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Numerical study of quantum percolation

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Abstract

We study the density of states and the optical conductivity of the classical double-exchange model on a site percolated cluster.

Keywords: Quantum percolation; Optical conductivity; Double-exchange

In a recent attempt [1] to describe the metal–insulator transition in CMR manganites we assumed a percolative coexistence of the two competing phases [2]. In the insulating phase doped holes are trapped by local Jahn–Teller or "breathing type" lattice distortions. The metallic phase consists of itinerant carriers whose hopping amplitude is coupled via double-exchange [3] to a background of localised spins.

To gain insight into the properties of the latter phase, we study the classical double-exchange model on a site percolated cluster,

$$H = \sum_{\langle kl \rangle} [t_{kl} c_k^\dagger c_l + h.c.]. \tag{1}$$

Here $c_l^\dagger$ creates a spinless fermion in the Wannier state at site l, and the summation is over neighbouring sites on a simple cubic lattice. The matrix element t_{kl} is nonzero only between sites of a cluster,

$$t_{kl} = \cos\frac{\theta_k}{2}\cos\frac{\theta_l}{2}\,e^{-i(\phi_k-\phi_l)/2} + \sin\frac{\theta_k}{2}\sin\frac{\theta_l}{2}\,e^{i(\phi_k-\phi_l)/2}, \tag{2}$$

where the angles $\{\theta_l, \phi_l\}$ parameterise the background of classical spins. Hence, in the present model there are two types of disorder which cause scattering or localisation of the involved fermions, namely, the random structure of the cluster and the disorder in the hopping matrix elements.

To construct a certain realization of model (1) with a given probability p we choose active sites from a simple cubic lattice. After labelling the resulting clusters [4] we keep only the largest (or the spanning) one for further calculations. To fix the hopping matrix elements a set $\{\theta_l, \phi_l\}$ is taken from an ensemble of thermalized classical spins in a magnetic field h_{eff}. This introduces the parameter $\lambda = \beta g \mu_B h_{\text{eff}}$.

Application of Chebyshev expansion and maximum entropy methods [5] yields the density of states, shown in Fig. 1 for different values of p and λ. For the ordered spin background ($\lambda = \infty$) with decreasing p a pseudo-gap feature appears close to the band centre, together with a distinct peak at $E = 0$. The weight W of this central peak (left-hand inset) increases continuously, and makes up more than 10% of the spectrum close to the classical percolation threshold $p_c \approx 0.3116$. On the other hand, increasing spin disorder, i.e., decreasing λ, transfers spectral weight to the band centre. It does not seem to affect the weight of the central peak. Of course, both types of disorder reduce the overall bandwidth.

What remains to be clarified is the nature of the involved eigenstates. Our calculations indicate that the states in the band centre show a chequerboard structure and are less localised compared to the rest of the spectrum. Similar behaviour was also found for lower dimensional systems, as discussed in Ref. [6].

Fig. 2 shows the regular part of the optical conductivity,

$$\sigma_{\text{reg}}(\omega) = \frac{1}{N}\sum_{m\neq 0}\frac{|\langle m|j_x|0\rangle|^2}{\omega_m}\delta(\omega-\omega_m) \tag{3}$$

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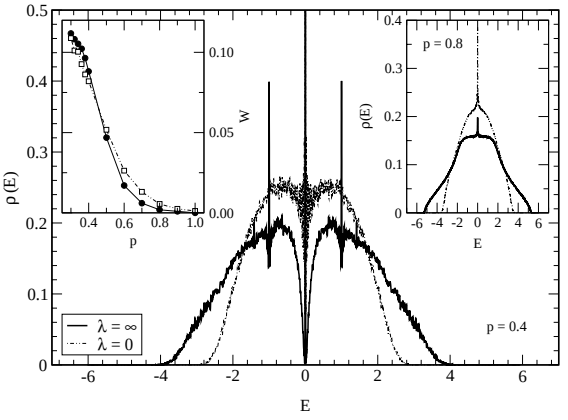

Fig. 1. Density of states obtained for $p = 0.4$ (right inset $p = 0.8$) and $\lambda = 0, \infty$ on a 100^3 site lattice with periodic boundary conditions; left inset: weight of the central peak as a function of p for $\lambda = 0, \infty$ and 64^3 sites.

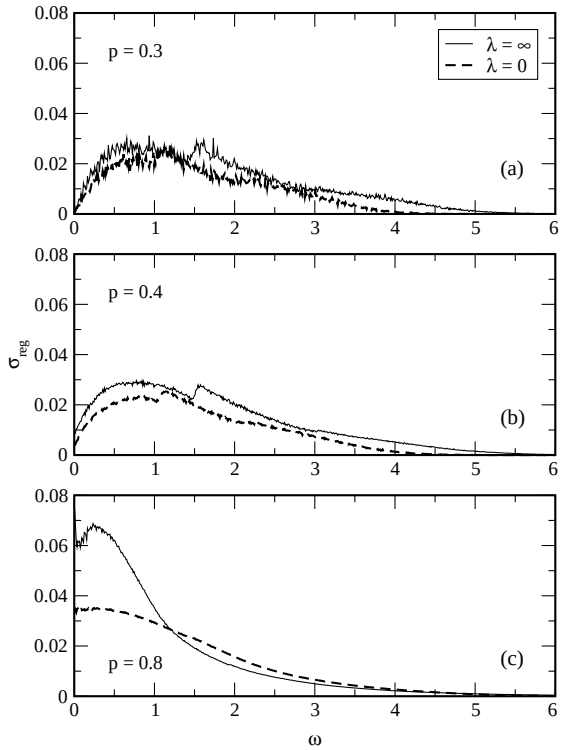

Fig. 2. Optical conductivity for $p = 0.3$, 0.4, 0.8 and $\lambda = 0, \infty$ averaged over 700 realizations on a 10^3 site lattice.

with $\omega_m = E_m - E_0$. The current j_x is given by

$$j_x = \sum_{\langle kl \rangle_x} [it_{kl} c_k^\dagger c_l + h.c.], \tag{4}$$

where the summation extends over neighbouring sites in x-direction only. Considering clusters on a 10^3 site lattice, we calculated the eigenstates of the hopping matrix and summed up the current matrix elements between empty and occupied eigenstates. We assumed zero (electron) temperature and a band filling of 0.2. Clearly, below the classical percolation threshold (panel (a)) we deal with finite size clusters which do not (or rarely) connect the boundaries. Hence, the averaged σ_{reg} is rather noisy and approaches zero in the limit $\omega \to 0$. For $p > p_c$ (panels (b) and (c)) the curves become smooth, and we obtain a finite DC conductivity. In panel (b) the hump between $\omega = 1$ and 2 is due to excitations into the central peak. With decreasing λ it is shifted to lower frequencies, because of the reduced bandwidth. Further studies of the model should clarify whether the quantum percolation threshold [7] $p_q > p_c$ is also visible in the optical conductivity.

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