Dynamical Aspects of Localisation in 2D Quantum Percolation

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Motivation

For classical percolation above a critical concentration of accessible sites, the so called percolation threshold p_c, a spanning cluster exists, allowing for transport. In the quantum case, the existence of a spanning cluster does not guarantee an extended wave function. Scattering and interference effects at the irregular boundaries of the cluster may lead to localisation (absence of diffusion) of a quantum particle. Then extended states may only exist above the quantum percolation threshold p_q. It is clear, that $p_c \leq p_q \leq 1$. The question is, whether p_q equals one of the boundaries. For the three-dimensional (3D) case, results in the literature agree on $p_c < p_q < 1$ (cf. Ref. [1]).

Controversy for the 2D case

In 2D, the situation is less clear. The physical community is divided in one group in favour of $p_q = 1$ and another claiming $p_q < 1$ (see [2] and references therein). The most striking argument against $p_q < 1$ is the one parameter scaling theory [3], according to which arbitrary small disorder leads to complete localisation in 2D. Several groups, however, presented results which are in favour of a quantum percolation threshold below unity. In this respect, the band centre states seem to be of particular importance. The bipartiteness of the lattice implies that for $E = 0$ extended states do not violate the one parameter scaling theory [4]. Renewed interest in 2D quantum percolation came up with recent experimental findings of metallic behaviour in dilute weakly disordered Si-MOSFETs [5]. Among other possible explanations, percolative scenarios are promising candidates to describe this effect. Quantum percolation models have also been applied for modelling the influence of an inhomogeneous charge density on the transport properties in graphene [6].

Model & Methods

We start from a generic tight-binding Hamiltonian

$$H = \sum_{i=1}^{N} \epsilon_i c_i^\dagger c_i - t \sum_{\langle ij \rangle} (c_i^\dagger c_j + \text{H.c.})$$

on a square lattice with $N = L^2$ sites and periodic boundary conditions. Drawing the on-site energies ϵ_i from the bimodal distribution

$$p[\epsilon_i] = p\,\delta(\epsilon_i - \epsilon_A) + (1-p)\,\delta(\epsilon_i - \epsilon_B)$$

we obtain the quantum percolation Hamiltonian in the limit $\epsilon_B \to \infty$. In this situation non-interacting electrons move on a random ensemble of $\bar{N}$ lattice points which, depending on p, may span the entire lattice or not. For this system we calculate the recurrence probability of a particle to a given site, $P_R(\tau)$, which for $\tau \to \infty$ may serve as a criterion for localisation [6]. While for extended states on the spanning cluster $P_R(\tau \to \infty) = 1/\bar{N}$, which scales to zero in the thermodynamic limit, a localised state will have a finite value of $P_R(\tau)$ as $\bar{N} \to \infty$. Following the time evolution of a localised initial state, $P_R(\tau)$ is given by the modulus square of the wave function at its starting position at time τ. We therefore expand the time evolution operator $U(\tau) = \mathrm{e}^{-\mathrm{i}H\tau}$ in Chebyshev polynomials [7] allowing for a very efficient method to calculate the dynamics of the system.

Chebyshev expansion

(Weiße, Wellein, Alvermann, Fehske, RMP **78**, 275 (2006))

As a first step, the Hamiltonian has to be rescaled ($H \to \tilde{H}$) to the definition interval of the Chebyshev polynomials $]-1, 1[$, leading to

$$U(\tau) = \mathrm{e}^{-\mathrm{i}(a\tilde{H}+b)\tau} = \mathrm{e}^{-\mathrm{i}b\tau} \left[c_0 + 2\sum_{k=1}^{M} c_k T_k(\tilde{H}) \right] .$$

The expansion coefficients c_k are given by

$$c_k = \int_{-1}^{1} \frac{T_k(x) e^{-\mathrm{i}ax\tau}}{\pi\sqrt{1-x^2}} \mathrm{d}x = (-\mathrm{i})^k J_k(a\tau) ,$$

where J_k denotes the Bessel function of kind k. Due to the fast asymptotic decay of the Bessel functions

$$J_k(a\tau) \sim \frac{1}{\sqrt{2\pi k}} \left(\frac{\mathrm{e}a\tau}{2k} \right)^k \quad \text{for} \quad k \to \infty ,$$

the higher-order expansion terms vanish rapidly. The order M at which we truncate the infinite series determines the accuracy of the algorithm and should be adapted according to the time step used (reasonable choice: $M \sim 1.5a\tau$). As compared to the standard Crank-Nicolson algorithm, the Chebyshev expansion permits the use of a considerably larger time step to achieve the same accuracy.

Local distribution approach

(Alvermann, Fehske, J. Phys. Conf. Series, **35**, 145 (2006))

While all characteristics of a certain material are determined by the corresponding distribution $p[\epsilon_i]$, each actual sample of this material constitutes only one particular realisation $\{\epsilon_i\}$. Hence, we have to focus on site-dependent quantities like the local density of states (LDOS) at lattice site i,

$$\rho_i(E) = \sum_{m=1}^{N} |\langle i|m\rangle|^2 \, \delta(E - E_m) .$$

The (energy resolved) LDOS measures the contribution of each eigenstate $|m\rangle$ to the local density at i,

$$n_i(\tau) = |\psi(\mathbf{r}_i, \tau)|^2 = \Big| \sum_{m=1}^{N} \mathrm{e}^{-\mathrm{i}E_m t} \langle m|\psi(0)\rangle \langle i|m\rangle \Big|^2 .$$

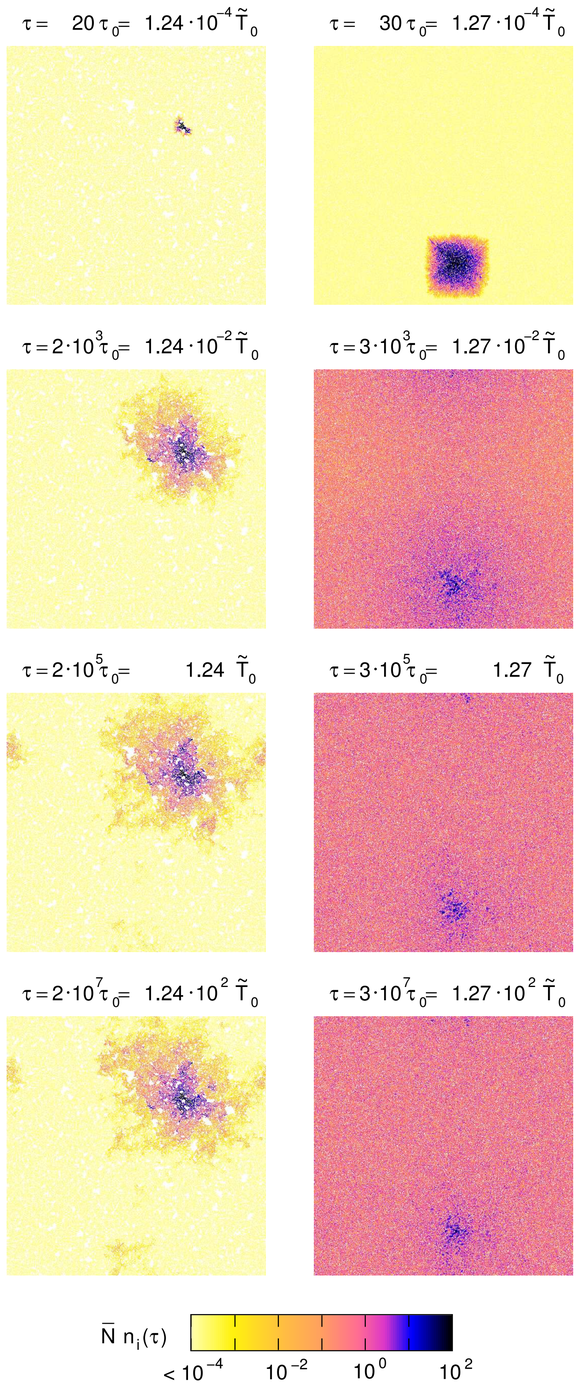
Evolving an arbitrary initial state in time, we only have access to $n_i(\tau)$, containing contributions of the whole spectrum. Probing different sites in the crystal and recording n_i results in the corresponding probability distribution $f[n_i]$. To alleviate the problem of statistical noise we consider the distribution function

$$F[n_i] = \int_0^{n_i} f[n_i'] \, \mathrm{d}n_i' .$$

In the thermodynamic limit, $f[n_i]$ (or $F[n_i]$) is independent of the actual realisation $\{\epsilon_i\}$ and the chosen sites, but depends solely on $p[\epsilon_i] \rightsquigarrow F[n_i]$ characterises $H(p[\epsilon_i])$, not only $H(\{\epsilon_i\})$. For an extended state the amplitude of the wave function is more or less uniform $\rightsquigarrow f[n_i]$ sharply peaked and symmetric around $1/\bar{N}$. For localised states n_i strongly fluctuates throughout the lattice $\rightsquigarrow f[n_i]$ is very asymmetric with a long tail and $\langle n_i \rangle \to 0$. The distribution function $F[n_i]$ steeply rises for extended states whereas for localised states the increase extends over several orders of magnitude. Note, that n_i takes into account the whole spectrum, and we may not examine localisation with energy resolution as by the LDOS. But, starting from p_c and increasing p, we may detect the first occurrence of an extended state somewhere in the spectrum and thus p_q.

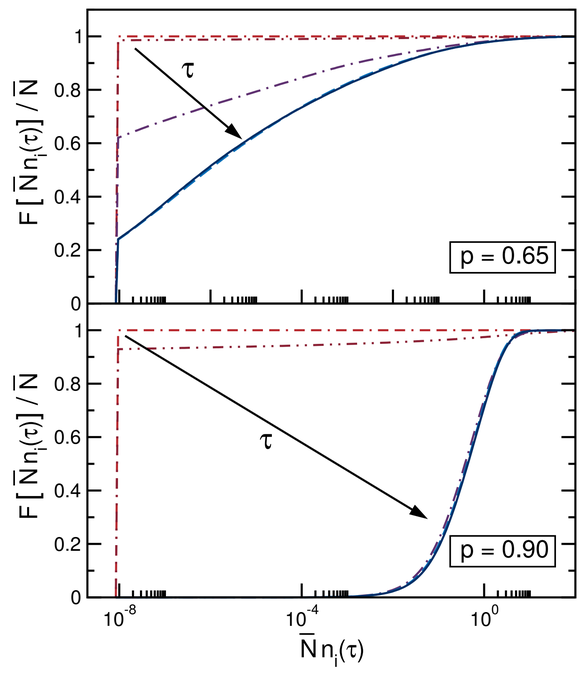
Results

Time evolution



Normalised local density $\bar{N}n_i(\tau)$ for an initially localised state on the spanning cluster of a $N = 512^2$ lattice for $p = 0.65$ (left) and $p = 0.90$ (right). Timescales: $\tau_0 = 1/t$, $\tilde{T}_0 = \bar{N}\tau_0$.

For small $p > p_c = 0.593$, the initially localised state spreads within a short time over a finite region of the cluster. Also for very long times, this extension does not change significantly anymore. For large p, the spreading is even faster, but here the state is not confined to some finite region, but n_i is transfered to the whole cluster. The darker spots in the vicinity of the initial position are due to contributions from localised states.

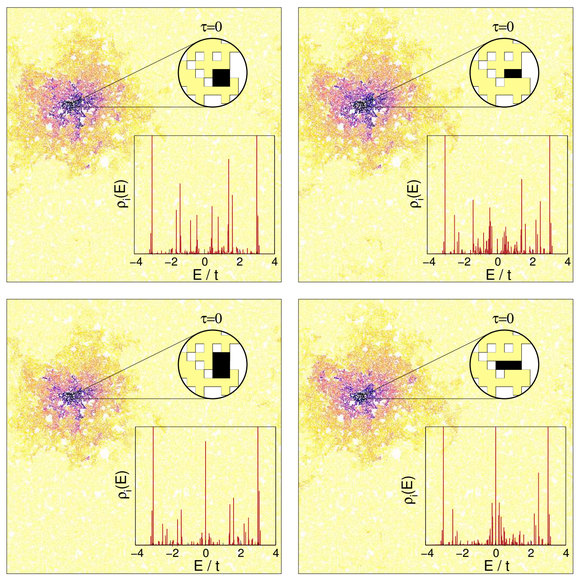


Distribution functions of the local density, $F[\bar{N}n_i]$. The curves correspond to the data in the previous figure.

The distribution function also substantiate the notion of a localised and an extended state.

Initial conditions

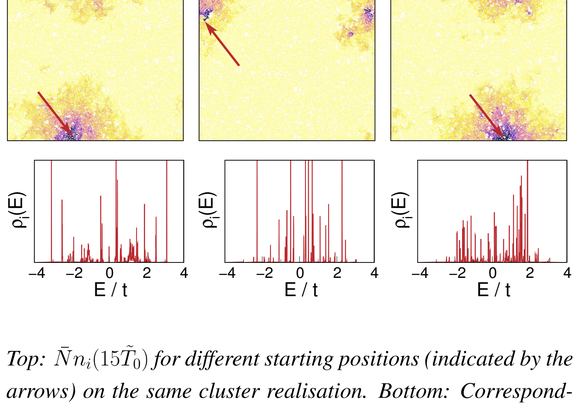
For one particular cluster realisation we fix the centre of the initial wave function. The configurations have the same energy $E = 0.5t$, but differ in the number of sites with non-vanishing amplitudes for $\tau = 0$ and thus in their LDOS.



$\bar{N}n_i(15\tilde{T}_0)$ for different initial states on one particular cluster realisation ($N = 512^2, p = 0.65$). Insets: Initial configurations and LDOS of the initial states.

Although the evolution of the states differs in detail, on a coarse grained scale they behave similarly. The detailed structure is determined by the LDOS at $\tau = 0$. Changing the energy of the initial state has a similar effect as changing the initial configuration. Thus the main characteristics of the time evolution is determined by the cluster structure, the initial state has only minor influence.

Clearly, at another position within the cluster, the local cluster structure differs and affects the evolution of ψ. The random nature of the cluster guarantees a similar structure above a certain scale. So we expect also only a minor effect of the starting position.

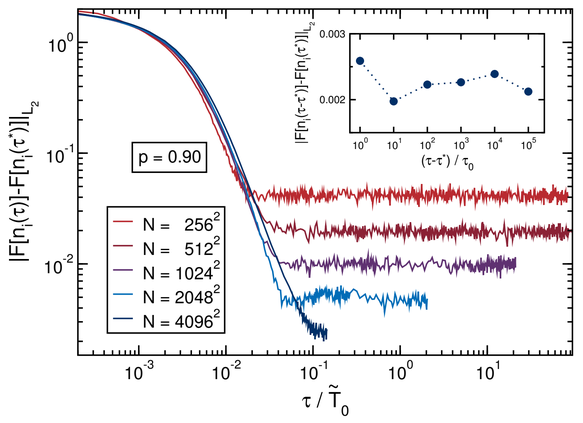


Top: $\bar{N}n_i(15\tilde{T}_0)$ for different starting positions (indicated by the arrows) on the same cluster realisation. Bottom: Corresponding LDOS at $\tau = 0$.

This reasoning also holds for different cluster realisations. Despite the variation from one configuration to the next, in the distribution sense, we may extract the basic features of the time evolution from one randomly chosen configuration.

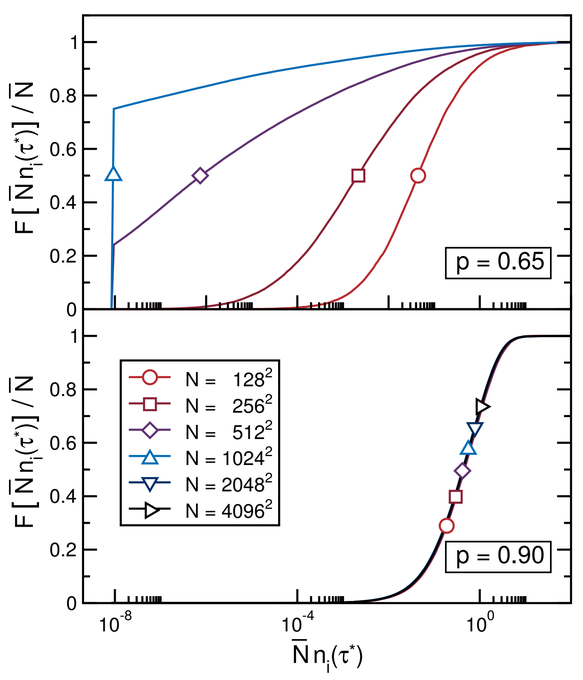
Finite-size scaling

In view of a finite-size scaling of the numerical data we first have to ensure that the obtained distribution function has already become quasi-stationary. To check this, we calculate the L_2 norm of the difference between two distribution functions at different times. Due to fluctuations, we cannot expect this quantity to vanish completely even for large times.



L_2 norm of the difference between the distribution function at time τ and time τ^*, for which $F[n_i(\tau^*)]$ is quasi-stationary. Inset: Fluctuations of $F[n_i(\tau)]$ in the quasi stationary regime ($N = 4096^2$; note the different time scale).

For $\tau \gtrsim 0.1\tilde{T}_0$ we have reached the quasi-stationary regime for all considered system sizes. At this time, the wave function has reached its maximum extension and the further development is governed by amplitude fluctuations from site to site. In this regime, the difference between the distribution functions does not depend on time anymore, which is a clear indication of random fluctuations without additional drift motion. This allows for a determination of a quasi-stationary distribution function together with an error estimation and enables us to compare different system sizes.



Finite-size scaling of $F[n_i(\tau^*)]$ in the quasi-stationary regime.

For the two different occupation probabilities, we get two completely different behaviours: While for $p = 0.65$ the distribution function shifts towards smaller values on increasing the system size, for $p = 0.90$ it is not affected by the change of system size at all. The latter is the behaviour one would expect for an extended state.

Conclusion

For any numerical investigation of finite systems, the extrapolation to the infinite system is difficult. The high efficiency of the Chebyshev expansion technique, however, allows us to study the time evolution of much larger systems than any others previously in the literature. To best of our knowledge, we conclude from our data after careful finite-size scaling, that for the 2D quantum percolation model $p_q < 1$.

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