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The non-universality of critical conductance in quantum site-percolation

A Kusy,[a]* A W Stadler,[a] G Hałdaś[a] and R Sikora[b], *[a]Department of Electronics Fundamentals, [b]Department of Physics, Rzeszów University of Technology, W. Pola 2, 35-959 Rzeszów, Poland*

The conductance in the quantum site-percolation on simple cubic lattice is numerically studied using Landauer–Büttiker formalism. Binary distribution of site energies $P(\varepsilon_n) = p\delta(\varepsilon_n) + (1-p)\delta(\varepsilon_n - \infty)$ *is assumed with* $p(1-p)$ *being concentration of metallic (insulating) sites. The metal-insulator transition is defined as such point* p_q *for which dimensionless conductance* g *changes its dependence on linear size* L *of the system from* $g \propto exp(-L/\xi_{loc})$ *for* $p < p_q$ *to* $g \propto L$ *for* $p > p_q$. *The critical conductance at the metal-insulator transition is estimated as* $g_c \equiv g(p_q)$. *It is found that* g_c *expressed in* $e^2/\hbar$ *units decreases from 1 at the center of each subband (E/U = 0) down to 0.002 in the vicinity of the subband edge (E/U = 6). This, almost three orders of magnitude, variation of the critical conductance vs electron Fermi energy* E *can be compared with the range 0.02–10.0 obtained for* g_c *by Kaveh and Mott.*[2] *They have concluded that critical conductance is not universal. Our data support this conclusion.*

1. Introduction

Abrahams *et al*[1] have developed a scaling theory for the zero-temperature dc dimensionless conductance, $g = G/(e^2/\hbar)$, of disordered electronic systems; where G is conductance (in Ω^{-1}) of disordered sample in the shape of the cube with side L, e is elementary charge and $\hbar$ Planck's constant. According to this theory in three dimensions there exists a critical conductance g_c that separates the extended states (metallic) phase $g > g_c$ from the localized states (insulating) phase. In the metallic phase conductance tends to increase linearly with the size L of the system. On the other hand, in the insulating phase, g exponentially decreases with L, $g \propto \exp(-L/\xi_{loc})$, where ξ_{loc} is localisation length of the electronic wave function. According to the scaling theory the critical conductance, g_c is independent of the material.[1] Estimation of g_c has been a subject of several theoretical and experimental elaborations (for a review see e.g. Ref. 2). Unfortunately the results obtained by different authors are not consistent. It is often suggested that g_c expressed in $e^2/\hbar$ units is of the order of unity.[1] Using a model of random scatterers for localisation problem, and a renormalisation group technique, Shapiro[3] has found $g_c \cong \pi/3.92$ that is in fact close to unity. More recently Lambrianides and Shore[4] have utilized Kubo–Greenwood formula to numerically evaluate the conductance for Anderson model of three-dimensional noninteracting electrons in a uniformly distributed random potential. They found $g_c = 0.1 \pm 0.01$. According to the calculation of Kaveh and Mott[2] localisation effects alone lead to $g_c = b/3\pi^2$ with $1 < b < 3$, which gives $0.03 < g_c < 0.1$. This is consistent with the value g_c of the order of π^{-2} as given by Lee and Ramakrishnan.[5] However Kaveh and Mott[2] discussion of both theoretical and experimental data gives a broad range 0.02–10 for g_c.

In this paper we present a numerical estimation of the critical conductance g_c in the site-percolation on a simple cubic lattice. We use Landauer–Büttiker formalism following the approach given in our recent paper.[6] We show that g_c strongly depends on the electron Fermi energy in the system.

2. Model

Let us consider one-electron tight-binding Hamiltonian with diagonal disorder defined on simple cubic lattice of sites

$$\mathbf{H} = \sum_{\mathbf{n}} |\mathbf{n}\rangle \varepsilon_{\mathbf{n}} \langle \mathbf{n}| + \sum_{\mathbf{n}} |\mathbf{n}\rangle U_{\mathbf{n},\mathbf{m}} \langle \mathbf{n}| \qquad (1)$$

where $U_{\mathbf{n},\mathbf{m}} = U$ are hopping matrix elements which vanish unless $\mathbf{n}$ and $\mathbf{m}$ are nearest neighbours, $|\mathbf{n}\rangle$ represents a wave function on the site $\mathbf{n}$ and the site energies $\varepsilon_{\mathbf{n}}$ are binary distributed following

$$P(\varepsilon_{\mathbf{n}}) = p\delta(\varepsilon_{\mathbf{n}}) + (1-p)\delta(\varepsilon_{\mathbf{n}} - \infty). \qquad (2)$$

$p(1-p)$ is concentration of metallic (insulating) sites.

We evaluate the dimensionless conductance of our model using Landauer–Büttiker formalism.[7] To perform the calculations we attach metallic ($p = 1$), semiinfinite electrodes to the opposite walls of the lattice. One way to estimate the conductance of the

* To whom correspondence should be addressed.

disordered system is to use the multichannel Landauer–Büttiker formula[6,7] that corresponds to four-point (four-probe) method of measurements

$$g_{4-p} \equiv \frac{G_{4-p}}{e^2/\hbar} = \frac{2}{\pi} \frac{\left(\sum_{i=1}^{L_0} T_i\right)\left(\sum_{i=1}^{L_0} v_i^{-1}\right)}{\sum_{i=1}^{L_0} (1+R_i-T_i)v_i^{-1}} \tag{3}$$

where L_0 is the number of quantum channels in the leads, T_i and R_i are calculated by summation of transmission and reflection matrices over L_0, v_i is velocity in the channel i and G_{4-p} is the sample conductance. The transmission and reflection matrices have been calculated with the help of Green's function method (see Ref. 6 and references therein). Conductance of the disordered system can also be calculated using another Landauer–Büttiker formula[7]

$$g_{2-p} \equiv \frac{G_{2-p}}{e^2/\hbar} = \frac{1}{\pi} \sum_{i=1}^{L_0} T_i \tag{4}$$

which corresponds to two-point electrical measuring. It gives roughly the same results as formula (3) for strongly disordered systems. However for weakly disordered samples the contact resistance has to be subtracted from g_{2-p}^{-1} as follows

$$g_1 = (g_{2-p}^{-1} - \pi L_0^{-1})^{-1}. \tag{5}$$

3. Results and discussion

We have performed numerical calculations of the dimensionless conductance for the model described in Section 2 using eqns (3)–(5). First, quantitative agreement between data obtained using eqns (3)–(5) have been tested (see Fig. 1). For weakly disordered samples, $g > 1$, the agreement can be observed only between eqn (3) and eqn (5) while in the strong disorder range, $g < 1$, all three formulas give approximately the same results. On this basis in the following we have used eqn (3) to calculate dimensionless conductance $g = g_{4-p}$.

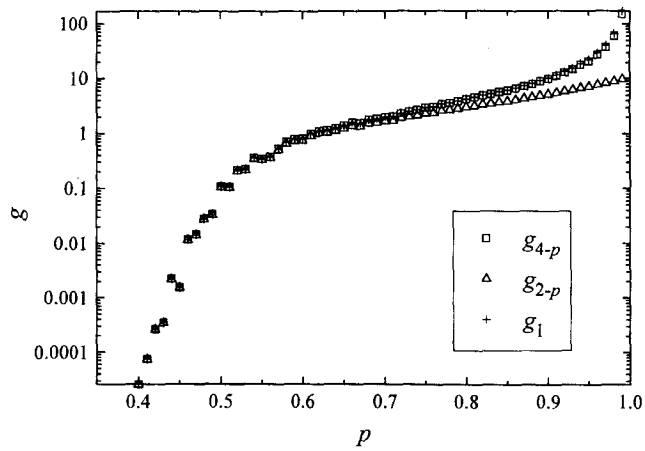

Figure 1. Dimensionless conductance of 3-D quantum site-percolation model calculated by eqns (3), (4) and (5) vs concentration p of the metallic sites. Calculation have been made for the lattice size $L = 6$ and Fermi energy $E/U = 0.001$. For strong disorder ($g < 1$) the results obtained by different formulas coincide.

Concentration p, Fermi energy E/U and sample size L have been varied to estimate mobility-edge trajectory. Only percolating samples in the regime $p > p_c \cong 0.312$ were taken into account. The extended states phase ($g \propto L$) and localized states phase ($g \propto \exp(-L/\xi_{loc})$) have been identified from g vs L behavior with the localization length ξ_{loc} diverging at critical point $g_c \equiv g(p_q)$

$$\xi \propto \left|\frac{p-p_q}{p_q}\right|^{-\nu} \propto \left|\frac{g-g_c}{g_c}\right|^{-\nu} \tag{6}$$

where $\xi = \xi_{loc}$ for $g < g_c$ while for $g > g_c$ ξ is such a characteristic length that for $L > \xi$ ohmic behavior $g(L) \propto L$ is observed.

The conductance [eqn (3)] has been averaged over 2000–10,000 configurations for L from 11 down to 3, respectively. In general geometric average, $e^{\langle \ln g \rangle}$, and arithmetic average have been used in the insulating and metallic regime, respectively. The localization-delocalization point has been estimated on the basis of two steps for each value of the Fermi energy. First g has been plotted vs metal concentration p for different lattice sizes L (Fig. 2). From these data critical concentration p_q and corresponding critical g_c have been estimated noting that for $p < p_q$ ($g < g_c$) the conductance decreases exponentially while for $p > p_q$ ($g > g_c$) it increases roughly linearly with the lattice size L. From Fig. 2 one finds $p_q \cong 0.6$ and $g_c \cong 0.002$. In the second step we have carefully studied the straight-line equation $\ln g = \ln g_c - (L/\xi_{loc})$ changing p from $p = 0.56$ to p close to the critical point with the step 0.005. The magnitude of the slope of this straight line has been found as continuously decreasing to zero as p approached p_q; it means that $\xi_{loc} \to \infty$ with $p \to p_q$ has been observed according to eqn (6). To evaluate g_c we have fitted the data $\ln g$ vs L to the straight line equation. By this approach we have found $p_q = 0.585 \pm 0.0005$, $g_c = 0.0016 \pm 0.00025$ for $E/U = 4$. Next using this value of p_q

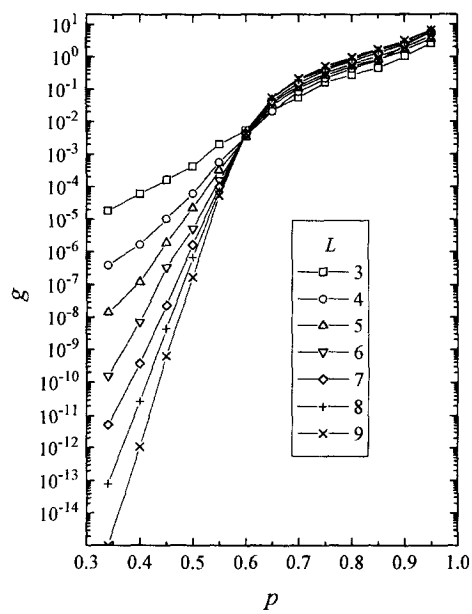

Figure 2. Dimensionless conductance g of 3-D quantum site-percolation model vs metal concentration p for the electron Fermi energy $E/U = 4$. The g values have been estimated as geometric average $e^{\langle \ln g \rangle}$, over 10,000–500 configurations for L 3–9 in the wide range of p, and over 10,000–2000 configurations for L 3–11, for p near p_q, respectively. Data in the vicinity of p_q have been omitted in this picture for clarity.

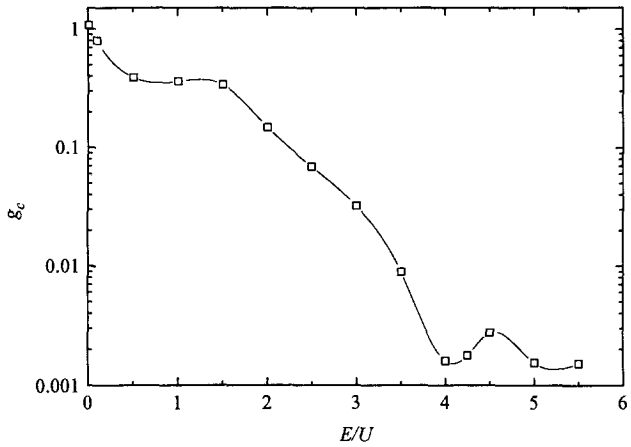

Figure 3. Mobility-edge trajectory in the conductance-energy plane for the quantum site-percolation problem on simple cubic lattice with the site energies distributed according to eqn (2). The points are results of numerical calculations described in the text and the line has been drawn to guide the eye.

the data $\ln \xi_{loc}$ vs $\ln|p-p_q|$ have been fitted to the straight line equation and from its slope critical exponent $\nu = 1.16 \pm 0.08$ has been found.

Using the above described method, critical concentration p_q and critical conductance g_c vs Fermi energy E/U have been calculated. The mobility-edge trajectory in the concentration vs energy plane has been published in our recent paper[6] and found to be in good agreement with the results of Soukoulis *et al*[8]. In Fig. 3 we have shown the critical conductance vs Fermi energy obtained from the calculation. As can be seen it decreases from $g_c \cong 1$ down to $g_c \cong 0.002$ when E/U increases from 0.01 up to 5.5. These three orders of magnitude decrease of g_c vs E/U is in contrast to the universality of the critical conductance predicted by one-parameter scaling theory of Abrahams *et al*.[1] This universality has been accepted and used in the studies of mesoscopic systems and nanoelectronic devices. In particular the value of $G \cong e^2/\hbar$ is often considered as an indication of the bound to which conductance of the nanoelectronic device can be decreased before it reaches the localized states phase behavior. Our data indicate that the critical conductance is not universal and remain in agreement with the result of the studies by Kaveh and Mott.[2] They have reported the range 0.02–10 for g_c in the same unit of $e^2/\hbar$ and have also concluded its non-universality. We think that the variation of critical conductance found in this paper may reflect the experimental observations of g_c over three orders of magnitude observed for different materials with different Fermi energies.

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