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Metal–insulator transition in anisotropic systems with both diagonal and spin-orientation-dependent off-diagonal disorder

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Abstract. The localization behaviour of the anisotropic extended double-exchange model with both diagonal and spin-orientation-dependent off-diagonal disorder is investigated using the transfer-matrix method. The anisotropy is described by different in-plane and inter-plane hopping integrals. By using a mean-field distribution of the spin orientation, the localization length of electrons is calculated as a function of temperature. It is found that the metal–insulator transition temperature t_{MIT} of the system increases with decreasing degree of anisotropy γ. On the insulating side, the localization length for t close to t_{MIT} varies as $\xi \propto (t - t_{\mathrm{MIT}})^{-\nu}$. We also calculate the value of ν for various γ-values. The comparison of the results obtained and the experimental measurements for the layered mixed-valence Mn oxides is discussed.

1. Introduction

The effects of anisotropy on the properties of disordered systems have received considerable attention [1–7] in recent years. This is due to the fact that there are a large variety of materials that are highly anisotropic, e.g., random superlattices, high-T_c superconducting materials, and layered magnetic compounds. From numerical calculations in the case of anisotropic systems with random on-site energies, Zambetaki *et al* [6] have shown that although the critical behaviour is the same in both the in-plane and inter-plane directions, the localization lengths are different. These results were used to explain the anisotropic normal-state behaviour of the high-T_c superconductors. Recently, Milde *et al* [7] studied the metal–insulator transition (MIT) in anisotropic systems by using multifractal analysis. Their results show that the eigenstates of the Hamiltonian exhibit multifractal behaviour at the MIT even for strong anisotropy.

Most of the previously investigated anisotropic systems are described by Anderson Hamiltonians with diagonal disorder. Recent studies on the isotropic double-exchange (DE) model show that off-diagonal randomness may play an important role in explaining the anomalous transport behaviour in the mixed-valence manganites [8, 9]. Since the off-diagonal disorder in such systems is related to the magnetic order parameter and is therefore temperature dependent, a disorder-driven metal–insulator transition is expected on increasing the temperature [9]. An interesting question to ask is that of what the critical behaviour of such systems is if the anisotropy is incorporated.

In the present paper, we study the localization behaviour of a three-dimensional (3D) disordered anisotropic system described by the simplified DE Hamiltonian with both diagonal and off-diagonal disorder. Anisotropy is introduced by taking different hopping integrals along perpendicular and parallel directions, labelled as $t_\perp$ and $t_\parallel$, respectively. The strength of the

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anisotropy is characterized by the parameter γ, defined as $1 - t_\perp/t_\parallel$. In the DE Hamiltonian the hopping integrals are related to the orientations of the local spins, which are governed by the ferromagnetic phase transition and thus are temperature dependent. Thus, the strength of the off-diagonal disorder is also temperature dependent. Under certain conditions this may lead to a MIT at a critical temperature. By using the transfer-matrix technique [10] and assuming a mean-field distribution for the spin orientation [9], the localization length is calculated as a function of temperature for different anisotropy strengths γ. It is found that the MIT temperature t_{MIT} increases with decreasing anisotropy γ and approaches its isotropic value in the limit $\gamma \to 0$. On the insulating side, the localization length for t close to t_{MIT} varies as $\xi \propto (t - t_{\mathrm{MIT}})^{-\nu}$. We also calculate the value of ν for various γ-values. From the finite-size scaling, the calculated exponent ν varies between 1.2 and 2 with rather large error bars. This work is also motivated by current experimental studies of layered mixed-valence Mn oxides with anisotropic exchange interactions, which exhibit some unusual properties [11, 12].

2. The model and formalism

The system that we consider is described by an anisotropic extended DE model [8, 9]:

$$H = -\sum_{ij} V_{ij} d_i^+ d_j + \sum_i \epsilon_i d_i^+ d_i. \tag{1}$$

Here the first term is the DE Hamiltonian, in which V_{ij} is the effective transfer integral for nearest-neighbouring Mn sites. It was proposed [13, 14] that V_{ij} has the form

$$V_{ij} = V'_{ij}\left\{\cos\left(\frac{\theta_i}{2}\right)\cos\left(\frac{\theta_j}{2}\right) + \sin\left(\frac{\theta_i}{2}\right)\sin\left(\frac{\theta_j}{2}\right)\exp[-\mathrm{i}(\phi_i - \phi_j)]\right\} \tag{2}$$

where (θ_i, ϕ_i) are the polar angles characterizing the orientations of local spins, and the V'_{ij} are the transfer integrals in the absence of Hund's rule coupling and depend on the directions of the ij-bonds. We assume that the easy axis lies in the magnetic sheets, so all of the local spins are always in the in-plane directions $\boldsymbol{x}$ and $\boldsymbol{y}$ and their orientations are specified by θ_i only [15] if the polar axis is chosen to be in the plane. The anisotropy is characterized by the difference of the in-plane and inter-plane values of V'_{ij}, which are assigned to be 1 and $1 - \gamma$, respectively, with the in-plane hopping integral being the energy unit. The parameter $\gamma \in [0, 1]$ describes the strength of the anisotropy. For $\gamma = 0$ we recover the isotropic 3D case, and $\gamma = 1$ corresponds to N independent planes. As in the usual treatment, we assume all the nonmagnetic randomness to be included effectively in the diagonal disorder in Hamiltonian (1), where the ϵ_i stand for random on-site energies distributed between $-W/2$ and $W/2$. Without the off-diagonal disorder the problem of Anderson localization in anisotropic systems has been solved by using the transfer-matrix method [6], and the results show that at the centre of the band the critical disorder W_c for $\gamma = 0.9$ is approximately 8.0. W_c decreases if the off-diagonal disorder is switched on in an isotropic system [8]. This value is expected to be further decreased if the anisotropy and off-diagonal disorder are both taken into account. So, in order to ensure the occurrence of a MIT in the present system we choose $W = 4$ for the strength of the diagonal disorder.

At the same time, the local spins are coupled with each other via the double-exchange interactions. In this paper we consider the case of ferromagnetic couplings. In using the mean-field theory the orientation of a local spin is governed by an effective field H_{eff} which is produced by the other spins in the absence of an external magnetic field. In this way the energy gain of a spin due to this field is $2\mu_B S_{eff} H \cos\theta$ where μ_B is the Bohr magneton, S_{eff} is the effective spin on a Mn site, and the polar axis for measuring angle θ is along the direction

of the field H_{eff}. Thus, at finite temperature the probability distribution of the orientations of local spins can be expressed in a Maxwell–Boltzmann form [9]:

$$f(\theta) = C \exp\left(-\frac{2\mu_B S_{eff} H_{eff} \cos\theta}{k_B T}\right) \tag{3}$$

where C is a normalization factor. From this distribution the thermal average $\langle\cos\theta\rangle$ can be calculated as

$$\langle\cos\theta\rangle = L\left(\frac{2\mu_B S_{eff} H_{eff}}{k_B T}\right) \tag{4}$$

where

$$L(x) = \coth x - \frac{1}{x}$$

is the Langevin function. In the mean-field scheme the effective field 'felt' by a local spin can be expressed as

$$H_{eff} = 2g\mu_B S_{eff} \langle\cos\theta\rangle \tag{5}$$

where g is a constant depending on the magnetic coupling and coordinate number. By combining equations (3), (4), and (5) one can solve for $H_{eff}(T)$ for a given temperature. In the absence of a magnetic field, $H_{eff}(T)$ vanishes if $T \geqslant T_C$, with

$$T_C = \frac{g(2\mu_B S_{eff})^2}{3k_B}$$

being the Curie temperature. We can rewrite the distribution in the form

$$f(\theta) = C \exp\left(-\frac{3m\cos\theta}{t}\right). \tag{6}$$

Here, $m = \langle\cos\theta\rangle$ and $t = T/T_C$ are the normalized magnetization and temperature, respectively. The normalized magnetization is a function of t and can be obtained by solving the following equation:

$$m = L\left(\frac{3m}{t}\right). \tag{7}$$

Figure 1 shows the probability distribution of the nearest-neighbour transfer integral $P(V_{ij})$ for different temperatures. It can be seen that the distribution is broadened on increasing the temperature in the range $T \leqslant T_C$, implying an increase of the off-diagonal disorder. In order to illustrate the temperature dependence of the strength of the off-diagonal disorder, in the inset to figure 1 we plot w, defined as the second-order moment of the distribution, as a function of temperature t. One can easily see that at $t = 0$ the local spins are completely ordered and there is no off-diagonal disorder ($w = 0$). With increasing t the off-diagonal disorder increases, but it saturates if $t \geqslant 1$ because above the Curie temperature the magnetization $m = 0$ and the off-diagonal disorder reaches its maximum. So, the contribution of the off-diagonal disorder to the electron localization increases with temperature only over the range $1 > t > 0$. In the range $\infty > t \geqslant 1$, the off-diagonal disorder becomes constant, corresponding to the strongest and saturated value.

In order to calculate the Lyapunov exponent and localization length within the scheme of finite-size scaling, we investigate an $N \times N \times L$ bar with L being extremely large. For such a quasi-1D bar-shaped system of cross section $N \times N$, the Schrödinger equation can be written in the form of the transfer-matrix equation

$$\begin{pmatrix} \psi_{i+1} \\ \psi_i \end{pmatrix} = \mathsf{T}_i \begin{pmatrix} \psi_i \\ \psi_{i-1} \end{pmatrix} = \begin{pmatrix} \mathsf{H}_i & -\mathsf{I} \\ \mathsf{I} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \psi_i \\ \psi_{i-1} \end{pmatrix} \tag{8}$$

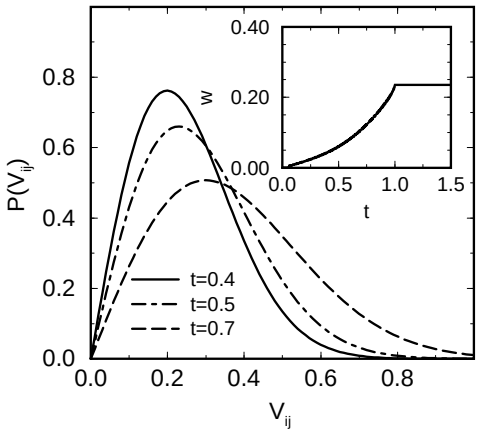

Figure 1. The probability distribution of the nearest-neighbour transfer integral $P(V_{ij})$. Inset: the off-diagonal disorder strength w (the second-order moment of the distribution) as a function of t.

where ψ_{i+1} and ψ_i are vectors with N^2 components describing the wave-function amplitudes of planes $i + 1$ and i, respectively, the $N^2 \times N^2$ matrix $\mathbf{H}_i$ is the sub-Hamiltonian within the ith plane, and $\mathbf{I}$ is a unit matrix. We calculate the Lyapunov exponents for this system using the transfer-matrix method, in which the Gram–Schmidt orthonormalization procedure is adopted [10]. The largest localization length $\lambda_N(E, t)$ for a system with finite width N is then given by the inverse of the smallest Lyapunov exponent. In our numerical calculation, we choose the sample length L to be over 10^4 so that the self-averaging effect automatically takes care of the ensemble statistical fluctuations.

According to the one-parameter scaling hypothesis [10], the rescaled localization length $\Lambda_N = \lambda_N/N$ should be a function of N for given energy E, anisotropy γ, and temperature t. It is expected that Λ_N should increase (decrease) on increasing N for the extended ($t < t_{\mathrm{MIT}}$) (localized ($t > t_{\mathrm{MIT}}$)) cases. At the critical point $t = t_{\mathrm{MIT}}$, an N-independent fixed-point value Λ_c is expected that defines the critical temperature t_{MIT}.

The localization length for infinite system ξ can be determined by using the finite-size scaling *ansatz* [10]

$$\lambda_N/N = F(\xi/N). \tag{9}$$

We make a further assumption that this scaling parameter $\xi(t, \gamma)$ for t close to t_{MIT} and $t > t_{\mathrm{MIT}}$ varies as $\xi \propto (t - t_{\mathrm{MIT}})^{-\nu}$. We may then expand the function F near the critical point Λ_c for a given γ:

$$\lambda_N/N \approx \Lambda_c + AN^{1/\nu}(t - t_{\mathrm{MIT}}) \tag{10}$$

where A is a constant and

$$AN^{1/\nu} = \left.\frac{\mathrm{d}F}{\mathrm{d}t}\right|_{t=t_{\mathrm{MIT}}}. \tag{11}$$

Therefore, $1/\nu$ can be obtained from the slope of the linear relationship between $\ln \mathrm{d}F/\mathrm{d}t$ and $\ln N$ at $t = t_{\mathrm{MIT}}$. In this paper we use four values of N (=4, 6, 8, and 10) to calculate the exponent ν for each γ. In the following, we restrict ourselves to calculation at the band centre ($E = 0$), for simplicity.

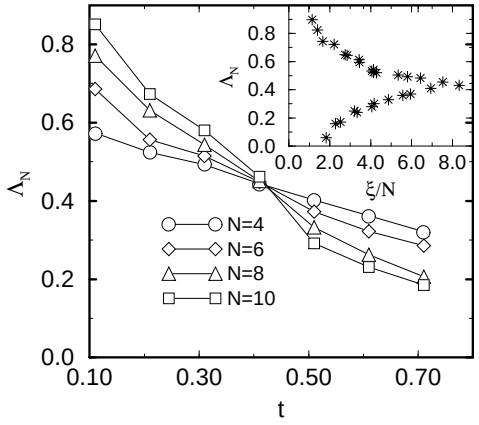

Figure 2. The rescaled localization length $\Lambda_N = \lambda_N/N$ as a function of t for $\gamma = 0.9$ with $W = 4$ for propagation in the perpendicular direction. Inset: the scaling function $\lambda_N/N = F(\xi/N)$ for $\gamma = 0.9$ in the perpendicular direction.

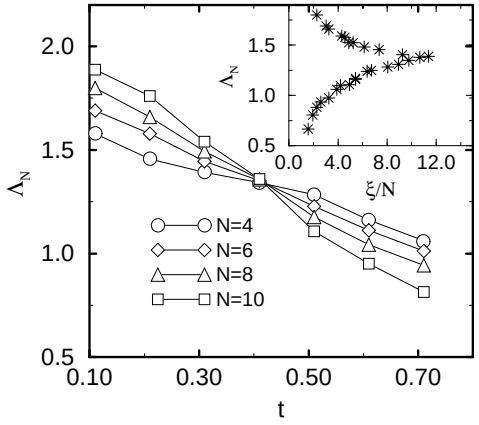

Figure 3. As figure 2, but for propagation in the parallel directions.

3. Numerical results and discussion

In figure 2 and figure 3 we display the rescaled localization length $\lambda_N(t)/N$ as a function of temperature t with $\gamma = 0.9$ and $W = 4$ for the perpendicular and parallel directions, respectively. The data are calculated for different bar widths N with a statistical accuracy of 0.25%. The MIT is indicated by the common crossing point which shows the same critical temperature $t_{\mathrm{MIT}} \simeq 0.4$ for both propagation directions. However, the N-independent fixed-point values Λ_c are different for these two directions. This confirms the conclusion from the single-parameter scaling theory, and coincides with the results for the anisotropic systems with only diagonal disorder [6]. It seems that electrons are less mobile in the perpendicular direction than in the parallel direction, corresponding to a larger localization length in the in-plane directions. By introducing the scaling parameter ξ, we have confirmed that λ_N/N is indeed a single-parameter function of ξ/N (see the insets of figure 2 and figure 3).

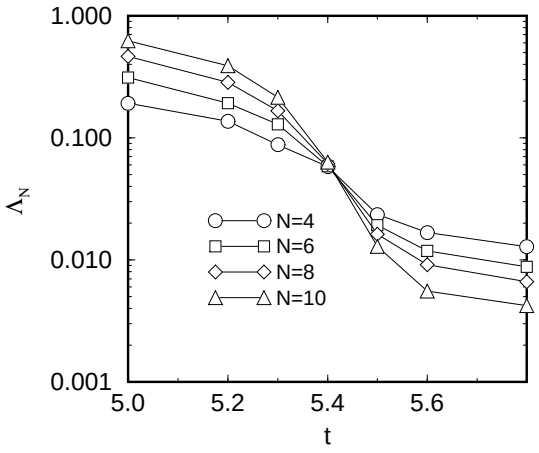

Figure 4. The rescaled localization length λ_N/N as a function of t for $\gamma = 0.5$ with $W = 4$ for propagation in the perpendicular direction.

Table 1. The MIT temperature t_{MIT} and exponent ν for systems with $W = 4$ and different anisotropies γ.

γ	0.9	0.7	0.5	0.3	0.1
t_{MIT}	0.4	0.46	0.54	0.66	0.73
ν	1.92 ± 0.10	1.63 ± 0.22	1.45 ± 0.25	1.32 ± 0.23	1.22 ± 0.18

It is expected that the critical temperature should be shifted to higher temperature by decreasing the anisotropy, because the extended states are more favourable in this situation. This is exactly what we observe in our calculation. Presented in figure 4 is the rescaled localization length λ_N/N versus t with $\gamma = 0.5$ and $W = 4$ for propagation along the perpendicular direction. We also perform the calculation of the critical temperature t_{MIT} and exponent ν for more values of γ. In table 1 we show the γ-dependence of t_{MIT} and ν. One can see that the critical temperature moves towards higher temperature as the anisotropy decreases for systems with fixed diagonal disorder W. However, the exponent ν slightly decreases with decreasing strength of anisotropy γ. As the localization length is related to temperature via the temperature dependence of the strength of the off-diagonal disorder, one may expect that the value of ν should be related to the exponent ν' in the zero-temperature transition defined by $\xi \propto (w - w_c)^{-\nu'}$. The value of ν' has been calculated previously for the anisotropic Anderson model with diagonal disorder and a similar γ-dependence has been found [2, 16]. The change of ν' has been attributed to the large error in such a finite-size scaling calculation [2] and to the dimensionality crossover between 2D and 3D that occurs on changing γ [16].

In the present model the off-diagonal disorder is temperature dependent over the range $1 > t > 0$, so we can find a critical temperature for the MIT. This is different from the case for the Anderson model with quenched disorder, in which the disorder is temperature independent and the MIT corresponds to a zero-temperature phase transition. Since the off-diagonal disorder becomes saturated for $t \geqslant 1$, the MIT temperature should be lower than the Curie temperature if $\gamma \neq 0$. At the same time, t_{MIT} will decrease when the diagonal disorder W increases because the localized states are more favourable in this situation. If W is large enough so that the states are already localized without off-diagonal disorder, as in the calculation in reference [6], t_{MIT} becomes zero. On the other hand, if the diagonal disorder W is too weak, the largest (saturated) off-diagonal disorder may be not able to localize the states, and also one cannot find a finite t_{MIT}.

For $t > t_{\mathrm{MIT}}$, the system is in the insulator phase which means:

(a) The localization length is smaller than the system size.
(b) The transmission of electrons decays exponentially and the conductivity is very low.
(c) The transport relies on the variable-range hopping mechanism or other thermal excitation mechanisms of the carriers.

Usually in this phase the conductivity increases with increasing temperature, but an opposite situation may arise for the range $t_{\mathrm{MIT}} \leqslant t \leqslant 1$, since the off-diagonal disorder increases with increasing temperature and suppresses the conductivity.

In contrast, for $t \leqslant t_{\mathrm{MIT}}$, the system is in the metallic phase which implies:

(a) The localization length is larger than the system size even in the thermodynamical limit.
(b) The transmission of electrons is large and the conductivity is high.
(c) The conductivity decreases with increasing temperature due to the thermal phonon scattering and also due to the increasing off-diagonal disorder.

It is interesting to note that at t_{MIT} the transport properties may be dramatically changed by applying a magnetic field, since it will change the alignment of the local spins and change the off-diagonal disorder. From this, some kind of 'colossal magnetoresistance' may be produced, and the behaviour of the anisotropic magnetic Mn oxides can be explained qualitatively.

4. Summary

In summary, we have numerically studied, by the transfer-matrix method technique, the localization properties of anisotropic systems described by the extended DE Hamiltonian. We found that the MIT temperature is independent of the propagation directions and increases with decreasing anisotropy γ. This behaviour is attributed to the temperature dependence of the off-diagonal disorder due to the exchange interactions among the local spins. We have also calculated the temperature dependence of the localization length near the critical temperature, and a slightly γ-dependent exponent ν is obtained from the calculation. This exponent is related to the localization length exponent in the zero-temperature transition of the anisotropic Anderson disorder model, for which a similar behaviour was found previously. The dimensionality crossover between 2D and 3D might be one of the reasons for the γ-dependence of t_{MIT} and ν. In spite of the temperature dependence of the off-diagonal disorder, the MIT in this model is eventually driven by the change of the disorder strength. As a result, it may be expected that the spectral behaviour and statistical distribution of quantities of a given phase (metal or insulator) will be similar to those of the corresponding phase of the Anderson model. It would interesting to perform level statistics and multifractality studies on this finite-temperature transition in the future.

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