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ANDERSON TRANSITION IN TWO-DIMENSIONAL DISORDERED LATTICES WITH LONG-RANGE COUPLING

A. RODRÍGUEZ[1]

[1] *GISC, Departamento de Matemática Aplicada y Estadística, Universidad Politécnica, Madrid, Spain*

V. A. MALYSHEV[2], F. DOMÍNGUEZ-ADAME[3] and J.P. LEMAISTRE[4]

[2] *National Research Center, "Vavilov State Optical Institute", Saint-Petersburg, Russia*
[3] *GISC, Departamento Física de Materiales, Universidad Complutense, Madrid, Spain*
[4] *Laboratoire des Milieux Dèsordonnés et Hétérogènes, Université P. et M. Curie, Paris, France*

Abstract

We provide arguments indicating that an Anderson transition may exist in two-dimensional disordered systems with long-range coupling. As a working example, a two-dimensional dipolar Frenkel exciton Hamiltonian is used in order to confirm the existence of a localization-delocalization transition. It is found that the states of one of the band tails, but not of the band center, undergo the continuous Anderson transition.

1 Model and motivations

The Anderson transition in disordered solids[1], despite its forty-year history, still excites great interest among researchers. After the pioneering work by Abrahams *et al.* for two-dimensional systems[2], a number of papers raised the general belief that in those systems all eigenstates were exponentially localized[3] and that the localization-delocalization transition no longer exists in the thermodynamical limit. In this work we show that extended states may appear in two-dimensional systems with a long-range intersite coupling even for moderately large diagonal disorder. In three and one dimensions, this fact has been outlined in Refs[4,5]. To this end, we consider a Frenkel exciton Hamiltonian on a regular $\mathcal{N} = N \times N$ lattice with diagonal disorder:

$$\mathcal{H} = \sum_{\mathbf{n}} \epsilon_{\mathbf{n}} |\mathbf{n}\rangle\langle\mathbf{n}| + \sum_{\mathbf{mn}} J_{\mathbf{nm}} |\mathbf{n}\rangle\langle\mathbf{m}| \; . \tag{1}$$

Here, $\epsilon_{\mathbf{n}}$ and $|\mathbf{n}\rangle$ are the energy and the state vector of the $\mathbf{n}$-th excited molecule, respectively; $\mathbf{n} = (n_x, n_y)$, $-N/2 \leq n_x, n_y \leq N/2$, with N even. The dipole-dipole inter-site interaction is taken in an isotropic form $J_{\mathbf{nm}} = J/|\mathbf{n} - \mathbf{m}|^3$, where $J > 0$, implying that the transition dipole moments of all molecules are perpendicular to the latice plane and all of them have the same magnitude. We assume that the on-site energies $\epsilon_{\mathbf{n}}$ are uncorrelated random variables distributed according to a Gaussian function of variance Δ^2.

In the Bloch-wave representation, assuming periodic boundary conditions, Hamiltonian (1) takes the form

$$\mathcal{H} = \sum_{\mathbf{K}} E_{\mathbf{K}} |\mathbf{K}\rangle\langle\mathbf{K}| + \sum_{\mathbf{KK'}} (\delta\mathcal{H})_{\mathbf{KK'}} |\mathbf{K}\rangle\langle\mathbf{K'}|, \tag{2}$$

where $\mathbf{K} = (2\pi/N)(k_x, k_y)$ runs over the first Brillouin zone, $(-N/2 \leq k_x, k_y < N/2)$. Here $E_{\mathbf{K}}$ is the unperturbed exciton eigenenergy

$$E_{\mathbf{K}} = J \sum_{\mathbf{n}\neq\mathbf{0}} \frac{1}{|\mathbf{n}|^3} e^{i\mathbf{K}\cdot\mathbf{n}}, \tag{3}$$

and $(\delta\mathcal{H})_{\mathbf{KK'}}$ is the inter-mode coupling matrix

$$(\delta\mathcal{H})_{\mathbf{KK'}} = \frac{1}{\mathcal{N}} \sum_{\mathbf{n}} \epsilon_{\mathbf{n}} e^{i(\mathbf{K}-\mathbf{K'})\cdot\mathbf{n}}. \tag{4}$$

It can be shown that in close proximity of the extreme points of the band $\mathbf{K} = \mathbf{0}$ (top) and $\mathbf{K} = \mathbf{\Pi} \equiv (\pi, \pi)$ (bottom) the exciton energy spectrum behaves linearly and parabolically, respectively[6]:

$$E_{\mathbf{K}} \sim \begin{cases} 9.03J - 2\pi J|\mathbf{K}|, & |\mathbf{K}| \ll 1, \\ -2.65J + 0.4J|\mathbf{K} - \mathbf{\Pi}|^2, & |\mathbf{K} - \mathbf{\Pi}| \ll \mathbf{1}. \end{cases} \tag{5}$$

Depending on the degree of disorder Δ/J and the lattice size, the operator $\delta\mathcal{H}$ may couple the extended excitonic states $|\mathbf{K}\rangle$ to each other (thus resulting in their localization) or not. The magnitude of the exciton inter-mode coupling is given by

$$\sigma \equiv \sqrt{\langle |(\delta\mathcal{H})_{\mathbf{K},\mathbf{K}'}|^2 \rangle} = \frac{\Delta}{N}\,, \tag{6}$$

which reflects the well-known exchange narrowing effect[7].

At the top of the band, the energy spacing between the unperturbed states with $\mathbf{K} = \mathbf{0}$ and $\mathbf{K}' = (2\pi/N, 0)$ is $\delta E = 4\pi^2 J/N$. When comparing δE and σ the most remarkable fact is that both quantities decrease on increasing N in the same manner as $N^{-1} = \mathcal{N}^{-1/2}$. Now take $\Delta \ll 4\pi^2 J$. Under this condition, the strength of the reduced degree of disorder $\sigma = \Delta/N$, governing the exciton state mixing and thereof localization, is of *perturbative* magnitude ($\sigma \ll \delta E$) and, what is most important, it will remain *perturbative* upon increasing the lattice size. Hence, these states will not be mixed by disorder and will remain extended over the entire lattice independent of its size. On the other hand, if $\Delta > 4\pi^2 J$ there will be mixing and thereof localization of the eigenstates.

At the bottom of the band, the level spacing decreases as $\mathcal{N}^{-1} = N^{-2}$ upon increasing the lattice size, i.e., faster than the reduced degree of disorder σ (the same behavior takes place for both edges of the band obtained within the NN approximation, namely taking $J_{\mathbf{nm}} = 0$ when $|\mathbf{n} - \mathbf{m}| > 1$). Now, even if one starts with a *perturbative* magnitude of Δ at a fixed lattice size (so that $\sigma \ll \delta E$), it becomes *non-perturbative* for larger sizes, resulting finally in localization of those eigenstates. This implies the existence of only *one* mobility edge separating delocalized and localized states. Its position is expected to depend on the degree of disorder Δ/J and to increase toward the top of the band as Δ/J raises.

2 Numerical results

To examine the character of the exciton eigenfunction (localized or extended) we have calculated the inverse participation ratio (IPR) of the exciton eigenstates, according to the standard definition $\mathrm{IPR}_\nu = \sum_{\mathbf{n}} |\Psi_{\nu\mathbf{n}}|^4$, where the sum runs over lattice sites and it is assumed that the eigenfunction $\Psi_{\nu\mathbf{n}}$ of the νth eigenstate is normalized to unity. For a completely delocalized state $\mathrm{IPR}_\nu = 1/\mathcal{N} = N^{-2}$ whereas for a state concentrated in one site $\mathrm{IPR}_\nu = 1$, so the smaller the value of the IPR, the more delocalized the state is. In fact, the participation ratio IPR_ν^{-1} is of the order of the number of sites over which the eigenfunction is spread.

We have used Lanczos and Householder algorithms to calculate the IPR of the uppermost eigenstate and of the complete set of eigenstates respectively. The IPR of the uppermost exciton state as a function of the lateral size N is shown in Fig. 1. The plots comprise the result of 20 averages over disorder realizations and $\Delta/J = 1$ in all cases. The IPR calculated within the NN approximation shows no scaling which is in perfect agreement with the well-known result stating that those exciton states are localized. On the contrary, the slope of the straight line obtained within the exact model is equal to -1.97 that almost matches the theoretical value -2. This scaling undoubtedly confirms the extended nature of the uppermost exciton state.

Figure 2 presents the IPR of the uppermost state as a function of Δ/J for different system sizes. At first glance, it seems that this state undergoes an abrupt Anderson transition at the

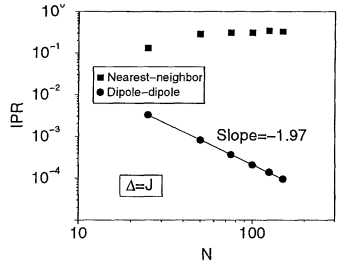

Figure 1: Lateral size scaling of the IPR of the uppermost exciton eigenfunction.

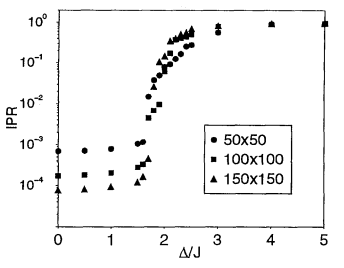

Figure 2: IPR of the uppermost exciton eigenfunction as a function of Δ/J.

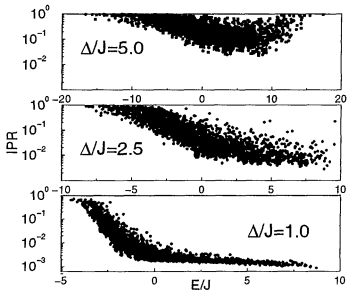

Figure 3: IPR as a function of energy for $\mathcal{N} = 50 \times 50$ and different values of Δ/J. Note the different scale of the E/J axis indicating the widening of the bandwidth with increasing Δ/J.

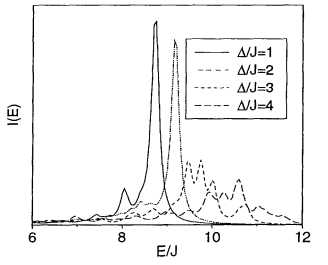

Figure 4: Absorption line shape in arbitrary units for 50×50 systems and different values of the degree of disorder Δ/J. Results comprise 20 realizations of disorder for each value of Δ/J.

critical value of Δ/J approximately equal to 2 independently of the system size. Nevertheless, this is not really true. The uppermost states whose IPR are shown in Figure 2 arise from large fluctuations in the on-site energies $\epsilon_{\mathbf{n}}$. Indeed, it is straightforward to verify that at $N \simeq 100$ and $\Delta/J > 2$, the probability of a large site-energy fluctuation giving an energy $\epsilon_{\mathbf{n}}$ outside of the band of the ordered system is of the order of unity. In Fig. 3, after the "transition" has occurred ($\Delta/J > 2$), it can be seen the dramatic increase in the IPR of the uppermost state whereas the increase in the IPR of the states actually coming from the top of the band of the ordered system is no so abrupt.

The width of the absorption spectrum σ_A can be proposed to indirectly measure the extension of the optically active exciton eigenstates (top band states in our case): $\sigma_A \sim \mathrm{IPR}_{\mathrm{top}}^{1/2}\Delta$.[8] We calculated the absorption spectra of the system at different degrees of disorder Δ/J. The results are shown in Fig. 4. The absorption line width σ_A presents a clear tendency to smoothly widen on increasing Δ/J, in correspondence with the fact that the IPR of the top band states smoothly go up. The uppermost eigenstate, being the only one coupled to the light in an ordered system, is now mixed with the other eigenstates, spreading its oscillator strength over them. As a result, the absorption spectrum widens.

3 Conclusions

In summary, we have found that a continuous Anderson transition may exist in two-dimensional systems with dipole-dipole intersite coupling in the vicinity of the band top. In our opinion, the failure of the one-parameter scaling theory for the conditions considered in the present paper originates from that this approach deals only with the size scaling of the energy spacing but pays no attention to the subsequent renormalization of the disorder (6). As it follows from our treatment, the latter effect may play a major role in localization phenomena, violating the one-parameter scaling and thus leading to the impossibility to match our numerical results by this theory.

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