Localisation delocalisation transition in disordered electron systems

Gerald Schubert[1], Alexander Weiße[2] and Holger Fehske[1]

[1]Institut für Physik, Universität Greifswald, Germany

[2]University of New South Wales, Sydney, Australia

A proper description of disordered systems should focus on distribution functions. Using the kernel polynomial method (KPM) – a refined Chebyshev expansion technique – we calculate the probability distribution of the local density of states (LDOS) for large finite clusters (up to 100^3). As the distribution of the LDOS shows a significant change at the disorder induced localisation-delocalisation (LD) transition, the so-called typical DOS, defined as the geometric mean, emerges as a natural order parameter.

Anderson transition

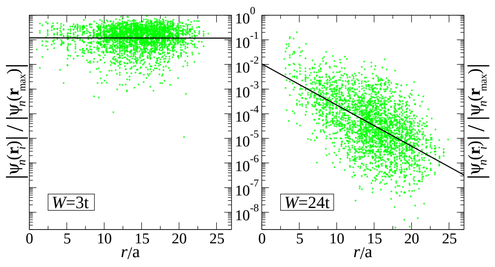
To underline the reliability and quality of our LDOS-KPM approach, we compare our findings with known results for the well examined Anderson model:

$$H = -t \sum_{\langle ij \rangle} [c_i^\dagger c_j + \text{H.c.}] + \sum_{j=1}^{N} \epsilon_j c_j^\dagger c_j \,,$$

$$p(\epsilon_j) = \frac{1}{W}\, \theta\left(\frac{W}{2} - |\epsilon_j|\right) \,.$$

For $d > 2$ a LD transition occurs at finite values of disorder W. Thus we concentrate on the $3d$ case (with periodic boundary conditions), where analytical treatments fail and numerical investigation is costly. Considering the wavefunction, localisation effects can be discussed in terms of the the localisation length λ, being finite for localised states and infinite otherwise:

$$|\psi_n(\mathbf{r}_i)| \sim f(\mathbf{r}_i) \exp\left(-\frac{|\mathbf{r}_i - \mathbf{r}_{\max}|}{\lambda}\right) \,.$$

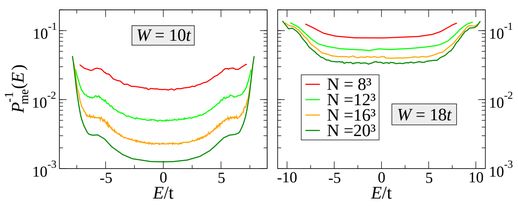


Decay of an electronic wavefunction ψ_n in the band centre as a function of distance $r = |\mathbf{r}_i - \mathbf{r}_{\max}|$. $N = 30^3$

Determining λ via ψ by exact diagonalisation (ED) restricts this method to small systems ($\lesssim 30^3$). Calculating ψ, also the inverse participation number (IPN)

$$P^{-1}(E_n) = \sum_{i=1}^{N} |\psi_n(\mathbf{r}_i)|^4 \,,$$

describing the number of sites with amplitudes markedly different from zero, is accessible. For localised states the IPN is independent of N, but vanishes for extended ones in the thermodynamic limit.



Mean IPN $P^{-1}_{\text{me}}(E) = \langle P^{-1}(E) \rangle$ for different system sizes.

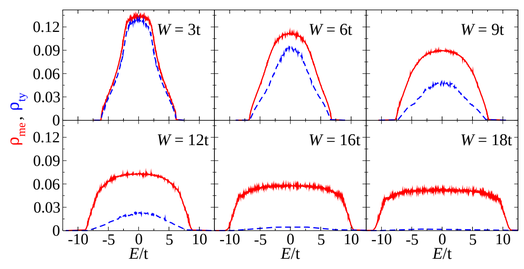
For the LD transition distributions of local quantities are of special interest [1]. We consider the LDOS,

$$\rho_i(E) = \sum_{n=1}^{N} |\psi_n(\mathbf{r}_i)|^2 \delta(E - E_n) \,,$$

connected with the local amplitudes of the wavefunctions at a given site i. Expanding the LDOS in a finite series of M Chebyshev polynomials and taking special care of the effects of the truncation, the calculation of $\rho_i(E)$ requires memory and CPU time scaling as $\mathcal{O}(N)$. The resolution of this approximation is $\sim M^{-1}$. Averaging over an ensemble of K_r realisations of disorder and K_s sites arithmetically and geometrically yields the mean and typical DOS:

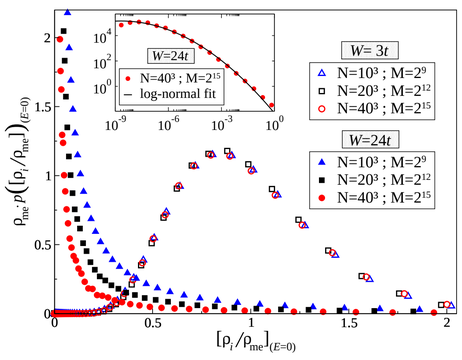
$$\rho_{\text{me}}(E) = \langle \rho_i(E) \rangle \,,$$
$$\rho_{\text{ty}}(E) = \exp\langle \ln(\rho_i(E)) \rangle \,.$$

While ρ_{me} is insensitive to localisation, ρ_{ty} allows for the distinction between localised ($\rho_{\text{ty}} \to 0$) and extended ($\rho_{\text{ty}} > 0$) states.



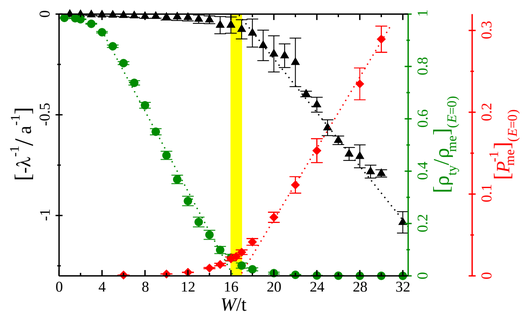
Mean and typical DOS for the Anderson model. $N = 50^3$, $M = 8192$, $K_s \times K_r = 32 \times 32$.

This behaviour of ρ_{ty} is due to different shapes of the probability densities $p(\rho_i)$ in the two regimes.



General shape and finite size scaling of the probability density of the LDOS $p[\rho_i(E = 0)]$ for the ratio $N/M = 1.95$. $K_s \times K_r = 10000 \times 100,\ 100 \times 100,\ 32 \times 32$ for $N = 10^3,\ 20^3,\ 40^3$.

For fixed N/M the shape of $p[\rho_i(E = 0)]$ is independent of the system size for low disorder. On the other hand, for strong disorder the distribution shifts towards smaller values with increasing N and becomes singular in the thermodynamic limit. In the localised regime the data agrees well with a log-normal fit.



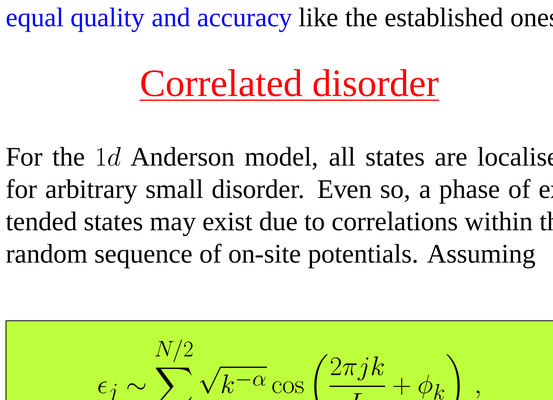
Comparing the obtained values for the critical disorder, it is obvious, that the LDOS yields a criterion of equal quality and accuracy like the established ones.

Correlated disorder

For the $1d$ Anderson model, all states are localised for arbitrary small disorder. Even so, a phase of extended states may exist due to correlations within the random sequence of on-site potentials. Assuming

$$\epsilon_j \sim \sum_{k=1}^{N/2} \sqrt{k^{-\alpha}} \cos\left(\frac{2\pi j k}{L} + \phi_k\right) \,,$$

we model a long-range correlated random sequence without any characteristic scale and with power-law decay of the Fourier transform of the two point correlation function [2]. While for small α the whole band is still localised, above a certain strength of correlation ($\alpha_c \gtrsim 2$), a phase of extended states exists, whose width saturates for $\alpha \gtrsim 5$.

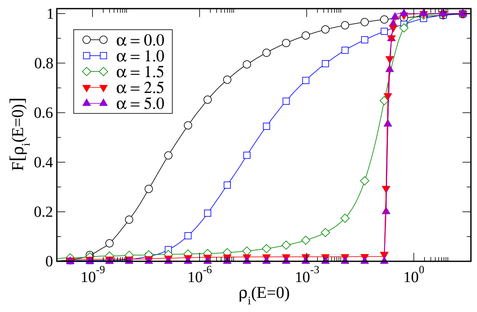


Mean and typical DOS for the Anderson model with correlated disorder. Lower panels: sequences of on-site potentials. $N = 125000, M = 32768, K_r \times K_s = 32 \times 32$.

Instead of analysing the probability density $p(\rho_i(E))$, it shows up, that the probability distribution

$$F[\rho_i(E)] = \int_0^{\rho_i(E)} p(\rho_i'(E)) d\rho_i'(E)$$

is the more suitable quantity, as due to the integration smaller ensembles are sufficient to extract the characteristics. While the smooth increase of $F[\rho_i]$ for localised states reflects a broad probability density $p(\rho_i)$, the extended regime is characterised by an almost steplike probability distribution which is due to $p(\rho_i)$ being sharply peaked at ρ_{me}.



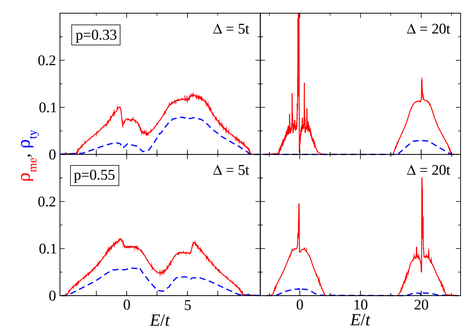
Probability distribution $F[\rho_i(E)]$ of the LDOS in the band centre for different values of correlation strength α. $N = 125000, M = 32768, K_r \times K_s = 32 \times 32$.

Quantum percolation

From the Anderson model, describing an alloy with an infinite number of composites, the class of site percolation models is obtained by assuming a binary distribution of on-site potentials [3]:

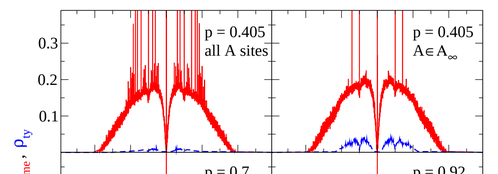
$$p(\epsilon_j) = p\, \delta(\epsilon_j - \epsilon_A) + (1 - p)\, \delta(\epsilon_j - \epsilon_B) \,.$$

For $\Delta = |\epsilon_A - \epsilon_B| > 4td$ the band separates into two sub-bands centred at ϵ_A and ϵ_B.



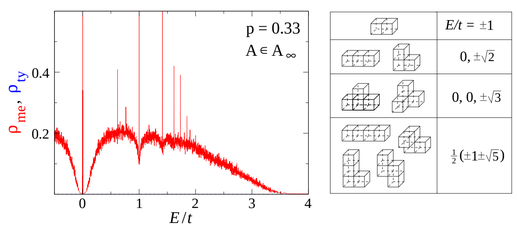
Mean and typical DOS for different occupation probabilities p and energy differences between the on-site potentials Δ. $N = 50^3, M = 32768, K_s \times K_r = 32 \times 32$.

In the limit $\epsilon_B \to \infty$ (keeping $\epsilon_A = 0$ fixed) the B-sites are completely inaccessible. In order to discuss localisation in this case, it is sufficient to consider the spanning cluster A_∞ only. Although many spikes in the spectrum are due to isolated islands, most of them persist even if the calculation is restricted to A_∞.



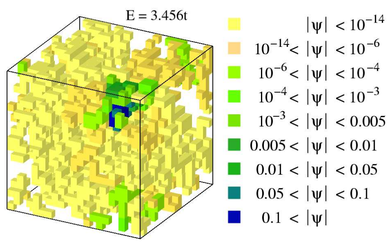
Mean and typical DOS in the limit $\epsilon_B \to \infty$ for different occupation probabilities p. $N = 50^3, M = 16384, K_s \times K_r = 32 \times 32$.

As the typical DOS vanishes at these special energies, these states are localised. It shows up, that they can be associated with localised states on some dead ends of the spanning cluster.

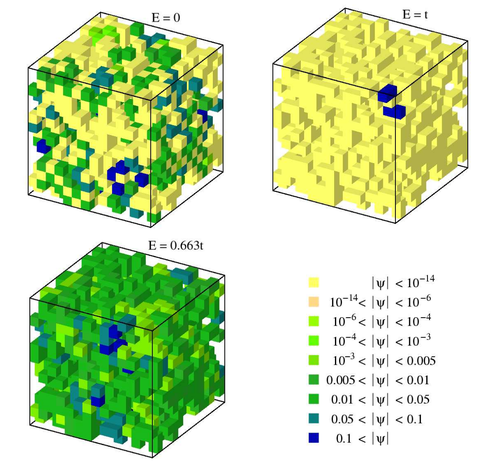


High resolution plot of the mean and typical DOS on A_∞ for $p = 0.33$. $N = 100^3, M = 32768, K_s \times K_r = 100 \times 100$. Right: Geometries of the dead ends and corresponding E_n.

To clarify the structure of these states, for some energies we calculate the amplitudes, comparing them with those for localised and extended states.

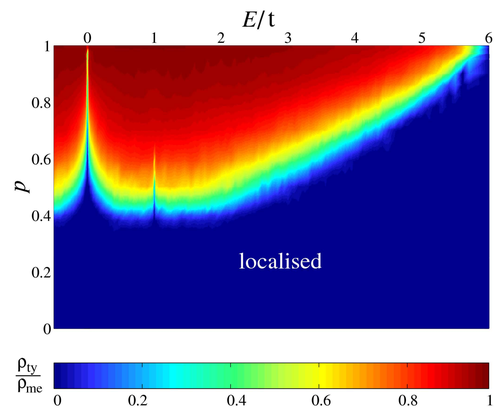


Amplitudes $|\psi_n(\mathbf{r}_i)|$ of a localised state. $N = 21^3$, $p = 0.33$.



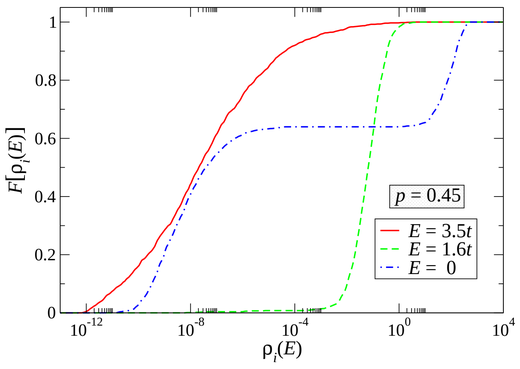
Amplitudes of the wavefunction $|\psi_n(\mathbf{r}_i)|$ on the spanning cluster of a 14^3 lattice with $p = 0.45$. Chequerboard state for $E = 0$, dead end state for $E = t$ and extended state for $E = 0.663t$.

Because of the high degeneracy of the $E = 0$ state, linear combinations are possible which span the whole cluster in a chequerboard structure of sites with vanishing and finite amplitudes. Although those states are extended in a sense, their alternating structure suppresses the conductance, giving rise to call them anomalously localised. Interestingly this pattern is rather robust and even persists if the boundary conditions are mismatched. In this case the chequerboard is connected to itself by sites of vanishing amplitudes. As the probability of finding specific dead end geometries, giving rise to special energies, decreases with their complexity, the spectral weight of more complicated clusters is reduced. Nevertheless, in principle they can be constructed for arbitrary values of E. Thus there exists a set of energies with localised states throughout the whole band and the spectrum seems to fragment into localised and extended states.



Normalised typical DOS $\rho_{\text{ty}}/\rho_{\text{me}}$ in the concentration energy plane. $N = 100^3$ (50^3) is used for $p \leq 0.5$ (> 0.5), $M = 16384, K_s \times K_r = 32 \times 32$.

Determining the value of p, below which all states are localised, fixes the quantum mechanical analogue p_q to the classical percolation threshold p_c, above which there exists a spanning cluster. As interference effects can lead to localisation, suppressing the conductance, it is not clear, if p_c and p_q are equal or differ. The obtained result confirms that $p_q(E) \gtrsim 0.4 > p_c \approx 0.31$. The most promising way to distinguish the different classes of states is again to look at the probability distribution of the LDOS $F[\rho_i(E)]$.



Probability distribution of the LDOS for three energies in the different regimes. $N = 53^3$, $M = 32768$, $K_s \times K_r = 32 \times 32$.

Differing either from those of localised states (smooth increase, corresponding to a very broad probability density) or from extended ones (steep increase at ρ_{me}, i.e. $p(\rho_i)$ being sharply peaked around its mean value), the special properties of the $E = 0$ state show up again. The two-step like function corroborates the assumption of a chequerboard structure of sites with vanishing and finite amplitudes.

[1] R. Abou-Chacra, P. W. Anderson and D. J. Thouless, J. Phys. C **6**, 1734 (1973).

[2] Francisco A. B. F. de Moura and Marcelo L. Lyra, Phys. Rev. Lett. **81**, 3735 (1998)

[3] C. M. Soukoulis, Qiming Li and Gary S. Grest, Phys. Rev. B. **45** 7724 (1992).

[4] G. Schubert, A. Weiße and H. Fehske, arXiv:cond-mat/0309015, cond-mat/0406212, cond-mat/0406750.