Level statistics and localization in a 2D quantum percolation problem

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A two dimensional model for quantum percolation with variable tunneling range is studied. For this purpose the Lifshitz model is considered where the disorder enters the Hamiltonian via the nondiagonal elements. We employ a numerical method to analyze 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 crossover from a GOE type behavior to a Poisson like distribution is indicated. The localization properties are calculated by using the sensitivity to boundary conditions and we find a strong crossover from localized to delocalized states.

The statistics of energy levels in complicated quantum systems has been a subject of research for several decades. It started with the study of energy levels in atomic nuclei \cite{1}, then the statistics of electronic states in atoms was investigated \cite{2}, and more recently the statistics of electrons in quantum dots (also known as “artificial” atoms) \cite{3}. A surprising result of most of these approaches was that the statistics of energy levels is 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, e.g., by the level spacing distribution \( P(s) \) which goes like \( s^\beta \) for small \( s \). The exponent \( \beta (=1,2,4) \) characterizes the universality class \cite{4}. In contrast to this repulsive behavior (Wigner–Dyson distribution) the assumption of statistically independent energy levels would lead to a Poisson distribution \( P(s) = e^{-s} \). 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 atoms like 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 due to Anderson localization \cite{5}. Approaches to the role of level statistics for the Anderson transition \cite{6} were presented by several authors, and a model for quantum percolation for nearest neighbor transfer was investigated in Ref. \cite{7}. Recently it was found \cite{8} that the divergence of the localization length \( \xi \) 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.

The purpose of this paper is to study a quantum percolation model where the transfer is not only between nearest neighbors but where the transfer rate decays exponentially with distance. Moreover, in contrast to Anderson’s model for localization we study disorder in the off-diagonal part of the Hamiltonian. This is also known as Lifshitz type of disorder. This model is motivated by physical systems. One example is a two-dimensional array of quantum dots \cite{9}. Our model is also motivated by the analogous picture of variable range hopping in solids \cite{10}. A third example for this model is the class of low doped high–\( T_c \) cuprates. Here the charge carriers are holes in two–dimensional CuO\(_2\) layers. It seems that disorder and phase separation play an essential role in these systems \cite{11,12}. The two–dimensional copper oxide plane is separated into hole rich conducting and magnetically correlated (insulating) areas. A possible origin for phase separation are polaronic states that are discussed in Refs. \cite{13,14}. Therefore our model can describe a transition or at least a crossover 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. \cite{14} of low doped \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) 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. \cite{15} for a sample with doping concentrations of \( x \approx 0.04 \) found a conductivity of hopping type near localization below 20 K.

Our model for quantum percolation corresponds to the Hamiltonian

\[
H = \sum_{i,j} (t_{ij} a_i^\dagger a_j + h.c.),
\]

with the following off–diagonal (hopping) matrix elements.
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 type disorder \[ \text{GOE}. \] The exponential decay of the localized wave functions leads to an exponentially decay of the hopping rate with distance on the inverse decay length $\alpha$. The spatial extension of the localized states, e.g., given by the size of a polaron, is expressed as Lifshitz type disorder [16]. The exponential decay of the hopping rate with distance on the inverse decay length $\alpha$.

For example, for $t_{ij} > r_0$, 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 $\alpha$, is the fact that the density of states is smoothed out in contrast to the sharp peaks found for nearest neighbor transfer [6]. The smooth density of states is easier to analyze with the methods of random matrix theory. The density of states is shown in fig. 2. It shows a broad peak near the lowest eigenvalue.

The numerical calculation is performed as follows. The $N$ (typically $N = 400$, $N < L^2$) localized states are randomly chosen with probability $c (c = N/L^2)$ on an $L \times L$ square lattice with lattice constant $a$. In this procedure periodic boundary 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 [6] with the hopping element [6]. The resulting matrix is diagonalized numerically using standard orthogonal decomposition methods. It is important to notice that in contrast to the corresponding matrix of the Anderson model we do not obtain a sparsely occupied matrices. This requires more numerical effort and leads to a limitation of the matrix size we can diagonalize to matrices not larger than $400 \times 400$. As a result the distribution curves fluctuate stronger than in the case of nearest neighbor hopping models, where the matrices can be significantly larger.

The level spacing distribution $P(s)$ of our model is analyzed and compared with the Poisson distribution and with the distribution of the Gaussian orthogonal ensemble (GOE, $P^G(s) = \pi s^2 e^{-\pi s^2}$). The choice of the GOE is due to the fact that our Hamiltonian obeys time reversal symmetry. As one can see in fig. 2 the level-statistics for the quantum percolation regime does not follow the GOE regime. In particular, for $s > 2$ the distribution decays slower than $P^G(s)$. This is in agreement with the prediction by Aronov et al. [4] 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 this is not only a feature near the metal insulator transition but it is present in the whole doping range. In general the level repulsion of the quantum percolation model is weaker than the one for the GOE.

In order to investigate this behavior in more detail we analyze the $\Delta_3$ statistics of the eigenvalue spectra. The latter is defined for a different number $n$ of levels as [4]

\[
\Delta_3(n) = \frac{1}{n} \min_{A,B} \int_0^n (St(x') - Ax' - B)^2 dx'.
\]

Here $St(x')$ is the staircase function. The result is shown in fig. 3. The $\Delta_3$ statistics indicates the following behavior 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 common 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 behavior 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 two-dimensional) system.

To investigate the transition between spatially localized states and extended states the sensitivity of the eigenvalues with respect to a change of the boundary conditions is considered [7]. The Peierls substitution of the hopping matrix elements $t \rightarrow te^{i\phi \Delta x}$ is used to vary continuosly the boundary conditions in the Hamiltonian. Expanding the exponential function enables us to use perturbation theory [18]

\[
H \rightarrow H + H_\phi
\]

\[
H_\phi = \sum_{ij} iH_{ij}(x_i - x_j)|\phi c_j^+ c_j + h.c.,
\]

where $x_j$ is the $x$-coordinate of site $j$. Since $H_\phi$ is purely imaginary the eigenvalues of the Hermitean Hamiltonian are affected only in second order perturbation theory

\[
\Delta E_M^2 = \sum_{N \neq M} \frac{|\langle \psi_M | H_\phi | \psi_N \rangle|^2}{E_M - E_N}.
\]

For the numerical calculation the average is taken over an ensemble of (typically 30) matrices. $N$ runs from $M - 10$
to \( M + 10 \) since the nearest energy levels contribute mainly to \( \Delta E \). \( \Delta E_M \) can be identified with the conductivity via the Kubo–Greenwood formula [19]. Eqn. (6) is also known as the Thouless formula for the conductivity.

A numerical investigation can only give information about localization lengths smaller or comparable with the system size [20]. The transition from localized to delocalized states, shown in fig. 1, 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, fig. 2 shows that with increasing \( \alpha \) the crossover from localized to extended states gets more abrupt while the absolute value of the energy shift decreases. \( \alpha^{-1} \), 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 the level statistics as we go through the percolation threshold as shown in figs. 1, 2. This effect depends on the strength of doping \( c \) as well as on the range of the transfer \( \alpha \). 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 experimental observations (see e.g. inelastic neutron scattering data of ErBa\(_2\)Cu\(_3\)O\(_{4-x}\) by Mesot et al. [21] which are interpreted with similar cluster sizes). Such polaronic states will give a percolation threshold for a doping concentration of \( c \approx 0.05 \). Therefore, the transition from localized to delocalized states will occur near this concentration if \( r_0 \approx 4a \).

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Figure captions

FIG. 1. 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 distribution. Note that for \( s > 2 \) the distribution decays slower than predicted by the Wigner distribution. The parameters for this plot are \( \alpha = 0.5/a \) with the lattice constant \( a \) and \( r_0 = a \) For comparison the inset shows the result for the GOE ensemble of the same size.

FIG. 2. For the same concentrations and parameters as in fig. 1 the results of the calculated \( \Delta_3 \) statistic is plotted. The transition from a more Poisson like to a 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 ensemble is shown in the inset.

FIG. 3. The density of states for two different concentrations is drawn. The increase of the density of states towards small energy values is due to the two-dimensionality of the system. Since \( \alpha = 0.5/a \) as in fig. 1 and in fig. 2 was chosen no peaks from parts separated from the percolation backbone occur.

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FIG. 4. For different values of $\alpha$ (in units of the inverse lattice constant) the sensitivity to the boundary conditions is shown in dependence of the doping concentration $c$. A transition from localized to delocalized states can be seen which for larger $\alpha$ gets more abrupt as can be seen in the inset. For this calculation $r_0$ is again $r_0 = a$.
fig. 1
fig. 2
fig. 3

![Graph showing the distribution of energy intervals](image)

- $c = 0.29$
- $c = 0.55$

no of energy intervals (100 $E/\Delta E_{Max}$)
fig. 4