x(i)$ is a real solution of the dispersion relation. Transmission and reflection probabilities T_i and R_i are calculated from the Fisher–Lee relations [10]

$$T_i = \sum_{j=1}^{N_0} v_i v_j \left|\boldsymbol{G}_{ij}(R,L)\right|^2, \quad R_i = \sum_{j=1}^{N_0}\left|i\sqrt{v_i v_j}\boldsymbol{G}_{ij}(L,L) - \delta_{ij}\right|^2,$$

where $\boldsymbol{G}_{ij}(r', r)$ is the one particle retarded Green's function (matrix) between the source at the position r in channel j and the destination r' in

channel i. In fact, R and L denotes blocks of the full Green's matrix related to sites in right (outgoing) and left (incoming) leads, respectively. Dyson equation in the form $\boldsymbol{G} = (\boldsymbol{I} - \boldsymbol{G}_0\boldsymbol{V})^{-1}\,\boldsymbol{G}_0$ is used to evaluate the Green's function, where $\boldsymbol{G}_0 = (E\boldsymbol{I} - \boldsymbol{H}_0)^{-1}$ is the resolvent of the unperturbed system, which is convenient to be evaluated analytically.

It should be mentioned at this point that in this approach the electron is restricted to be scattered elastically everywhere inside the model. It looses its phase information only as it enters the leads. The latter are a distance L away, which in that way becomes a phase coherence length L_ϕ — the distance over which the electron keeps its phase. Since L_ϕ is known to be a strong function of temperature, $L_\phi \propto T^{-\gamma}$, where the exponent γ is of the order of unity and characterizes the dominant scattering mechanism, varying the size of the model corresponds to changes in temperature.

Quantum conductance needs to be averaged over the number of realizations of the system since it is the random variable. Therefore 1000 realizations of the system with randomly distributed scattering centers were generated for every set of parameter like magnetic field B, concentration p, and size of the model L.

3. Results

Results of numerical simulations performed at fixed energy of electron $E = 0.5$ for magnetic flux α from 0.001 up to 0.5 and for sizes L of the system from 3 up to 12 are depicted in Fig. 1. The concentration p changes from 0.4 up to 0.9. Such range of p was chosen in order to cover both regimes of localized states, for $p < p_{\mathrm{q}} \cong 0.44$ and of delocalized states for $p > p_{\mathrm{q}}$, where p_{q} is the quantum percolation threshold [11]. For extreme values of concentration (Figs 1(b) and 1(c)) where magnetoconductance Δg keeps its sign, and hence log–log scale is possible to use, additional lines marked asymptotic behavior predicted by theories are added as a reference. Furthermore, arrows denoted by T point the tendency while temperature increases. It can be seen from Fig. 1(a) that for $p = 0.4 < p_{\mathrm{q}}$ magnetoconductance Δg is positive and in the low field limit it follows the relation $\Delta g \propto B^2$ whereas for larger magnetic flux it tends to $\Delta g \propto B^{1/2}$. The apparent behavior is in accordance with weak localization theory. In contrast to that, magnetoconductance is negative for high concentration of metallic phase (see Fig. 1(d)), $p = 0.9$, and it follows Kohler's rule $\Delta g \propto -B^2$ at least for small B. It may be expected that for intermediate values of p behavior of Δg would be superposition of the above two. Indeed, for $p = 0.6$ (Fig. 1(b)) and $p = 0.7$ (Fig. 1(c)) the magnetoconductance changes its sign when magnetic flux increases. The value of α at which this change takes place depends on p. Namely, the larger p the smaller α at which Δg changes its sign. In these

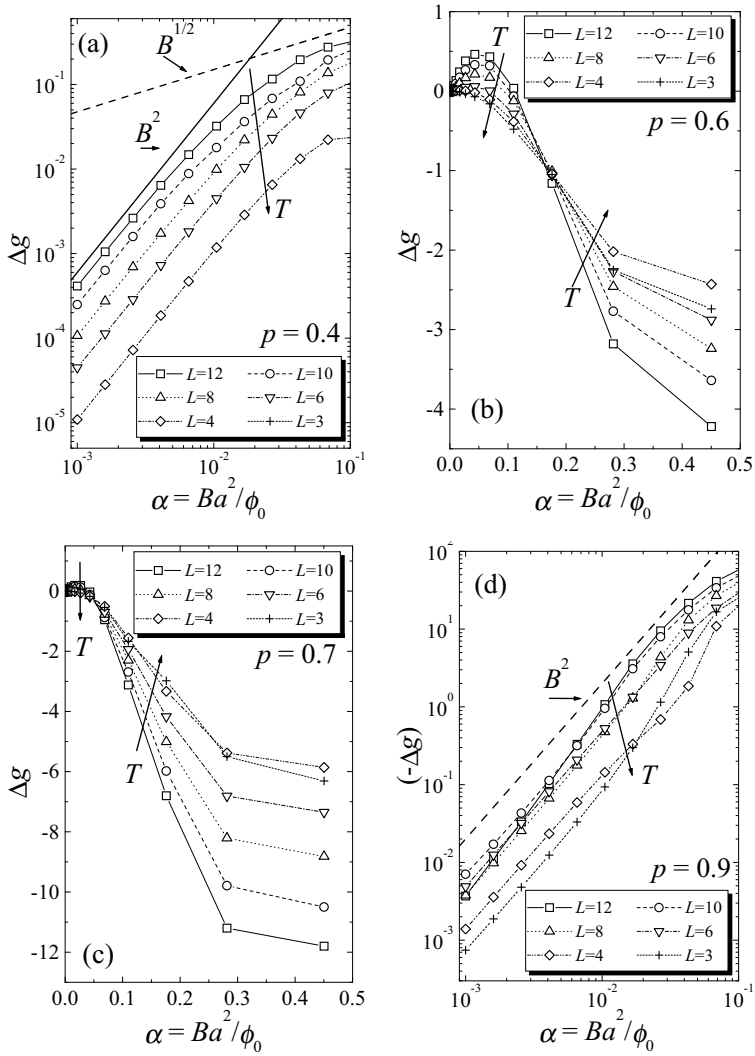

Fig. 1. Magnetoconductance Δg versus magnetic flux α for various content of metallic phase: (a) $p = 0.4$, (b) $p = 0.6$, (c) $p = 0.7$, (d) $p = 0.9$. Series for different sizes L of the system are shown. Lines marked as being proportional to B^2 and $B^{1/2}$ are included as a reference. Arrows point tendency when temperature T increases. Magnetoconductance is positive for $p = 0.4$ (Fig. 1(a)) and negative for $p = 0.9$ (Fig. 1(d)) in studied span of magnetic flux. It changes its sign for intermediate values of concentration p (Figs 1(b) and 1(c)) hence the scales are linear in these cases. Lines connecting points are added to guide an eye.

two cases (Figs 1(b) and 1(c)) localized-like behavior is observed for small α whereas for large α metallic-like behavior is dominated. Such behavior manifests due to the fact that magnetic field destroys constructive interference and because of that localization disappears as well.

4. Conclusions

We have shown that quantum-percolation model gives result in accordance to weak localization theory. Namely for small values of metallic phase content, the relation $\Delta\sigma \propto B^2$ and $\Delta\sigma \propto B^{1/2}$ hold for small and large B, respectively. On the other hand for high metal concentration, $p \approx 1$, magnetoconductance follows Kohler's rule, $\Delta\sigma \propto -B^2$.

As it was mentioned earlier, the larger L the smaller the temperature (Fig. 1). Therefore it is interesting to find size dependence of magnetoconductance. Fig. 2 presents Δg versus L for $p = 0.4$ (a) and $p = 0.6$ (b) depicted for various (but small) magnetic fluxes. The strength of this relationship is expressed as a slope of linear approximation in log–log scale for $\alpha = 0.001$. Note that this value of α was chosen in order to illustrate behavior of the system in weakly localized regime. We get the slope of 3.3 for $p = 0.4$ and 4.4 for $p = 0.6$. These values bring us up to on interesting conclusion. Provided that for both concentrations the exponent in L_ϕ on T

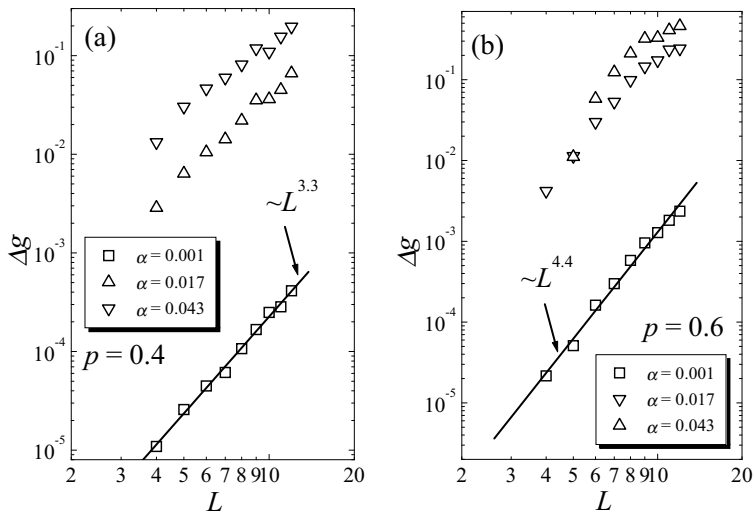

Fig. 2. Magnetoconductance Δg versus system size L for different content of metallic phase: (a) $p = 0.4$, (b) $p = 0.6$. Results for various magnetic fluxes α are shown. Data for $\alpha = 0.001$ (weak magnetic field) are fitted by the straight line. The slopes of the fitting lines are: 3.3 for $p = 0.4$, 4.4 for $p = 0.6$.

dependence is kept the same, we conclude that for smaller p the influence of temperature on magnetoconductance is weaker. It may be useful in practical applications since it points out the direction in development of temperature and/or magnetic field sensors based on highly disordered materials.

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REFERENCES

[1] P.W. Anderson, *Phys. Rev.* **109**, 1492 (1958).

[2] B. Kramer, A. MacKinnon, *Rep. Prog. Phys.* **56**, 1469 (1993).

[3] E. Abrahams, P.W. Anderson, D.C. Licciardello, T.V. Ramakrishnan, *Phys. Rev. Lett.* **42**, 673 (1979).

[4] A. Kawabata, *Solid State Commun.* **34**, 431 (1980).

[5] D.V. Baxter, R. Richter, M.L. Trudeau, R.W. Cochrane, J.O. Strom-Olsen, *J. Phys. I* **50**, 1673 (1989).

[6] N.W. Ashcroft, N.D. Mermin, *Solid State Physics*, Holt, Rinehart and Winston, 1976.

[7] A. Kusy *et al., Ann. Phys.* **8**, 589 (1999).

[8] S. Datta, *Introduction to Mesoscopic Physics*, Cambridge University Press, 1995; M.J. McLennan, Lee Yong, S. Datta, *Phys. Rev.* **B43**, 13846 (1991).

[9] M. Buttiker, Y. Imry, R. Landauer, S. Pinhas, *Phys. Rev.* **B31**, 6207 (1985).

[10] D.S. Fisher, P.A. Lee, *Phys. Rev.* **B23**, 6851 (1981).

[11] C.M. Soukoulis, E.N. Economou, G.S. Grest, *Phys. Rev.* **B36**, 8679 (1987); C.M. Soukoulis, Li Qiming , G.S. Grest, *Phys. Rev.* **B45**, 7724 (1992).