Available online at www.sciencedirect.com
SCIENCE DIRECT®
Journal of Luminescence 108 (2004) 269–272
JOURNAL OF LUMINESCENCE
www.elsevier.com/locate/jlumin

Universal parameter at the Anderson transition on a one-dimensional lattice with non-random long-range coupling

A.V. Malyshev[a,1], V.A. Malyshev[b,2], F. Domínguez-Adame[b], A. Rodríguez[c,*]

[a] *Departamento de Física Aplicada, Universidad de Salamanca, E-37008 Salamanca, Spain*
[b] *Departamento de Física de Materiales, Universidad Complutense, E-28040 Madrid, Spain*
[c] *Departamento de Matemática Aplicada y Estadística, Escuela Universitaria de Ingenieria Tecnica Aeronautica, Plaza del Cardenal Cisneros s/n, Universidad Politécnica, E-28040 Madrid, Spain*

Abstract

We study numerically the localization–delocalization transition in a class of one-dimensional tight-binding Hamiltonians $\mathscr{H}$ with *non-random* power-law inter-site coupling $\mathscr{H}_{mn} = J/|m-n|^{\mu}$ and *random* on-site energy. This model is critical with respect to the magnitude of disorder at one of the band edges, provided $1<\mu<\frac{3}{2}$. We demonstrate that at some value of the magnitude of disorder Δ_c, interpreted as the critical one, the ratio of the standard deviation to the mean of the participation number distribution is a size-invariant parameter: all curves of this ratio versus the magnitude of disorder, plotted for different system sizes, have a joint intersection point at Δ_c. This value is finite for $1<\mu<\frac{3}{2}$ implying the existence of the transition, while in the marginal case (at $\mu=\frac{3}{2}$) the intersection point is at $\Delta_c = 0$ implying localization of all the eigenstates.

Keywords: Anderson localization; Disordered solids; Metal–insulator transition

1. Introduction

In recent years, a vast amount of work has been devoted to studies of Frenkel excitons in low-dimensional molecular aggregates, where the interplay of disorder and long-range dipole–dipole coupling determines fundamental physical properties [1]. It has been argued, for example, that two-dimensional Frenkel excitons display anomalous localization properties of the states, which determine the linear absorption spectra of the aggregates [2]. To deepen our understanding of these underlying phenomena, we consider a general tight-binding Hamiltonian $\mathscr{H}$ on a regular one-dimensional (1D) lattice with *non-random* long-range inter-site coupling $\mathscr{H}_{mn} = J/|m-n|^{\mu}$ with $1<\mu\leqslant\frac{3}{2}$ and uncorrelated diagonal disorder [3,4]. We find a localization–delocalization transition (LDT) *with respect to the magnitude of disorder* at the upper band edge provided $1<\mu<\frac{3}{2}$; this transition resembles the one in the standard three-dimensional Anderson model [5]. In the

*Corresponding author. Departamento de Matemática Aplicada y Estadística, Escuela Universitaria de Ingeniería Técnica Aeronáutica, Plaza del Cardenal Cisneros s/n, Universidad Politécnica, E-28040 Madrid, Spain. Tel.: +34-91-336-74-86; fax: +34-91-336-74-85.

E-mail address: amesas@euita.upm.es (A. Rodríguez).

[1] On leave from Ioffe Physico-Technical Institute, 194021 Saint-Petersburg, Russia.

[2] On leave from "S.I. Vavilov State Optical Institute", 199034 Saint-Petersburg, Russia.

0022-2313/$ - see front matter © 2004 Elsevier B.V. All rights reserved.
doi:10.1016/j.jlumin.2004.01.057

marginal case ($\mu = \frac{3}{2}$), all eigenstates are found to be localized. In this case, the considered model is similar to the two-dimensional Frenkel Hamiltonian (see Ref. [4] for details) where the states are weakly localized. Thus, higher dimensional models can be mapped onto the considered one.

Level and eigenfunction statistical properties at criticality (both the mobility edge or LDT) reveal specific features due to the critical nature of the eigenstates [6]. Therefore, analysis of these properties provides a tool to detect a critical point. In this work, we show, in particular, that the relative fluctuation of the participation number is scale-invariant at the transition within the considered model. We argue that this invariance is a general property at criticality and propose to use this invariance for calculation of the critical magnitude of disorder. To the best of our knowledge, this general property has never been used for such a purpose. To test the validity of the proposed method, we compare the results with those obtained from the traditional level statistics analysis and find a good agreement.

2. Model Hamiltonian and monitoring tools of a LDT

We consider a general tight-binding Hamiltonian $\mathscr{H}$ on a 1D regular lattice with N sites. In the site representation, the diagonal elements of the Hamiltonian (site energies) $\mathscr{H}_{nn} = \varepsilon_n$ are stochastic variables, uncorrelated for different sites and distributed uniformly around zero within an interval of width Δ. Off-diagonal elements (hopping integrals) are $\mathscr{H}_{mn} = J/|m-n|^{\mu}$ with $1 < \mu \leqslant \frac{3}{2}$ and $m \neq n$. Hereafter we assume that $J > 0$, thus the LDT is expected to occur at the upper band edge provided $1 < \mu < \frac{3}{2}$ (see Refs. [3,4] for details).

We perform numerical analysis of size and disorder scaling of the first two momenta of the participation number (PN) distribution: the mean participation number (MPN) and the standard deviation (SDPN). The PN is defined as $P_v = [\sum_{n=1}^{N} |\psi_{vn}|^4]^{-1}$, where ψ_{vn} is the vth normalized eigenstate of the Hamiltonian $\mathscr{H}$. As the LDT occurs at the top of the band, we analyze disorder and size scaling of the two momenta for the uppermost state. Open boundary conditions are used in all calculations. We take advantage of the Lanczos method to calculate the extreme eigenfunctions and eigenvalues for large system sizes (up to $N \sim 6 \times 10^4$ sites) and two particular values of the interaction exponent: $\mu = \frac{4}{3}$ (the LDT is expected to occur) and $\mu = \frac{3}{2}$ (the marginal case; all states are expected to be localized).

Fig. 1 shows the disorder scaling of the ratio SDPN/MPN for $\mu = \frac{4}{3}$ and different system sizes. The figure demonstrates that all SDPN/MPN curves have a non-trivial joint intersection point at $\Delta_c = 10.0 - 10.5\ J$ (see below for the discussion of the slight dependence of the intersection point on the system size). At this point the ratio SDPN/MPN is a size-invariant parameter, so we conjecture that this is the transition point. Note also that, at this point, both the MPN and the SDPN are of the same order of magnitude for any system size, as was found for the case of power-law random banded matrices [7]. The size invariance of the relative fluctuation is a direct consequence of the general multifractal nature of wave functions at criticality and therefore this invariance is also a general property. This provides grounds to claim

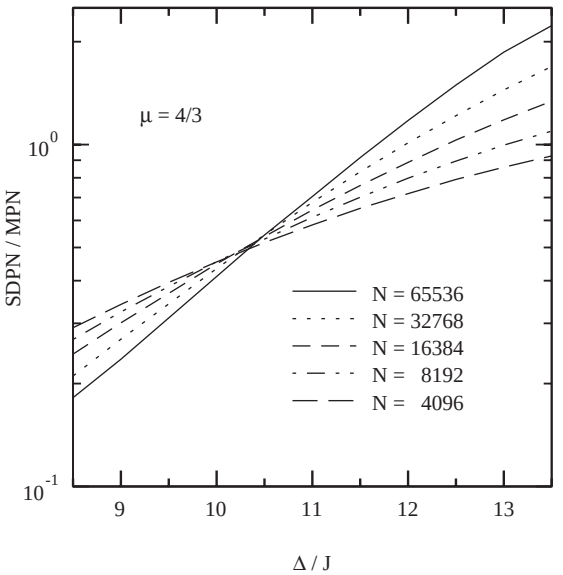

Fig. 1. Disorder scaling of the ratio SDPN/MPN for different system sizes at $\mu = \frac{4}{3}$.

that the proposed method of the critical point detection is applicable for other LDTs.

We have also computed the ratio SDPN/MPN for the marginal case ($\mu = \frac{3}{2}$) and found that the only joint intersection point of all SDPN/MPN curves is at $\Delta_c = 0$. Thus, no signatures of the LDT appear in the marginal case. Recall here that at $\mu = \frac{3}{2}$, the relationship between the level spacing at the upper edge of the bare band and the effective disorder (reduced by the quasi-particle motion) is exactly the same as in the center of the 2D band within the standard Anderson model [4], where the states are weakly localized [8]. This analogy provides support for the localized nature of the states and hints also that the localization length may be very large in this case.

Contrary to the standard Anderson model, the contribution of off-diagonal terms to the Hamiltonian $\mathscr{H}$ converges slowly on increasing the system size. This results in the dependence of the band width (actually, the upper edge) on the system size: the band is wider for larger systems. This means that the same disorder is effectively stronger for smaller systems. This effect introduces a regular dependence of the critical point on the system size. Fig. 2 shows both the upper band edge $E(N)$ in units of its asymptotic value $E(\infty)$, and the intersection point $\Delta(N)$ [with its maximum value fitted to $E(N)/E(\infty)$] as a function of N for $\mu = \frac{4}{3}$. The values $\Delta(N)$ are intersection points of the pairs of SDPN/MPN scaling curves from Fig. 1 for subsequent system sizes; each point is attributed to the maximum system size of the intersecting pair of curves. The figure demonstrates that the band edge shift provides the dominant contribution to the size dependence of the intersection point for large systems. It allows also to determine the limiting value of the intersection point, in other words, the critical point in the thermodynamic limit. This value can be estimated as $\Delta_c \approx 10.9\ J$. More detailed analysis of finite-size effects are to be published elsewhere.

To test our predictions against traditional techniques of critical-point detection, we focus also on the level statistics analysis. To this end, we calculate numerically the energy spacing of the two uppermost states for different realizations of disorder. After normalizing by the mean level spacing (MLS), we obtain the standard deviation of the normalized distributions (SDLS/MLS). At the LDT this distribution should be independent of the system size [9]. Consequently, the disorder scaling curves of the normalized standard deviation plotted for different values of N are expected to intersect at the transition point. Fig. 3 shows such curves for $\mu = \frac{4}{3}$ and demonstrates that all the curves have a non-trivial joint intersection point at $\Delta_c = 10.7 - 11.4\ J$. This value is slightly larger on average than that obtained by the PN statistics analysis method. This difference is related to the finite size effects partly discussed above (see discussion of Fig. 2). The critical points obtained by the two methods are in good agreement. Compared to traditional level statistics analysis, the proposed method appeared to be more efficient in terms of the number of realizations we had to consider to obtain reliable results.

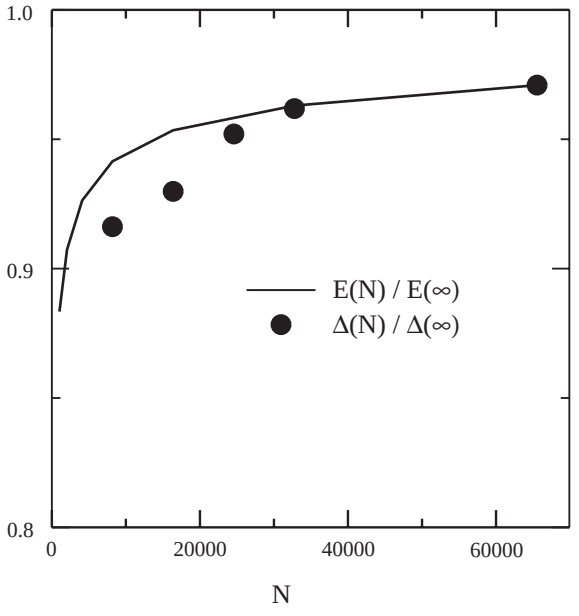

Fig. 2. Size dependence of the upper-band edge $E(N)$ [in units of its asymptotic value $E(\infty)$] and the normalized intersection point, $\Delta(N)/\Delta(\infty)$, at $\mu = \frac{4}{3}$.

In summary, we studied numerically the 1D Anderson model with *non-random* long-range power-like coupling, $J_{nm} = J/|n-m|^{\mu}$, $J > 0$. Our simulations confirm the prediction that this model is critical for the range $1 < \mu < \frac{3}{2}$ and

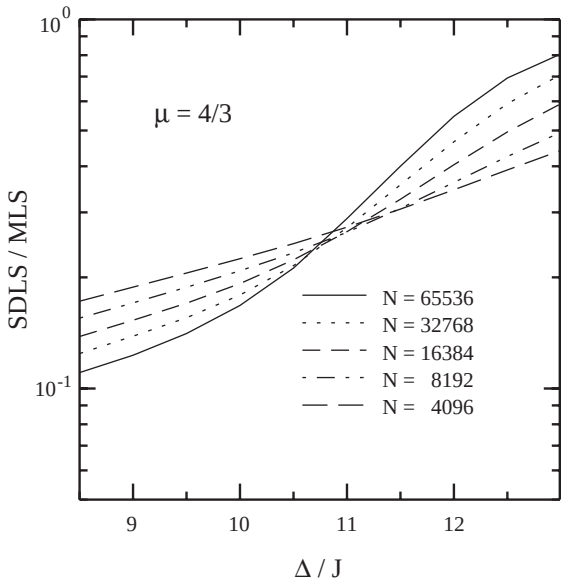

Fig. 3. Disorder scaling of the standard deviation of the distribution of normalized level spacing for different system sizes and $\mu = \frac{4}{3}$.

undergoes the localization–delocalization transition at the upper band edge [3,4]. We prove numerically the general conjecture that the ratio of the standard deviation to the mean of the participation number distribution is a scale-invariant parameter at criticality. This finding provides a new general efficient method to monitor a LDT: the joint intersection point of the SDPN/MPN disorder-scaling curves, plotted for different system sizes, yields the transition point. We find, in particular, that at $\mu = \frac{4}{3}$ the critical point is $\Delta_c = 10.9 \pm 0.5\ J$. In the marginal case ($\mu = \frac{3}{2}$), the only joint intersection point is at $\Delta_c = 0$, indicating that all states are localized. The marginal case is the most relevant one in the context of molecular aggregates since it can be mapped onto the two-dimensional Frenkel Hamiltonian [4]. We can then conclude that two-dimensional Frenkel excitons are localized.

Acknowledgements

The authors thank M.A. Martín-Delgado and G. Sierra for discussions. This work was supported by DGI-MCyT (MAT2000-0734) and MECyD (SB2001-0146). V.A.M. acknowledges support through a NATO Fellowship.

References

[1] T. Kobayashi (Ed.), J-Aggregates, World Scientific, Singapore, 1996.
[2] A. Rodríguez, M.A. Martín-Delgado, J. Rodríguez-Laguna, G. Sierra, V.A. Malyshev, F. Domínguez-Adame, J.P. Lemaistre, J. Lumin. 94–96 (2001) 359.
[3] A. Rodríguez, V.A. Malyshev, F. Domínguez-Adame, J. Phys. A: Math. Gen. 33 (2000) L161.
[4] A. Rodríguez, V.A. Malyshev, G. Sierra, M.A. Martín-Delgado, J. Rodríguez-Laguna, F. Domínguez-Adame, Phys. Rev. Lett. 90 (2003) 27404.
[5] P.W. Anderson, Phys. Rev. 109 (1958) 1492.
[6] A.D. Mirlin, Phys. Rep. 326 (2000) 259.
[7] A.D. Mirlin, Y.V. Fyodorov, F.-M. Dittes, J. Quezada, T.H. Seligman, Phys. Rev. E 54 (1996) 3221.
[8] E. Abrahams, P.W. Anderson, D.C. Licciardello, T.V. Ramakrishnan, Phys. Rev. Lett. 42 (1979) 673.
[9] V.E. Shklovskii, B. Shapiro, B.R. Sears, P. Lambrianides, H.B. Shore, Phys. Rev. B 47 (1993) 11487.