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1989 J. Phys. A: Math. Gen. 22 L345

(http://iopscience.iop.org/0305-4470/22/8/007)

J. Phys. A: Math. Gen. **22** (1989) L345-L351. Printed in the UK

LETTER TO THE EDITOR

A model for competition between 'classical' and 'quantum' percolation effects in disordered electronic systems†

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Received 21 November 1988

Abstract. A simple model of a diluted lattice is proposed to discuss the interplay between classical percolation and quantum localisation effects on electronic transport properties in disordered media. 'Absent' sites act as infinite barriers, while interference effects at 'occupied' sites are assumed to be negligible at random with probability α. The limits $\alpha = 0$ and $\alpha = 1$ are respectively 'quantum' and 'classical' percolation. The phase diagrams of conducting and insulating phases are discussed through a small-cell position-space renormalisation group in space dimensionalities $d = 2$ and 3; in $d = 2$ there is crossover from 'classical' to 'quantum' percolation, while in $d = 3$ the phase structure exhibits a multicritical point and a 'classically insulating' phase which are not present in $d = 2$.

It is well known that a simple (classical) percolation model cannot account for all the complex features of the transition between localised and extended one-electron wavefunctions in disordered materials. Such a transition is believed to be properly described by the Anderson model or its variants (Anderson 1958, see also Kirkpatrick and Eggarter 1972, Abrahams *et al* 1979, Anderson *et al* 1980, Lee and Ramakrishnan 1985). The Anderson model as originally proposed displays a wealth of interesting physical aspects; however, its treatment on a first-principles basis is so involved that often adaptations are made, which are thought to include some essential physical features of the model, yet render it more tractable in practice. One such scheme is quantum percolation (Kirkpatrick and Eggarter (1972); for a recent review see e.g. Odagaki (1986) and references therein). For a tight-binding Hamiltonian

$$\mathscr{H} = -\sum_i \varepsilon_i |i\rangle\langle i| + \sum_{\langle ij\rangle} V_{ij} |i\rangle\langle j| \tag{1}$$

while in the usual Anderson model the site self-energies ε_i are continuously distributed, (e.g. according to a flat distribution of width W) for the (site) quantum percolation problem one assumes the bimodal distribution

$$P(\varepsilon_i) = x\delta(\varepsilon_i) + (1-x)\delta(\varepsilon_i - \infty) \tag{2}$$

i.e., a fraction $1-x$ of the sites is forbidden (analogously to empty sites in classical percolation). For bond quantum percolation, the nearest-neighbour hopping parameter V_{ij} is zero with probability $1-p$, and $V \neq 0$ with probability p. Here, we shall be concerned only with the site problem.

† Work partially supported by FINEP, CAPES and CNPq.

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0305-4470/89/080345+07$02.50

Quantum percolation differs fundamentally from the standard Anderson problem in that all moments (of order greater than zero) of the distribution diverge (for the bond problem, which corresponds to off-diagonal disorder, the relevant distribution is that of $\log V$ (Odagaki 1980, Soukoulis and Economou 1981, Puri and Odagaki 1981)). In such a case, usual arguments regarding the Anderson problem would lead one to conclude that all states are localised, for any space dimension d and any degree of disorder (x or $p \neq 1$). Instead, at least in $d = 3$ evidence shows that there is a finite quantum percolation threshold x_q (or p_q) < 1 at which the localisation transition takes place (Chang and Odagaki 1987a and references therein). In $d = 2$ it seems that all states are localised for any disorder, as obtained for the Anderson problem from the scaling approach of Abrahams *et al* (1979); direct evidence for this, however, is not conclusive. For example, Chang and Odagaki (1987a) obtain $x_q > 0.94$ in $d = 2$ from a large-cell Monte Carlo renormalisation group; large fluctuations prevent those authors from making a more precise statement. The existence of these fluctuations is consistent with the idea that $d = 2$ is a marginal dimension in this case, as for the Anderson problem (Abrahams *et al* 1979). See also Raghavan (1984) for similar results, and Chaturvedi and Srivastava (1983) for arguments in favour of $x_q < 1$ in $d = 2$.

An attempt to make the rules of quantum percolation more flexible, in order to encompass a wider range of possible physical situations, was made by Chang and Odagaki (1987b) by incorporating tunnelling effects through finite barriers. They only consider $d = 3$ and find, for the site problem, an extrapolated $x_q \simeq 0.26$ for infinite barrier height, *smaller* than the classical percolation threshold $x_c = 0.3118$ (Stauffer 1985). In an altogether different direction, the work of Shapiro (1982) discusses the interplay between quantum localisation and classical percolation through the introduction of a diluted lattice of random quantum scatterers. He finds no localisation transition in $d = 2$, and in $d = 3$ a transition with the same exponents of the usual Anderson problem. Although this model is not equivalent to quantum percolation, the resistance ρ assigned to each scatterer (which may be present or absent with respective probability p or $1 - p$, absent sites corresponding to total reflection of the incident wave) to some extent measures the strength of (quantum) interference effects. For $\rho = 0$ the problem is identical to classical percolation; at $p = 1$ and $\rho \neq 0$ one expects to have the usual Anderson problem. While the parameter ρ is supposed to represent the existence of microscopic disorder, it does so in an average way: each random scatterer is in fact a 'supersite', approximating a region with linear size at least equal to the electron's phase coherence length (this is essential for the random scattering assumption), which may contain many actual atoms. It is thus interesting to check whether results similar to Shapiro's will emerge when microscopic disorder (i.e. interference effects) is dealt with from a viewpoint similar to that used in quantum percolation, where no random-phase assumptions are made about nearest-neighbour hopping.

In order to do this, we propose a simple model of a diluted lattice, where empty sites act as infinite barriers, such as in quantum percolation or Shapiro's model, but occupied sites may exhibit either classical behaviour (i.e. transmission coefficient = 1 for any incoming particle) with probability α, or quantum behaviour (an incoming particle may be reflected or transmitted, according to the laws of wave mechanics) with probability $1 - \alpha$. To make contact with the 'binary alloy' interpretation of Kirkpatrick and Eggarter (1972), we keep the forbidden sites (type B) with infinite energy, and now allow the self-energies of allowed sites (type A) to vary, and approximate the distribution of type-A site energies by a binary form: 'low' barriers, with zero reflectance, and 'high' ones (or height comparable to the electron's energy), at which

the reflection probability is not negligible. For a fixed distribution of site self-energies, one can think of α as related to the diffusing electron's energy: highly energetic electrons are unlikely to be reflected from allowed sites by any but the highest finite barriers, so in this case α is close to 1; the propagation of low-energy electrons is simulated by a small value of α. Thus the model incorporates, albeit crudely, an energy scale, making room for the definition, for example, of a mobility edge; in standard quantum percolation, such a scale does not exist, since the only barriers are infinite (empty sites). The $p=0$ limit of Shapiro's model corresponds to $\alpha=1$ here (classical percolation); however, while the present model changes over to quantum percolation as $\alpha \to 0$, that author obtains, at $p=1$ and $\rho \neq 0$, the standard Anderson problem formulated in terms of random scatterers. Although the two models are therefore not strictly equivalent, both incorporate an interplay between 'classical' and 'quantum' disorder.

The aim of this letter is to study the effects of space dimensionality on the phase diagram of insulating and metallic regions for the mixed classical-quantum percolation model proposed above. For this, we have used a small-cell position-space renormalisation group (PSRG) already developed separately for each extreme: classical (Reynolds *et al* 1977, 1980) and quantum (Odagaki and Chang 1984), with suitable adaptations for intermediate situations. As seen below, there is in this case a marked difference between $d=2$ and 3 (the only dimensions considered here) which parallels that found for the Anderson problem, but is not identical to it; overall, our study is complementary to others in this field, in that it shows that no matter how one chooses to incorporate disorder effects in electronic transport problems, qualitative differences arise between two- and three-dimensional systems.

Classical percolation effects are defined by a geometric rule (namely, a particle can jump, with probability 1, only between two adjacent occupied sites), while the quantum percolation aspects are obtained through the analysis of Hamiltonians like equation (1) above. In PSRG, one can take both into account as follows:

(i) For the renormalised site occupation probability x', specify all configurations in the original cell in which one can 'get across' the cell through a path of occupied sites (percolating configurations).

(ii) In addition to its intrinsic probability $x^n(1-x)^{N-n}$ for a configuration with n $(N-n)$ present (absent) sites, each percolating configuration has a weight related to the probability that a particle will diffuse through it: this is 1 in the classical problem, and, for purely quantum percolation (following Odagaki and Chang 1984)

$$W_{\text{conf}} \propto \lim_{t\to\infty} \sum_{\alpha\beta} |\langle\beta| \exp(-\mathrm{i}H_{\text{conf}}t)|\alpha\rangle|^2 \tag{3}$$

where α are sites on one edge of the cell, β are those on the opposite edge (already in the next cell; see figure 1(b) of Odagaki and Chang (1984)), and H_{conf} is the Hamiltonian of the particular configuration (with hopping allowed only between nearest-neighbour present sites). Note that $W_{\text{conf}}<1$, since it is normalised by the weight of the configuration with all sites present, through which one assumes that an electron will certainly percolate, in analogy with Bloch waves in the infinite pure crystal (Odagaki and Chang 1984).

In our case, where configurations with both 'classical' and 'quantum' sites are allowed:

(a) we have given weight 1 to percolating configurations in which it is possible to cross the cell stepping only on 'classical' sites;

(b) configurations whose crossing is necessarily made through at least one 'quantum' site are given the same weight as if all present sites in that configuration were 'quantum' (thus W_{conf} would be calculated by equation (3)). Although these criteria incorporate a certain degree of arbitrariness, rule (a) reflects the physically relevant fact that, if a particle can choose between propagating freely or subject to reflections, it will follow the easiest path; rule (b) is based on the idea that a chain is as weak as its weakest link. It is expected that all reasonable rules will give the same qualitative results; we have confirmed this through slight variations of the above-mentioned criteria.

We have obtained a set of two combined recursion relations for x' (probability of a renormalised site being occupied) and $x'\alpha'$ (probability of an occupied renormalised site being of 'classical' character). We consider only configurations where the cell can be crossed along a given direction, say horizontally (this is rule R_1 of Reynolds *et al* (1977)). Configurations that contribute for α' are those which conform to rule (a) above. For examples, see figure 1. We also tried writing an equation for $x'(1-\alpha')$, taking into account configurations which obey rule (b), having obtained the same qualitative results. For a two-dimensional square lattice, with rescaling parameter $b=2$, we have:

$$x' = x^4 + x^3(1-x)[4\alpha^3 + 10.5624\alpha^2(1-\alpha) + 9.8436\alpha(1-\alpha)^2 + 3.2812(1-\alpha)^3] + x^2(1-x)^2[2\alpha^2 + 2.625\alpha(1-\alpha) + 1.3125(1-\alpha)^2] \tag{4a}$$

$$x'\alpha' = x^4[\alpha^4 + 4\alpha^3(1-\alpha) + 2\alpha^2(1-\alpha)^2] + x^3(1-x)[4\alpha^3 + 4\alpha^2(1-\alpha)] + 2x^2(1-x)^2\alpha^2. \tag{4b}$$

Note that, for $\alpha = 1$ both equations degenerate into the recursion relation given in table 2 of Reynolds *et al* (1980) for the corresponding classical percolation problem; for $\alpha = 0$, equation (4*a*) reproduces that given by Odagaki and Chang (1984) for quantum percolation. As both $\alpha = 0$ and $\alpha = 1$ are fixed points of 4(*b*), the purely classical and purely quantum problems are transformed each into itself, as they should be. The equations for the simple cubic lattice, also with $b = 2$, behave similarly at the limits $\alpha = 0$ and $\alpha = 1$. However, the phase diagrams which emerge from the iteration of the recursion relations are very different from each other, as seen in figure 2.

In $d = 2$ there are only three attractors (fully stable fixed points), namely $(x, \alpha) = (1, 1)$, $(1, 0)$ and $(0, 0)$; their domains of attraction are respectively termed 'classical conducting' (CC), 'quantum conducting' (QC) and 'quantum insulating' (QI) phases. In addition to these, in $d = 3$ there is a fourth attractor at $(0, 1)$, whose domain of attraction is the 'classical insulating' (CI) phase (not present in $d = 2$). Physically, a

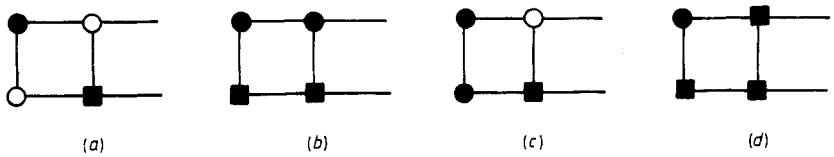

Figure 1. Examples of configurations in $d = 2$ indicating empty sites (○), occupied 'classical' sites (●), and occupied 'quantum' sites (□). (*a*) does not percolate (cell cannot be crossed from left to right). (*b*) counts as a renormalised 'classical' site; weight 1; intrinsic probability $x^4\alpha^2(1-\alpha)^2$. (*c*) counts as a renormalised 'quantum' site; weight 0.8750; intrinsic probability $x^3(1-x)\alpha^2(1-\alpha)$. (*d*) counts as a renormalised 'quantum' site; weight 1 (because all sites are occupied; see text); intrinsic probability $x^4\alpha(1-\alpha)^3$.

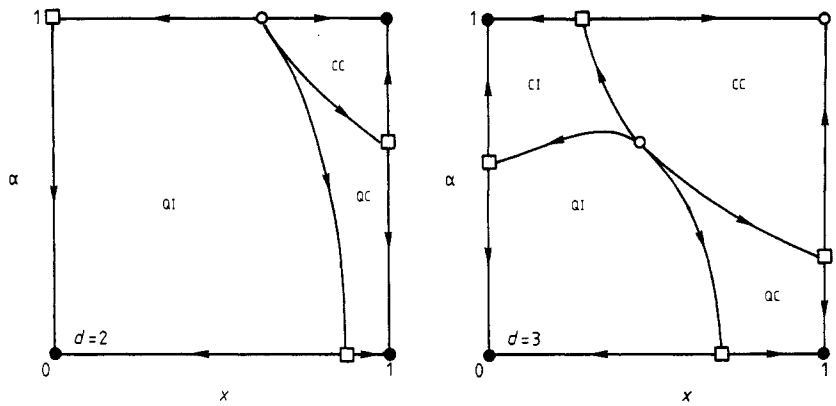

Figure 2. Phase diagrams in $d=2$ and $d=3$ obtained from the recursion relations $(x, \alpha) \rightarrow (x', \alpha')$, indicating flow directions along the phase boundaries, fully stable fixed points (attractors) (●), semi-stable fixed points (□), fully unstable fixed points (○) and domains of the quantum insulator (QI), classical insulator (CI), quantum conductor (QC) and classical conductor (CC) (see text).

system represented by a point in the CC phase will conduct mainly through classical diffusion mechanisms, whereas in a QC system, quantum intersite hopping is the dominant characteristic of conduction. Similarly, QI stands for a system in which it is quantum interference which essentially blocks conductivity; for a CI, low geometric connectivity is the decisive factor to disrupt macroscopic conduction.

It is clear that quantum effects are much stronger in $d=2$ than in $d=3$, as seen from the fact that the QI phase extends itself up to $\alpha=1$ in $d=2$; also, the direction of flow lines at the classical percolation point indicates that it is unstable relative to quantum perturbations in $d=2$ (implying crossover from classical to quantum behaviour), and stable in $d=3$.

In $d=2$ the quantum percolation critical point is at $(x_q, \alpha_q)=(0.867, 0)$ (Odagaki and Chang 1984), thus the QC phase occupies a finite fraction of phase space. For more realistic calculations (e.g. larger scaling factor b), this critical point is expected to move closer to $x=1$, so the QC phase will shrink accordingly. Whether its size will go down to zero depends on whether the quantum percolation threshold is exactly 1 in $d=2$ (see e.g. Chaturvedi and Srivastava 1983). On the other hand, we note that in this simple version of our model, the CC phase will always be present both in $d=2$ and $d=3$. This is because, as there is a finite probability (α) for a site to display exactly *zero* interference effects (i.e. to behave classically), for $x>x_c$ and α sufficiently close to 1 it will always be possible to have an infinite cluster of 'classical' sites (which will be classically conducting); at $x=1$, α just has to exceed the (classical) percolation threshold. Thus, the non-trivial fixed points along the 'classical' axis $\alpha=1$ and along the full lattice axis $x=1$ are located respectively at $(x, \alpha)=(0.618, 1)$ and $(1, 0.618)$ for $d=2$, and $(0.282, 1)$ and $(1, 0.282)$ for $d=3$ (compare respectively to $x_{c,d=2}=0.593$ (Reynolds *et al* 1980) and $x_{c,d=3}=0.3118$ (Heermann and Stauffer 1981)). We are at present discussing the effects, on the CC phase, of having a continuous distribution of interference strengths (instead of a distribution with a delta function at the 'classical', zero-interference strength, point).

The origin of the CI phase in $d=3$ (and its non-existence in $d=2$) is related to the fixed point at $\alpha \neq 0, 1$ on the $x=0$ axis. For $x \rightarrow 0$, only the lowest powers of x

enter the recursion relations, and one obtains:

$$\alpha' = a_d\alpha^2[a_d\alpha^2 + b_d\alpha(1-\alpha) + c_d(1-\alpha)^2]^{-1} \tag{5}$$

as the recursion relation for α in that limit. The subscripts d stand for space dimension, and $(a_d, b_d, c_d) = (2, 2.625, 1.3215)$ in $d = 2$ and $(4, 2.9404, 1.4702)$ in $d = 3$ respectively. The fixed points of (5) are $(0, 1)$ and

$$\alpha^* = c_d(a_d - b_d + c_d)^{-1}. \tag{6}$$

For $d = 2$, $\alpha^* = 1.91$ (unphysical) and for $d = 3$, $\alpha^* = 0.581$, as shown in the $d = 3$ phase diagram of figure 2. This difference arises essentially because $a_2 = 2$ and $a_3 = 4$, and these in turn are the numbers of distinct straight-line paths accross the cell along a given direction for each space dimension. The fact that for low concentrations, quantum interference effects must be finite in order to block conduction in $d = 3$, while in $d = 2$ they always dominate, is then directly related to the simple geometric fact that there are more paths between two sites in $d = 3$ than in $d = 2$.

We note that for the three-dimensional problem, the quantum percolation threshold is at $x_q \simeq 0.70$, the same as estimated by Odagaki and Chang (1984), while there is a doubly unstable (multicritical) point $(x, \alpha) = (0.444, 0.635)$. At this point, conduction takes place through a mixture of classical diffusion and quantum hopping. Since it is expected that $x_q \neq 1$ in $d = 3$ (although somewhat smaller than the above estimate; Chang and Odagaki (1987a) quote $x_q \simeq 0.42$), the QC phase must be present also in a more precise treatment (e.g. larger scaling factor b) of the present model. The same can be said about the CI phase: with the weak assumption that, in $d = 3$, the normalised weight (given by equation (3)) of a one-dimensional path goes to zero faster than b^{-1}, it can be shown that the derivative $\partial\alpha'/\partial\alpha$ of the recursion relation analogous to (6) for general b is always zero at $\alpha = 0$ and less than 1 at $\alpha = 1$, implying the existence of a non-trivial fixed point $0 < \alpha < 1$ on the $x = 0$ axis. Hence, the multicritical point and the four-phase structure for the three-dimensional problem are not small-cell artifacts.

In summary, we have proposed a simple model which is able to account for the competition between 'classical' and 'quantum' aspects of disorder. Differently from the model proposed by Shapiro (1982), 'quantum' disorder is incorporated directly from a viewpoint similar to that used in 'quantum percolation'. We have found essential differences between the phase diagrams for the two- and three-dimensional versions of the model, once again showing the essential role played by space dimensionality (especially as d goes from 2 to 3) in electronic transport problems. Our model has the advantage, over, for example, standard 'quantum percolation', of being 'tunable'; thus the distribution of interference effects (here approximated by a binary one) can be made continuous, and the influence of this over the corresponding phase diagrams (particularly over the 'classical conducting' phase) can be studied. Work along these lines is currently in progress.

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