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Level statistics and localization in a two-dimensional quantum percolation problem

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ABSTRACT

A two-dimensional model for quantum percolation with variable tunnelling range is studied. For this purpose the Lifshitz distribution is considered where the disorder enters the Hamiltonian via the non-diagonal hopping elements. We employ a numerical method to analyse the level statistics of this model. It turns out that the level repulsion is strongest around the percolation threshold. As we go away from the maximum level repulsion a cross-over from a Gaussian orthogonal ensemble type of behaviour to a Poisson-like distribution is revealed. The localization properties are calculated by using the sensitivity to boundary conditions and we find a cross-over from localized to delocalized states.

§1. INTRODUCTION

The statistics of energy levels in complicated quantum systems have been the subject of research for several decades. It started with the study of energy levels in atomic nuclei (Wigner 1951, 1958) then the statistics of electronic states in atoms was investigated (Rosenzweig and Porter 1960), and more recently the statistics of electrons in quantum dots have been studied (also known as 'artificial' atoms) (Efetov 1996). A surprising result of most of these approaches was that the statistics of energy levels are quite universal regardless of the specific system; systems can be classified according to their symmetry properties as orthogonal, unitary and symplectic. These universality classes represent strong correlations between the energy levels due to level repulsion. This is indicated, for example, by the level spacing distribution $P(s)$ which goes like s^{β} for small s. The exponent β $(= 1, 2, 4)$ characterizes the universality class (Metha 1991). In contrast with this repulsive behaviour (the Wigner–Dyson distribution) the assumption of statistically independent energy levels would lead to a Poisson distribution $P(s) = \exp(-s)$. The correlation in nuclei or atoms is so strong because their corresponding states have usually a large overlap, except perhaps for the ground state. The situation is less clear if we consider a macroscopic system of as atoms as in solid-state physics where disorder can be present. Depending on the latter there are extended electronic states and also states which are localized in space owing to Anderson localization (Efetov 1996). In terms of level statistics the localized states are expected to obey a Poisson distribution,

whereas the extended states are expected to have strong level repulsion characterized by a Wigner–Dyson distribution. Since there is a metal–insulator transition from extended to localized states driven by disorder (the Anderson transition), it is natural to study this in terms of the statistics of energy levels.

Approaches to the role of level statistics for the Anderson transition (Evangelou 1997) were presented by several workers, and a model for quantum percolation for nearest-neighbour transfer was investigated by Berkovitz and Avishai (1996). Recently it was found (Aronov *et al.* 1994, 1995) that the divergence of the localization length ξ at the metal–insulator transition leads to a deviation from the Wigner–Dyson statistics for $\xi > L$, L being the system size. In particular it was found that the decay of the level spacing density is weaker than that of the Wigner–Dyson statistics. This is also found in our investigation where we look at a different system with long-range hopping and off-diagonal disorder.

The purpose of this paper is to study a quantum percolation model where the transfer is not only between nearest neighbours but where the transfer rate decays exponentially with distance. Exponentially localized states (e.g. Wannier states) form a natural basis for a system close to a localization transition. Moreover, in contrast with Anderson's model for localization we study disorder in the off-diagonal part of the Hamiltonian.

This model is motivated by various physical systems. One example is a two-dimensional (2D) array of quantum dots (Duruöz 1995) where electrons can tunnel between the individual quantum dots. The imperfections of the fabricated array leads to disordered tunnelling rates. Numerical studies of such an array (Whan *et al.* 1996) have shown that the overlap of the electronic wavefunctions is not only between nearest neighbours but over a much longer range. Our model is also motivated by the analogous picture of variable-range hopping in solids (Mott 1974).

A third example for this model is the class of low doped high-T_c cuprates. Here the charge carriers are holes in 2D CuO_2 layers. The antiferromagnetically ordered parent materials show a charge-transfer (CT) gap between states of mainly oxygen p character and states of mainly copper $d_{x^2-y^2}$ character. Upon doping, states occur in the CT gap which are thought to originate from localized states. There are now two possible scenarios why disorder also plays an essential role in the insulator to metal transition. The first scenario (I) is that dopant atoms which are added in between the CuO_2 layers (e.g. Strontium in $La_{1-x}Sr_xCuO_4$ or excess oxygen) localize additional holes in their vicinity. The additional dopant atoms are randomly distributed and nearly immobile at low temperatures. The second scenario (II) would be that even without additional dopant atoms a doped hole can form a self-trapped polaronic state (Bulaevskii *et al.* 1968) and should therefore have a very low mobility. Again such states could be distributed in a random way.

In such a disordered state (which quickly loses its long-range order because of doping,) one has exponentially localized wavefunctions for each hole. With further doping, these states start to overlap more and more while disorder seems to play an essential role (spin-glass phase) until one finally reaches the conducting state (Hizhnyakov and Sigmund 1988, Sigmund and Müller 1994). The 2D copper oxide plane may be separated into hole-rich conducting and magnetically correlated (insulating) areas. A possible origin for phase separation are polaronic states more (I) or less (II) tightly bound to dopant atoms that have been discussed by Gooding (1991) and Kleimer *et al.* (1994). Therefore our model can describe a transition or at least a cross-over from strongly insulating (localized) states to states with infinite or

at least very large localization length. This picture can be applied to the physics of the normal state in the low-doped high-T_c materials. Indeed, conductivity measurements by Chen *et al.* (1995) of low-doped $La_{2-x}Sr_xCuO_4$ with $x \approx 0.002$ have shown that for temperatures below 50 K the transport properties are governed by a hopping-type conduction. Also earlier measurements by Keimer *et al.* (1992) for a sample with doping concentrations of $x \approx 0.04$ found a conductivity of hopping type near localization below 20 K. Further the origin of the so-called pseudogap phase in the underdoped cuprates has been discussed among other origins also as a result of disorder (Abrahams *et al.* 1970, Huscroft and Scalettar 1997).

§ 2. The model

Our model for quantum percolation corresponds to the Hamiltonian

$$H = \sum_{i,j} (t_{ij} a_i^\dagger a_j + \text{hc}), \tag{1}$$

with the following off-diagonal (hopping) matrix elements:

$$t_{ij} = \begin{cases} t \exp\left[-\alpha(r_{ij} - r_0)\right] & \text{for } r_{ij} > r_0, \\ t & \text{for } r_{ij} \leqslant r_0, \end{cases} \tag{2}$$

between the lattice sites r_i and r_j (with $r_{ij} = |r_i - r_j|$). The lattice sites i and j can be randomly occupied with quasiparticles in Wannier states, leading to random hopping elements t_{ij}. This type of randomness is also known as Lifshitz (1965) type disorder. The exponential decay of the localized wavefunctions leads to an exponential decay of the hopping rate with distance on the inverse decay length α. The spatial extension of the localized states, for example given by the size of a polaron, is expressed by r_0. A hopping matrix element t_{ij} is non-zero only if the sites i and j of the 2D lattice are both occupied by localized states.

An advantage of the long-range hopping of our model, at least for small enough α, is the fact that the density of states is smoothed out in contrast with the sharp peaks found for nearest-neighbour transfer (Berkovits and Avishai 1996). The reason for this is that in a system with nearest-neighbour hopping only configurations of $1, 2, \ldots$ localized states can occur completely disconnected from the percolation backbone. The energy levels of such configurations show up as sharp peaks in the density of states in a model with short range transfer only. Owing to the long-range nature of our transfer such disconnected configurations are rare in our model.

The smooth density of states is easier to analyse with the methods of random matrix theory. The density of states is shown in figure 1. It shows a broad peak near the lowest eigenvalue. This peak is due to the 2D nature of the system. For infinite α and all lattice sites occupied, only a nearest-neighbour transfer remains. In this case the density of states is the elliptical integral with the logarithmic singularity at the centre. For finite α, also next-nearest-neighbour and further transfers are included. This shifts the peak in the density of states to the lower band edge. The density of states drawn in figure 1 shows a remnant of this peak.

§ 3. Numerical results

The numerical calculation is performed as follows. The N (typically $N = 400$, $N < L^2$) localized states are randomly chosen with probability c $(= N/L^2)$ on an $L \times L$ square lattice with lattice constant a. In this procedure, periodic boundary

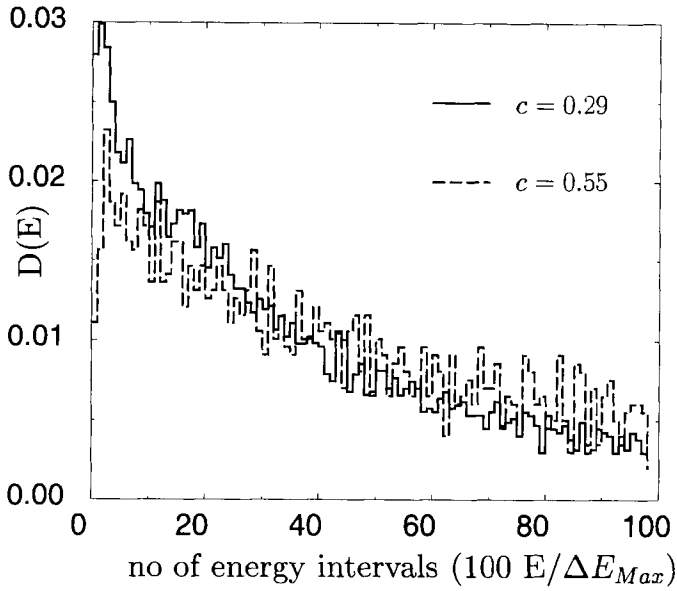

Figure 1. The density of states for two different concentrations is drawn. The increase in the density of states towards small energy values is due to the two-dimensionality of the system. Since $\alpha = 0.5/a$ (as in figure 1 and in figure 2) was chosen, no peaks arising from dangling bonds occur.

conditions are used. The coordinates of the localized states are distributed randomly while multiple occupation is prohibited.

For example, for $r_0 = a$ the classical (bond) percolation threshold is near $c \approx 0.5$. For any combination of pairs the off-diagonal elements have to be computed for the Hamiltonian (1) with the hopping element (2). The resulting matrix is diagonalized numerically using standard orthogonal decomposition methods. It is important to note that, in contrast with the corresponding matrix of the Anderson model, we do not obtain sparsely occupied matrices. This requires more numerical effort and leads to a limitation of the matrix size. We diagonalized matrices not larger than 400×400. As a result the distribution curves fluctuate more strongly than in the case of nearest-neighbour hopping models, where the matrices can be significantly larger. However, in order to improve the statistics, we performed an average over typically 30 diagonalizations.

3.1. *Level spacing distribution*

The level spacing distribution $P(s)$ of our model is analysed and compared with the Poisson distribution and with the distribution of the Gaussian orthogonal ensemble (GOE) ($P^{G}(s) = (\pi s/2)\exp(-\pi s^2/4)$). The choice of the GOE is because our Hamiltonian obeys time reversal symmetry. As one can see in figure 2 the level statistics for the quantum percolation regime do not follow the GOE regime. In particular, for $s > 2$ the distribution decays more weakly than the GOE. This is in agreement with the prediction by Aronov *et al.* (1994, 1995) for the situation near the Anderson-type metal–insulator transition. It can be interpreted as the domination of the statistics for larger level spacings by weakly overlapping states. According to our results not only is this a feature near the metal–insulator transition but it is present in

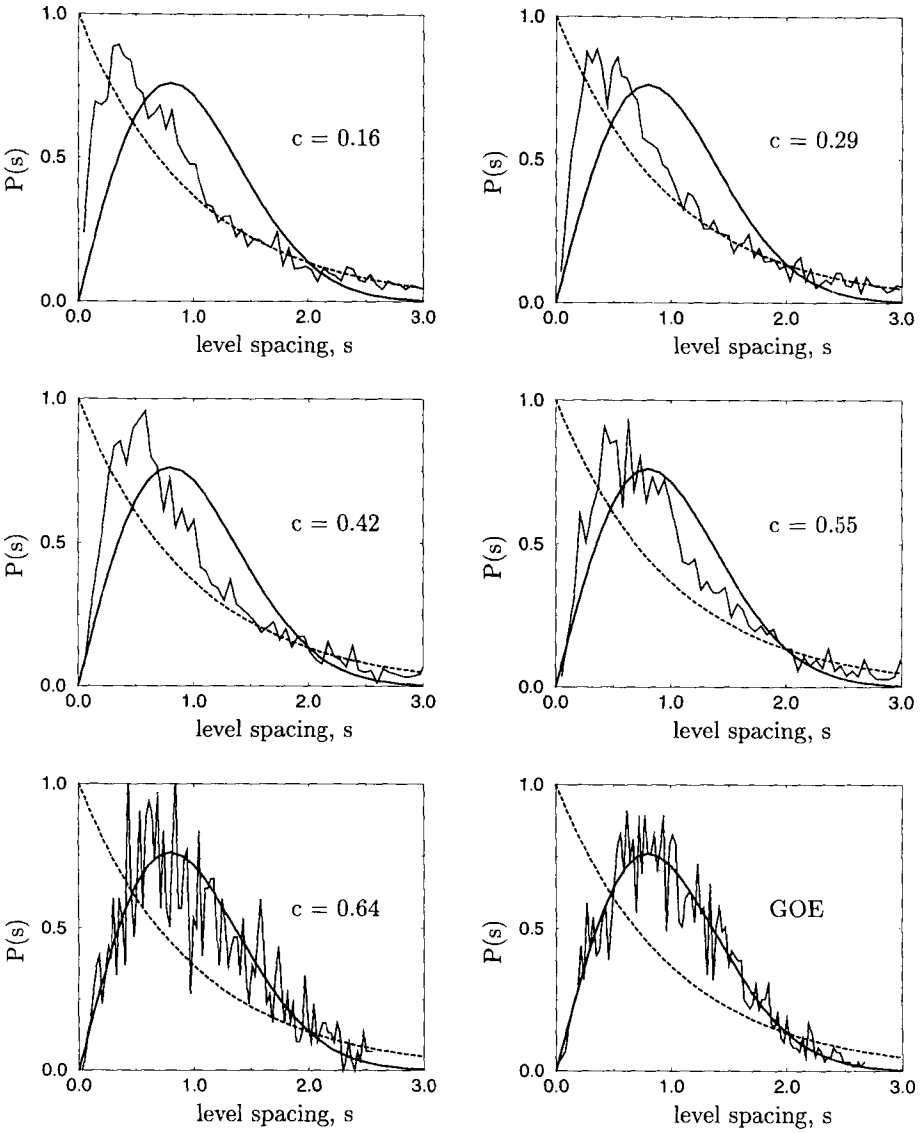

Figure 2. For different concentrations, below and above the classical percolation threshold, the level spacing distribution is drawn. It is compared with the Wigner and the Poisson distributions. Note that for $s > 2$ the distribution decays slower than predicted by the Wigner distribution. The parameters for this plot are $a = 0.5/a$ with the lattice constant a and $r_0 = a$. For comparison we show the result for the GOE of a matrix of the same size.

the whole doping range. In general the level repulsion of the quantum percolation model is weaker than that for the GOE. In order to investigate this behaviour in more detail we analyse the Δ statistics of the eigenvalue spectra. The latter is the mean square deviation of the energy levels from a straight line and is defined for a different number of levels n as (Metha 1991)

$$\Delta(n) = \frac{1}{n} \min_{A,B} \left(\int_0^n [N(E) - AE - B]^2 \, dE \right). \tag{3}$$

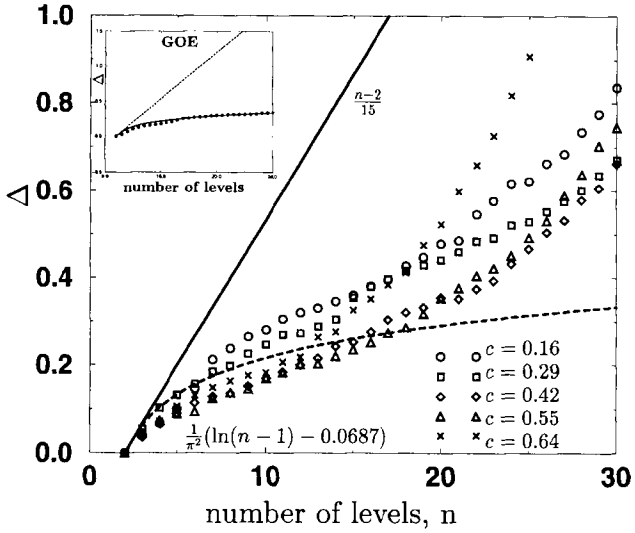

Figure 3. For the same concentrations and parameters as in figure 2 the results of the calculated Δ statistic are plotted. The transition from more Poisson like to more Wigner like and back to a Poisson-like distribution can be clearly seen in this plot. The level repulsion is strongest near the classical percolation threshold. Again for comparison the GOE is shown in the inset.

Here $N(E)$ is the integrated density of states. The result is shown in figure 3. The Δ statistics indicate the following behaviour for the doping dependence of the system. For low doping, far below the classical percolation threshold, the system shows only weak level repulsion and a tendency towards Poisson statistics. This is expected from usual arguments because well separated localized states are almost independently distributed, leading to a Poisson distribution. For moderate doping, in the vicinity of the classical percolation threshold, the level repulsion increases and the system shows a tendency towards the Wigner statistics. This behaviour indicates the beginning of the formation of overlaps between the states. As a result the eigenvalues experience level repulsion. However, this tendency is reversed when the doping concentration is further increased above the percolation threshold. A possible explanation is a tendency towards uncorrelated k-space states of the fully doped (pure 2D) system.

3.2. *Localization properties*

To investigate the transition between spatially localized states and extended states the sensitivity of the eigenvalues with respect to a change in the boundary conditions is considered (Hatsugai and Lee 1993). The Peierls substitution of the hopping matrix elements $t \rightarrow t\exp(\mathrm{i}\phi\,\Delta x)$ is used to vary continuously the boundary conditions in the Hamiltonian. Expanding the exponential function enables us to use perturbation theory (Edwards and Thoules 1974):

$$\mathbf{H} \rightarrow \mathbf{H} + \mathbf{H}_\phi, \tag{4}$$

$$\mathbf{H}_\phi = \sum_{ij} [\mathrm{i}t_{ij}(x_i - x_j)\phi c_i^\dagger c_j + \mathrm{hc}], \tag{5}$$

where x_j is the x coordinate of site j. Since $\mathbf{H}_\phi$ is purely imaginary, the eigenvalues of the Hermitian Hamiltonian are affected only in second-order perturbation theory:

$$\overline{\Delta E_M} = \sum_{N \neq M} \overline{\frac{|\langle \psi_M | \mathbf{H}_\phi | \psi_N \rangle|^2}{E_M - E_N}}. \tag{6}$$

For the numerical calculation the average is taken over an ensemble of (typically 30) matrices. N runs from $M - 10$ to $M + 10$ since mainly the nearest energy levels contribute to ΔE. $\overline{\Delta E_M}$ can be identified with the conductivity via the Kubo–Greenwood formula (Thouless 1974). Equation (6) is also known as the Thouless formula for the conductivity.

§4. Discussion

A numerical investigation can give only information about localization lengths smaller or comparable with the system size (Montambaux 1995). The transition from localized to delocalized states, shown in figure 4, may indicate a real transition to delocalized states in the infinite system. At least it will indicate a transition from exponentially to algebraically decaying states. Furthermore, figure 4 shows that with increasing α the cross-over from localized to extended states becomes more abrupt while the absolute value of the energy shift decreases. α^{-1}, the characteristic length scale of the hopping processes, is always much smaller than the system size.

In conclusion, we find a clear indication of a qualitative change of the system in terms of the level statistics as we go through the percolation threshold as shown in figures 2 and 3. This effect depends on the strength c of doping as well as on the range α of the transfer. To explain the onset of delocalization for the normal state of the high-T_c cuprates with our model the diameter of the polaronic states should be chosen as $r_0 \approx 4a$. This size is motivated by spatial inhomogeneities seen in experi-

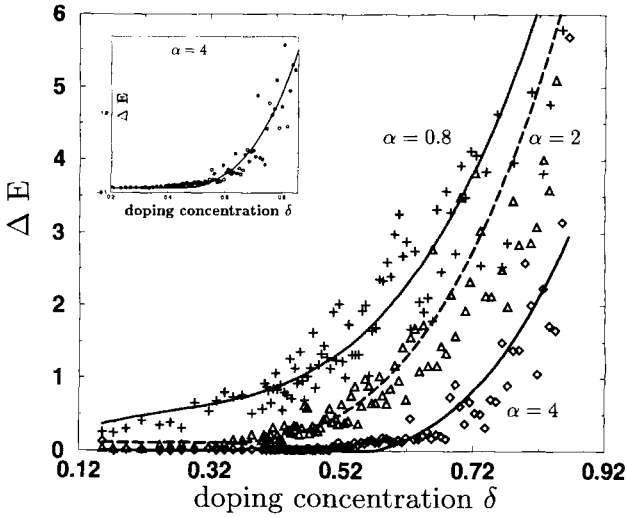

Figure 4. For different values of α (in units of the inverse lattice constant) the sensitivity to the boundary conditions is shown as a dependence on the doping concentration c. A transition from localized to delocalized states can be seen, which for larger α becomes more abrupt as is shown in the inset. For this calculation, again $r_0 = a$.

mental observations (see for example the inelastic neutron scattering data on $ErBa_2Cu_3O_x$ obtained by Mesot *et al.* (1993) which were interpreted with similar cluster sizes). Such polaronic states will give a percolation threshold for a doping concentration $c \approx 0.05$. Therefore, the transition from localized to delocalized states will occur near this concentration if $r_0 \approx 4a$. We note that the size r_0 of the localized states can always be chosen in a way such that the insulator–metal transition can be explained. Therefore the major aim of this paper is not to describe this transition in the cuprate superconductors but to investigate the level statistics around such a transition.

§ 5. Conclusion

A quantum percolation model realized with disorder of Lifshitz type which differs from the intensively investigated Anderson model owing to the inclusion of long-range transfer and non-diagonal disorder shows interesting aspects when its level statistics are investigated. We find level repulsion which is largest near the classical percolation threshold and also upon doping a cross-over from weak to strong dependence of the energy levels on the boundary conditions.

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