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Physica A 241 (1997) 403–408

PHYSICA A

Quantum percolation in electronic transport of metal–insulator systems: numerical studies of conductance

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Abstract

The quantum site-percolation problem defined by a tight-binding one-electron Hamiltonian on regular simple cubic lattice with binary probability distribution of site energies $P(\varepsilon_{\mathbf{n}}) = p\delta(\varepsilon_{\mathbf{n}}) + (1-p)\delta(\varepsilon_{\mathbf{n}} - \infty)$ is studied using the Landauer–Büttiker formalism and Green's function method. The dimensionless conductance g according to Landauer–Büttiker formula is calculated for a finite system of size $L \times L \times L$. The arithmetic and geometric ($e^{\langle \ln g \rangle}$) averages of g over many realizations of the disordered system are calculated. Plotting g for different L as a function of concentration p has enabled to find a critical $p = p_q$ such that g decreases (exponentially) with L for $p < p_q$ and it increases (linearly) with L when $p > p_q$. Thus, we have demonstrated the Anderson metal–insulator transition at critical concentration p_q from the behaviour of the conductance itself. We have also estimated the critical conductance, g_c as $g_c \equiv g(p_q)$. By estimating the critical point for different values of electron Fermi energy E we have estimated the mobility-edge trajectory and it has been found to be consistent with the corresponding line in the p–E plane obtained by Soukoulis et al. (1987; 1992).

PACS: 05.70.Jk; 71.30.+h; 72.15.Rn

Keywords: Quantum percolation; Localization; Metal–insulator transition

The estimation of conductance of disordered electron systems has attracted much theoretical interest for more than three decades. Perhaps, most attention has been devoted to the Anderson model [1]. It uses the one-electron tight-binding Hamiltonian on regular lattice with "diagonal" disorder

$$H = \sum_{\mathbf{n}} |\,\mathbf{n} > \varepsilon_{\mathbf{n}} < \mathbf{n}\,| + \sum_{\mathbf{n},\mathbf{m},\mathbf{n}\neq\mathbf{m}} |\,\mathbf{n} > U_{\mathbf{nm}} < \mathbf{m}\,|\,, \tag{1}$$

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PII S0378-4371(97)00115-5

where $U_{\mathbf{nm}}$ are hopping matrix elements which vanish unless **n** and **m** are nearest neighbours, $| \mathbf{n} >$ represents a wave function on the site **n** and the site energies $\varepsilon_{\mathbf{n}}$ are assumed to be uniformly distributed over some width W being the measure of the disorder degree. It has been shown both theoretically and by numerous computer experiments that in three-dimensional (3D) systems there exists some critical value of W, W_c, above which all eigenstates of the Hamiltonian are localized in the sense that the asymptotic decay is exponential with the distance [2,3].

Another interesting class of models involves substitutional (binary) disorder and they are usually called quantum percolation models. They provide zero-order descriptions for the electrical transport properties in binary metal alloys [4–6] and recently also in metal–insulator nanocomposites [7–9]. For the site-percolation problem the distribution $P(\varepsilon_{\mathbf{n}})$ of site energies is binary and for an alloy A_pB_{1-p} [4] it takes the form

$$P(\varepsilon_{\mathbf{n}}) = p\delta(\varepsilon_{\mathbf{n}}) + (1 - p)\delta(\varepsilon_{\mathbf{n}} - \varepsilon)\,, \tag{2}$$

where atoms labeled A and B are situated on the sites of a regular lattice with concentrations p and $(1 - p)$, respectively. From Eq. (2) it is seen that the energies of sites A and B are $\varepsilon_A = 0$ and $\varepsilon_B = \varepsilon$, respectively. When $\varepsilon > 2zU$, where z is the number of nearest neighbours at any site of the lattice and $U_{\mathbf{nm}} = U$ is a constant, the spectrum of Eq. (1) splits into two subbands, centered approximately about the energies 0 and ε [4]. A case of particular importance concerns “strong-scattering limit” in which $\varepsilon \to \infty$. In this case the sites B are completely inaccessible for an electron and can formally be removed from the problem.

The model of binary alloy, in which the sites of the lattice are occupied by atoms has been extended by Sheng and Zhang [7] to different disordered electron systems, namely to granular metal films, e.g. Au–Al_2O_3 films, being metal–insulator nanocomposites. In this case, sites of the lattice are occupied by nanometer-size metallic particles with probability p and by an insulator with probability $(1 - p)$. Because of the ultrasmall, mezoscopic size of the metallic particles, typically 10 nm, an electron is scattered during its travel through the system and at temperatures low enough, such that its phase coherence length L_ϕ is greater than this mezoscopic size, the interference and resulting localization phenomena are present also in this scale. Since the sites of the lattice occupied by an insulator form perfect barriers, the distribution of site energies for these systems corresponds to that given by Eq. (2) in the strong scattering limit, i.e. with $\varepsilon = \infty$. Sheng and Zhang [7] have presented numerical studies of such a model for a two-dimensional (2D) system using the Landauer–Büttiker formula [10] to calculate the dimensionless conductance g, showing that $g \sim \exp(-L/\xi_{\mathrm{loc}})$ where ξ_{loc} the localization length of the electron wave function, has been found as an increasing function of metal concentration p up to $p = 0.95$ with no sign of divergence.

We have extended the Sheng and Zhang model to a 3D system. We have demonstrated the Anderson transition from the localized-states phase ($g \sim \exp(-L/\xi_{\mathrm{loc}})$) to the extended-states phase ($g \sim L$) at two values of the critical metal concentration $p = p_q$ estimated for two different values of electron Fermi energy $E = 0.01$ [8] and $E = 2.0$ [9] (the values of E are expressed in the transfer energy U units).

In this paper we present numerical results for the quantum site-percolation problem with the distribution of site energies given by Eq. (2) in the strong scattering limit ($\varepsilon = \infty$). Using the Landauer–Büttiker formula to estimate the conductance we have calculated the mobility-edge trajectory, i.e. the line in the concentration–energy plane below which a state at an arbitrary energy from the band is localized. Such data have already been published by Soukoulis et al. [5,6], but they were based on the determination of the critical point from the scaling behaviour of the localization length itself and used the well-known numerical approach called transfer matrix method [2]. As opposed to that, we first estimate conductance and from its scaling behaviour we evaluate data for the mobility-edge trajectory. Therefore, our approach allows direct determination of critical conductance $g_c \equiv g(p_q)$ vs electron Fermi energy. Furthermore, Soukoulis et al. [5,6] start from a slightly different distribution of site energies, $P(\varepsilon_\mathbf{n}) = p\delta(\varepsilon_\mathbf{n} - \varepsilon_A) + (1-p)\delta(\varepsilon_\mathbf{n} - \varepsilon_B)$ with $\varepsilon_B = -\varepsilon_A$. However, they present the results for various values of ε_A including $\varepsilon_A = 10^7$ (in the energy U units) which can be considered as the strong scattering limit as in our model.

Now we describe briefly the algorithm of our calculations (for more details refer to Refs. [8,9]). We evaluate the dimensionless conductance using Landauer-Büttiker formula [10]:

$$g = \frac{G}{e^2/h} = \frac{4(\sum_{i=1}^{L_0} T_i)(\sum_{i=1}^{L_0} v_i^{-1})}{\sum_{i=1}^{L_o}(1 + R_i - T_i)v_i^{-1}}, \tag{3}$$

where L_0 is the number of quantum channels in the leads, i.e., ideal-metal electrodes attached to the sample, T_i and R_i are calculated by summation of transmission and reflection matrices over L_0, v_i is the channel velocity and G is the sample conductance. The transmission and reflection matrices have been calculated with the help of Green's function method [11]. At each value of the Fermi energy E assumed in the studies, the solutions k_x^i of the dispersion relation

$$E/U = 2(\cos k_x a + \cos k_y a + \cos k_z a) \tag{4}$$

have been found for discrete transverse wave vector values $k_y = \pi l/(L+2)$ and $k_z = \pi m/(L+2)$ with l, m taking the values $1, 2, \ldots, L+1$, i.e., the hard-wall boundary condition is assumed here. Lattice constant a was taken to be equal to 10 nm, i.e., typical size of metallic grains in granular metal films; in our numerical calculations the length is calibrated in untis of a. Each solution k_x^i of Eq. (4) determines one conducting channel with the Fermi velocity $v_i = \partial E/\partial k_x$ evaluated at $k_x = k_x^i$. The number of conducting channels L_0 used in the summations of Eq. (3) is the number of solutions k_x^i (or v_i) just defined.

We have performed numerical calculations of the dimensionless condutance g for the above described quantum site-percolation problem on a simple cubic lattice in which concentration p and electron Fermi energy E were varied in order to estimate the data for the mobility-edge trajectory. We have considered only percolating samples in the regime $p > p_c \simeq 0.312$, the classical percolation threshold for this

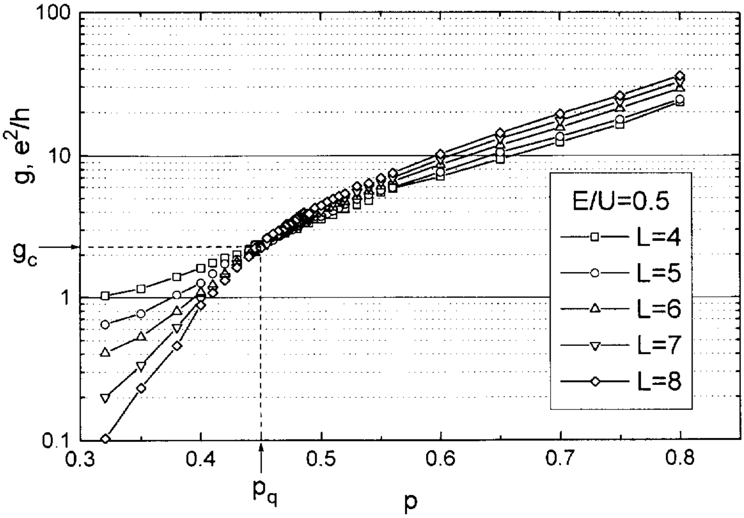

Fig. 1. Dimensionless conductance g (Eq. (3)) of a 3D quantum site-percolation model vs. metal concentration p for the electron Fermi energy $E = 0.5$ (in the transfer energy U units). The g value has been estimated as the geometric average $\langle g\rangle = e^{\langle \ln g\rangle}$ over 5000 and 1000 configurations for $L = 4$ and 5, respectively, and over 500 configurations for $L = 6, 7, 8$.

lattice. The calculations made for different lattice sizes L have allowed to distinguish between extended-states phase ($g \sim L$) and localized states phase ($g \sim \exp(-L/\xi_{\text{loc}})$) with localization length ξ_{loc} diverging at critical point p_q. The conductance (Eq. (3)) has been calculated as both geometric average, $e^{\langle \ln g\rangle}$, and arithmetic average over $5000, 1000, 500, 500$ and 500 configurations for $L = 4, 5, 6, 7$ and 8 respectively. In general, geometric average has been used to estimate the dimensionless conductance in the localized regime, where the self-averaging quantity is $\ln g$. On the other hand, the arithmetic average has been used in the extended-states regime, where dimensionless conductance itself appears as the self-averaging quantity.

The transition point for each value of the Fermi energy has been estimated on the basis of two steps. In the first step, g has been plotted vs. metal concentration p for different lattice sizes L. In Fig. 1 we have shown, as an example, g vs. p relations obtained for the Fermi energy $E = 0.5$. From this set of data the critical concentration p_q and the corresponding critical conductance g_c can be defined in such a way that in the range where $p < p_q$ (or equivalently $g < g_c$) the conductance decreases while when $p > p_q$ (or $g > g_c$) it increases with the lattice size L. We have verified the exponential conductance decay and linear conductance increase with L for $p < p_q$ and $p > p_q$, respectively. From Fig. 1 we can see that $p_q \simeq 0.45$ and $g_c \simeq 2.2$ in the units of e^2/h (see Eq. (3)) or $g_c \simeq 0.35$ in the units of $e^2/\hbar$. In the second step we have estimated the critical values of p_q (and g_c) more carefully. In the range where $p < p_q$ the straight-line relationship of the form $\ln g = \ln g_c - L/\xi_{\text{loc}}$ has been verified close to the critical point increasing p from $p = 0.40$ with the step 0.01. The magnitude of the straight-line slope has been observed as continuously decreasing to

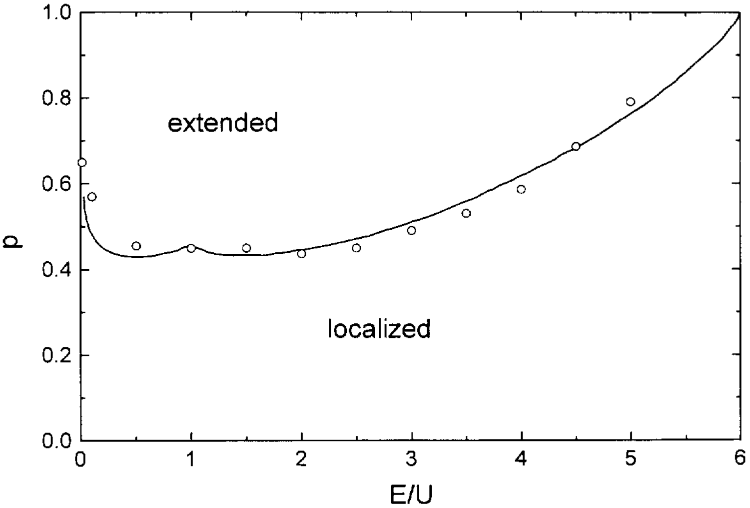

Fig. 2. Mobility-edge trajectory in the concentration–energy plane for the quantum site-percolation problem on the simple cubic lattice with the site energies distributed according to Eq. (2) in the strong scattering limit, i.e., with $\varepsilon = \infty$. The points are the results of the numerical calculations described in this work and the line is the trajectory found by Soukoulis et al. [5,6] for a similar binary system (see text) with $\varepsilon = 10^7$.

zero as p approached p_q from below; thus $\xi_{\mathrm{loc}} \to \infty$ with $p \to p_q$ has been noticed. This divergence of ξ_{loc} at p_q (g_c) is described by the fromula

$$\xi \propto \left|\frac{p-p_q}{p_q}\right|^{-\nu} \propto \left|\frac{g-g_c}{g_c}\right|^{-\nu}, \tag{5}$$

where $\xi = \xi_{\mathrm{loc}}$ for $p < p_q$ and for $p > p_q$, it is such a characteristic length that for $L > \xi$ Ohmic behaviour $g(L) \propto L^{d-2}$ (d being the dimensionality of the system) is observed. To evaluate p_q more exactly we have fitted the data ξ_{loc} vs. p to Eq. (5). By this approach we have found $p_q = 0.45 \pm 0.01$. Next, using this value of p_q the data have been fitted to the straight-line equation and from its slope $\nu = 1.2 \pm 0.2$ has been found. The obtained value of ν can be compared with $\nu = 1.5 \pm 0.1$ found by Kramer and MacKinnon [2]. We consider our estimation of the critical exponent as a rather rough one and give these data here only as resulting together with p_q from fitting the data to Eq. (5).

Using the method described above we have estimated the critical concentration for the following values of the electron Fermi energy $E = 0.01$, $0.1, 0.5, 1.0$, $1.5, 2.5$, $3.0, 3.5$, $4.0, 4.5$ and 5.0. They are shown as points in Fig. 2 together with the line being the mobility-edge trajectory found by Soukoulis et al. [5,6]. Because of the relatively small number L_0 of quantum channels estimated for $E > 5.0$, and from this resulting limitation of linear lattice size to the two or three largest L values, we have not been able to estimate the mobility-edge in this range of E with satisfactory accuracy. From Fig. 2 it is seen that the results obtained here are in good agreement with the data found by Soukoulis et al. [5,6]. The value of percolation threshold p_q below which all eingenstates are localized that can be estimated from our data is $p_q = 0.44 \pm 0.01$ and it corresponds to the energy $E = 2.0$. Soukoulis et al. obtained the same value of p_q, but for energy $E = 0.5$ and for this energy our calculation gives $p_q = 0.45 \pm 0.01$. The values of critical conductance g_c estimated in our studies as $g(p_q)$ depend strongly on the electron energy E. Namely, the critical conductance expressed in $e^2/\hbar$ units decreases from $g_c \simeq 1$ for $E = 0.01$ down to $g_c \simeq 0.003$ for $E = 5.0$. This more than two orders of magnitude variation of g_c can be compared with the range 0.02–10.0 as given by Kaveh and Mott [12]. However we do not know of any publication dealing with the dependence of the critical conductance on the Fermi energy.

This work was supported by the State Committee of Scientific Research (KBN), grant No 8 T11 B 038 09. Calculations have been performed using Sun Spare 1000 in the Computer Center of Rzeszów University of Technology.

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