Available online at www.sciencedirect.com
SCIENCE DIRECT®
Physica B 359–361 (2005) 801–803
PHYSICA B
www.elsevier.com/locate/physb

Delocalisation transition in chains with correlated disorder

Gerald Schubert[a], Alexander Weiße[b], Holger Fehske[a,*]

[a]*Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald, 17487 Greifswald, Germany*
[b]*School of Physics, The University of New South Wales, Sydney, NSW 2052, Australia*

Abstract

We show that in the one-dimensional (1D) Anderson model long-range correlations within the sequence of on-site potentials may lead to a region of extended states in the vicinity of the band centre, i.e., to a correlation-induced insulator–metal transition. Thus, although still disordered, the 1D system can behave as a conductor.

PACS: 71.23.An; 32.15.Rn; 71.30.+h

Keywords: Disordered electron systems; Anderson metal–insulator transition

In the context of electronic transport in quasi-1D binary solids, polymer chains or biological molecules, recently, systems with correlations in the sequence of on-site energies attracted increasing attention [1]. The examination of models with correlated disorder is also challenging from a theoretical point of view. In 1D noninteracting electron systems with independent random atomic potentials all states are exponentially localised at any amount of disorder [2]. Internal correlations within the potential landscape, however, might cause a breakdown of the Anderson localisation phenomenon in 1D and 2D [3,4]. Such long-range correlated random sequences without any intrinsic scale are observed in several stochastic processes in nature [5]. One of their characteristics is the power-law decay of the Fourier transform of the two-point correlation function with the wavenumber of the random fluctuations, $\mathcal{F}(\langle\varepsilon_i\varepsilon_j\rangle) \sim 1/k^{\alpha}$. Based on these findings de Moura and Lyra [4] proposed an Anderson type model, $H = \sum_j \varepsilon_j c_j^{\dagger} c_j - t\sum_{\langle ij\rangle}[c_i^{\dagger} c_j + \text{h.c.}]$, with the following ansatz for the on-site potentials,

$$\varepsilon_j = v(\alpha)\sum_{k=1}^{N/2} k^{-\alpha/2}\cos(2\pi jk/N + \phi_k), \tag{1}$$

where the $N/2$ random phases ϕ_k are uniformly distributed in the interval $[0, 2\pi]$ and α controls the strength of the correlation. The case $\alpha = 0$ corresponds to strongest disorder and is almost

*Corresponding author. Tel.: +49 3834 86 4760; fax +49 3834 86 4701.
E-mail address: fehske@physik.uni-greifswald.de (H. Fehske).

0921-4526/$ - see front matter © 2005 Elsevier B.V. All rights reserved.
doi:10.1016/j.physb.2005.01.232

equivalent to the uncorrelated Anderson model with Gaussian distributed on-site potentials. In order to obtain comparable results each disordered sequence is normalised to variance $\sigma^2 = 1$, i.e. $v(\alpha) = (\sum_{k=1}^{N/2} k^{-\alpha}/2)^{-1/2}$. This ensures that both disorder and bandwidth remain finite in the thermodynamic limit.

In the theoretical investigation of disordered systems it turned out that distribution functions for the random quantities of interest take the centre stage [6]. Of particular importance is the probability density $p(\rho_i(E))$ of the local density of states (LDOS)

$$\rho_i(E) = \sum_{n=1}^{N} |\psi_{n,i}|^2 \, \delta(E - E_n). \tag{2}$$

For a given energy E, $\rho_i(E)$ measures the local amplitude of the wave function at Wannier site i and therefore contains direct information about the localisation properties. Contrary to the mean (arithmetically averaged) density of states, $\rho_{\mathrm{av}}(E) = \langle \rho_i(E) \rangle$, the LDOS becomes critical at the localisation transition. Concurrently, $p(\rho_i(E))$ was found to have essentially different properties for localised and extended phases [7]. Of course, the study of entire distributions is a bit inconvenient, and for practical calculations the so-called "typical DOS" (geometric average) $\rho_{\mathrm{ty}}(E) = \exp\langle \ln \rho_i(E) \rangle$ is frequently used. Since $\rho_{\mathrm{ty}}(E)$ vanishes at the Anderson transition it acts as a kind of "order parameter".

Numerically the LDOS distribution can be easily calculated with the kernel polynomial method [8]. The corresponding arithmetic and geometric averages ρ_{av} and ρ_{ty} are shown in Fig. 1. In contrast to the uncorrelated Anderson model we observe the following effects: (i) most notably, while for small finite values of α the typical DOS vanishes within numerical accuracy for the entire band, with stronger correlation a region of extended states appears near the band centre; (ii) for larger values of α a dip in ρ_{av} develops at the band centre, which might be a signature of the 1D DOS of the completely ordered system that is expected for infinitely strong correlation; (iii) even though on average the model is symmetric with respect to $E \to -E$ in Fig. 1 the averaged density

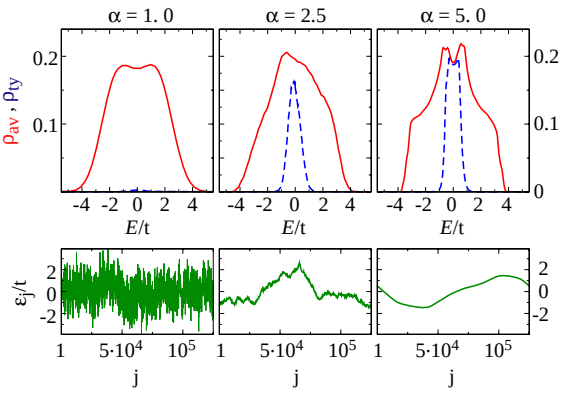

Fig. 1. Average (solid) and typical (dashed) DOS for the Anderson model with correlated disorder on a linear chain with 125,000 sites and different correlation strengths α. The typical DOS was calculated at $K_s = 32$ sites for $K_r = 32$ realisations of disorder using 32,768 Chebyshev moments, whereas for the average DOS only 256 Chebyshev moments and a random initial vector were used. Note that for $\alpha = 1$ $\rho_{\mathrm{ty}} < 10^{-4}\,\forall E$. The lower panels show one characteristic sequence of atomic potentials ε_j for each value of α.

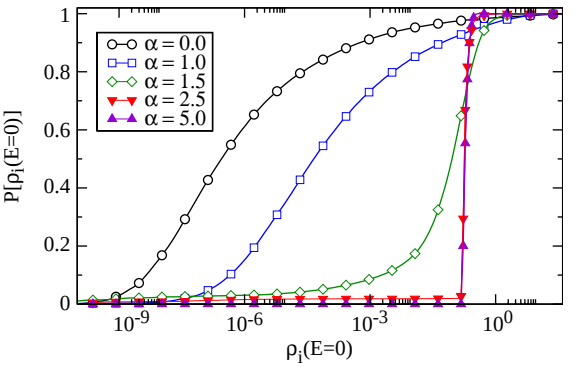

Fig. 2. Probability distribution $P(\rho_i)$ in the band-centre for different correlation strengths α (again $N = 125,000$, $M = 32,768$, $K_r \times K_s = 32 \times 32$).

of states shows a noticeable asymmetry for intermediate values of α. We fear that, due to the longer ranged fluctuations within the on-site potentials for increasing α, the considered rather large ensemble (32×32 realisations) is still insufficient to achieve a proper statistics.

Fig. 2 illustrates the behaviour of the probability distribution $P(\rho_i) = \int_0^{\rho_i} p(\rho_i') \, \mathrm{d}\rho_i'$. At small values of α, $P(\rho_i)$ reflects the characteristics of the LDOS distribution of localised states, i.e. large weight on

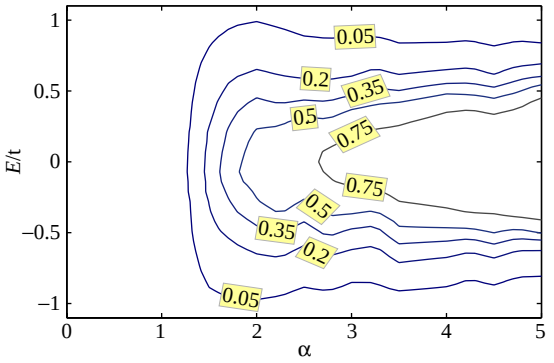

Fig. 3. Contour plot of R in the correlation-energy plane for the Anderson model with correlated disorder on a linear chain with 125,000 sites. In the calculation 32,768 Chebyshev moments and $K_r \times K_s = 128 \times 32$ realisations were used.

small values of ρ_i and a long tail. The jump-like increase of $P(\rho_i)$ for $\alpha \gtrsim 2$ signals the occurrence of a very narrow symmetric distribution centred around ρ_{av} and describes extended states. Finally Fig. 3 shows contours of the ratio $R(E) = \rho_{ty}(E)/\rho_{av}(E)$. Apparently all states become localised for $\alpha \lesssim 2$, whereas the width of the region of extended states saturates for $\alpha \gtrsim 5$.

In conclusion, we analysed the effect of impurity correlations on the localisation properties of 1D electron systems and showed that our model exhibits an insulator–metal transition with increasing correlation strength.

Work was supported by NIC Jülich, HLRN Berlin-Hannover, and DFG under SPP 1073 (FE 398/1-3).

References

[1] P. Carpena, et al., Nature 418 (2002) 955.
[2] V.L. Berezinskii, Zh. Eksp. Theor. Fiz. 65 (1973) 1251.
[3] J.C. Flores, J. Phys. Condens. Matter 1 (1989) 8471;
M. Hilke, Phys. Rev. Lett. 91 (2003) 226403.
[4] F. de Moura, M.L. Lyra, Phys. Rev. Lett. 81 (1998) 3735.
[5] M. Paczuski, S. Maslov, P. Bak, Phys. Rev. E 53 (1996) 414.
[6] R. Abou-Chacra, P.W. Anderson, D.J. Thouless, J. Phys. C 6 (1973) 1734;
A.D. Mirlin, Y.V. Fyodorov, Phys. Rev. Lett. 72 (1994) 526.
[7] F.X. Bronold, A. Alvermann, H. Fehske, Phil. Mag. 84 (2004) 673;
A. Alvermann et al., Physica B, this issue, doi:10.1016/j.physb.2005.01.228.
[8] G. Schubert, A. Weisse, G. Wellein, H. Fehske, in: S. Wagner, W. Hanke, A. Bode, F. Durst (Eds.), High Performance Computing in Science and Engineering, Springer, Berlin, 2005.