EUROPHYSICS LETTERS

Europhys. Lett., (), pp. ()

Anti-Localisation to Strong Localisation: The Interplay of Magnetic Scattering and Structural Disorder

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(received ; accepted )

PACS. 72.10.Bg – Electronic transport theory.
PACS. 72.15.Qm– Scattering mechanisms.
PACS. 72.15.Rn– Localisation effects.

Abstract. – We study the effect of magnetic scattering on transport in a system with strong structural disorder, using exact finite size calculation of the low frequency optical conductivity. At weak electron-spin coupling, spin disorder leads to a decrease in resistivity, by weakening the quantum interference precursors to Anderson localisation. However, at strong electron-spin coupling, the ‘double exchange’ limit, magnetic scattering increases the effective disorder, sharply increasing the resistivity. We illustrate the several unusual transport regimes in this strong disorder problem, identify a re-entrant insulator-metal-insulator transition, and map out the phase diagram at a generic electron density.

Introduction. – The physics of transport and localisation in the presence of structural disorder has been extensively studied [1]. In three dimension (3d) increasing disorder leads to a monotonic increase in the fraction of localised states, and the resistivity in the extended regime, leading finally to the Anderson metal-insulator transition (MIT).

The interplay of scattering from ‘paramagnetic’ moments with scattering from structural disorder leads to several new transport regimes, whose character is poorly understood. The presence of weak magnetic scattering actually weakens the localising effect of disorder, as discovered by Lee [2] and by Hikami et al. [3], while strong magnetic coupling, the ‘double exchange’ limit, enhances the localising effect of structural disorder [4]. There is no understanding of how these two endpoints are connected. This experimentally relevant “middle” is wide, unexplored, and beyond the reach of standard Boltzmann transport theory [5]. In this paper we present essentially exact results on the conductivity and MIT considering the combined effect of structural disorder and magnetic scattering, and illustrate the novel transport regimes in the problem.

An understanding of transport properties of disordered magnetic systems is of particular relevance now because of intense experimental activity in diluted magnetic semiconductors [6, 7, 8] (DMS), amorphous magnetic semiconductors [9, 10], e.g GdSi, and the manganites...
Some of these systems, notably those where the magnetic coupling arises from Hund’s rule, as in d electron systems, require an understanding beyond the ‘weak magnetic scattering' studies in the localisation literature. A quick look at the resistivity in the paramagnetic phase in these materials reveal that they are all ‘poor metals’. The resistivity at 300K in the DMS, Ga$_{1-x}$Mn$_x$As, at $x \sim 0.08$, is $\approx 4 - 6$ mΩcm [8]. For α-GdSi, in its ‘metallic regime’ this is $\sim 3$ mΩcm [9]. For the manganite La$_{1-x}$Sr$_x$MnO$_3$ (LSMO), at large doping, $x > 0.3$, where electron-phonon coupling effects are expected to be weak, the room temperature resistivity is $> 5$ mΩcm [12]. To put these numbers in perspective, let us use the Mott ‘minimum metallic conductivity' [13] as reference. The Mott ‘minimum’ conductivity is $\sim 0.03 (e^2/h\alpha_0)$ and if we use a lattice constant $a_0 = 3Å$ then $\sigma_{Mott} \sim 2.5 \times 10^4 (Ωm)^{-1}$, i.e., the ‘Mott resistivity’ $\rho_{Mott}$ is approximately 4 mΩcm. Comparing with the experimental data quoted above, for all the systems concerned, $\rho/\rho_{Mott} \sim O(1)$ in the paramagnetic phase. There is no standard theory for analysing the scattering from structural and magnetic disorder in this regime.

A complete theory of transport, for example the temperature dependence, in any of these systems would of course have to deal with annealed spin disorder. We will discuss these effects in the future, but focus here on the simpler case of scattering from a combination of quenched structural and magnetic disorder. Our principal results are contained in Fig.1, showing the ‘global’ behaviour of the resistivity, and the phase diagram in Fig.3.

**Model.** We study transport in the following model:

$$H = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{\sigma} (\epsilon_i - \mu)n_{i\sigma} - J' \sum_{i} \sigma_i S_i$$

(1)

This is the ‘Anderson disorder’ problem, with the electrons being coupled additionally to spins, $S_i$, through $J'$. We use $J' > 0$. The hopping is only between nearest neighbour sites in a simple cubic lattice. The random on site potential, $\epsilon_i$, is uniformly distributed between $\pm \Delta/2$. The dimensionless parameters in the problem are disorder $\Delta/t$, magnetic coupling $J'S/t$ and the electron density $n$, controlled by $\mu$. We absorb $S$ in our magnetic coupling $J'$, assuming $|S_i| = 1$. $W = 12t$ is the bandwidth. We assume that the spin distribution is uncorrelated between sites, and isotropic on site, i.e. each spin can point anywhere on the surface of a unit sphere. The energies are measured in units of $t$, set to 1.

**Conductivity calculation.** We estimate the d.c conductivity, $\sigma_{dc}$, by using the Kubo-Greenwood expression [14] for the optical conductivity. In a disordered non interacting system:

$$\sigma(\omega) = \frac{A}{N} \sum_{\alpha, \beta} (n_{\alpha} - n_{\beta}) \frac{|f_{\alpha\beta}|^2}{\epsilon_{\beta} - \epsilon_{\alpha}} \delta(\omega - (\epsilon_{\beta} - \epsilon_{\alpha}))$$

(2)

The constant $A = (\pi e^2)/h\alpha_0$. The matrix element $f_{\alpha\beta} = \langle \psi_{\alpha} | j_z | \psi_{\beta} \rangle$ and the current operator in the tight binding model is $j_z = it\alpha_0 \sum_{i, \sigma} (c_{i+dx, \sigma} c_{i, \sigma} - h.c.)$. The $\psi_{\alpha}$ etc are single particle eigenstates, for a given realisation of disorder, and $\epsilon_{\alpha}, \epsilon_{\beta}$ etc are the corresponding eigenvalues. The $n_{\alpha} = \theta(\mu - \epsilon_{\alpha})$ etc are occupation factors.

The conductivity above is prior to disorder averaging. We work in a $L_T \times L_T \times L$ geometry and, given the finite size, the $\delta$ function constraint in $\sigma(\omega)$ cannot be satisfied for arbitrary $\omega$. However, we can still calculate the average ‘low frequency’ conductivity, defined below, and extract the d.c. conductivity by studying a sequence of system sizes.

We set $L_T = 6$, and sum over the $\delta$ functions to compute the low frequency average $\sigma_{\alpha\nu}(\mu, \Delta\omega, L) = (\Delta\omega)^{-1} \int_{\Delta\omega} \sigma(\mu, \omega, L)d\omega$, for $\{L : 24, 28, 32, 36, 40\}$, using periodic boundary condition in all directions. The averaging interval is reduced with increasing $L$, with $\Delta\omega \sim$
Transport Regimes and Insulator-Metal Transitions. - The qualitative features in transport are immediately visible in the resistivity, Fig.1, panels (a) – (b), the most noteworthy being the strongly non monotonic behaviour of $\rho(J')$ at large $\Delta$. To set the stage for discussing the interplay of structural disorder and magnetic scattering, let us quickly review the individual effects arising from each of them.

Analytic approaches to the structural disorder problem, beyond Born scattering, consider the weak localisation (Cooperon) contributions to the conductivity in a $(k_F l)^{-1}$ expansion, with $k_F$ and $l$ being the Fermi wavevector and mean free path respectively. Beyond this one can use the approximate self-consistent theory (SCT) of localisation [16], or depend on numerical results. With growing disorder the resistivity, at fixed electron density, increases monotonically, finally diverging at the Anderson transition.

For magnetic disorder, the lowest order effect arises from Born scattering, with $\rho(J') \propto J'^2$. Beyond this regime the resistivity shows a dependence [15] of the form $\rho(n, J') \sim b_1(n) J'^2 + b_2(n) J'^4$, up to moderate coupling, $J'/t \sim 3$, with $b_1, b_2$ being electron density dependent.
Our interest is in the combined effect of these two scattering mechanisms. There are tentatively five different transport regimes in the problem, and, except for (i) below, all of them are beyond the reach of standard transport theory. These are: (i) the weak scattering regime, where Mathiessen's rule holds, (ii) spin flip correction to weak localisation (WL), with the \( \Delta \) dependence showing WL corrections and spin flip increasing the conductivity, (iii) spin dephasing driven insulator-metal transition (IMT), occurring over a window in \( \Delta \), (iv) the disordered double exchange (DE) limit, and (v) the intermediate coupling 'metal'. We analyse our data in the spirit of this classification.

(i) **Weak scattering, obeying Mathiessen's rule:** The regime of weak structural disorder and weak electron-spin coupling can be understood in terms of additive Born scattering, with the net scattering rate, \( \Gamma(\Delta, J') \approx a_1 \Delta^2 + b_1 J'^2 \). The resistivity is additive and both contributions are described by lowest order perturbation theory. This corresponds to the bottom left hand corner in Fig. 1(a). The 'parallel' curves in Fig. 2(a) for \( \Delta \) upto 4, and the regime \( J' \leq 3 \) broadly identify the domain of 'Mathiessen's rule'. The net resistivity in this regime, Fig. 2(a), is \( \rho < 0.1 \rho_{\text{Mott}} \), i.e., a few hundred \( \mu \Omega \text{cm} \).

(ii) **Spin flip correction to weak localisation:** In the structural disorder problem the quantum corrections to the conductivity become important with growing \( \Delta \), and show up via the WL effect. This effect is already beyond standard transport theory. The leading corrections to \( \sigma(\Delta) \) in three dimensions, beyond Boltzmann transport, have been worked out [17]. Exact numerical calculations [15, 18] suggest that the Boltzmann result and the low order quantum corrections describe the resistivity up to \( \Delta/W \approx 1 \). In this regime, with \( \Delta/W \sim 1 \), the effect of magnetic scattering, with \( J'/W \ll 1 \) is non trivial. Spin flip scattering of the electrons [2, 3], by the random magnetic moments serves to suppress the localising effect of structural disorder, Fig. 1(a) and Fig. 2(a), as we discuss below.

Just as inelastic scattering leads to decoherence, and a suppression of quantum interference,
spin flip scattering of the electrons, arising from processes of the form \((S_{zi} + iS_{yi})c_{i}^{\dagger}c_{t}\) etc, leads to **spin decoherence** and a corresponding cutoff to WL corrections. If the dephasing time is \(\tau_s\), then the spin diffusion length is \(l_s = \sqrt{D\tau_s}\), with the diffusion constant \(D \propto \Delta^{-2}\), and \(\tau_s^{-1} \propto J'^2\). The WL correction gets corrected \([1]\) by \(\delta \sigma \propto l_s^{-1} \propto \Delta|J|\). If the WL correction to the conductivity scales as \(\sim (k_F l)^{-1} \sim \Delta^2\), then the corresponding spin flip correction to the **resistivity** should behave as \(\delta \rho \sim -\Delta^2|\Delta|\).

Fig.2.(a) shows \(\rho(\Delta, J')\) in the moderate \(J'\) region, with \(\Delta\) increasing beyond the Born scattering regime. At weak disorder the resistivity has the expected form \(\rho(\Delta, J') \propto a_1 \Delta^2 + b_1 J'^2\), while at larger disorder we expect the \(\Delta\) dependence to be stronger, and **simultaneously a positive contribution to the conductivity** \(\delta \sigma \propto |J'|\) to show up. The coefficient of the \(J'^2\) term could also be renormalised at large \(\Delta\). Taking these possibilities into account we fit the low \(J'\) resistivity to the form: \(\rho(\Delta, J')|_{J'\to 0} \approx \rho_1(\Delta) + b_1 J'^2 + c_1(\Delta)|J'| + f(\Delta) J'^2\), where the coefficients would depend on electron density. \(\rho_1(\Delta)\) tracks the localising effect of structural disorder, \(c_1(\Delta)\) measures the ‘antilocalising’ effect of spin flip scattering, and \(d_1 = b_1 + f(\Delta)\) monitors the renormalised ‘Born scattering’ from spins.

For \(n = 0.5\), the resistivity from structural disorder, \(\rho_1(\Delta) \approx a_1 \Delta^2 + a_2 \Delta^4 + a_3 \Delta^6\), as we fit in Fig.2.(b), with \(a_1 = 0.408\), \(a_2 = 3 \times 10^{-4}\), and \(a_3 = 4 \times 10^{-5}\). The coefficient of the ‘anti-localisation’ term, Fig.2.(c) is \(c_1(\Delta) \approx c_0 \Delta^\alpha\), with \(c_0 = -3.4 \times 10^{-4}\), and \(\alpha \sim 5.16\). The (renormalised) coefficient of the \(J'^2\) term, \(d_1 = b_1 + f(\Delta)\), has the form indicated in Fig.2.(d). While Fig.2.(b) highlights the rapid growth in resistivity due to structural disorder, Fig.2.(c) indicates how this growth is cut off via the spin flip scattering effected by \(J'\). This affects the metal-insulator phase boundary as we discuss next.

(iii) **Spin dephasing driven IMT:** There is no perturbative scheme as the disorder increases beyond the weak localisation regime. The SCT provides a guide and of course there is extensive numerical work on the Anderson transition. Unfortunately, the SCT has no equivalent that includes magnetic scattering as well (although there were early attempts in two dimensions \([19]\)), and we do not know of even numerical work probing the MIT including magnetic scattering.

As \(\Delta\) drives the system towards localisation, the effect of *weak* \(J'\) is dramatic. The small increase in conductivity, correcting the weak localisation contribution, now develops into a full fledged anti-localisation effect, enlarging the domain of the metallic phase, see phase diagram in Fig.3.(a), and pushing up the critical disorder needed for localisation. The critical disorder now depends on \(J'\) and increases from \(\Delta \approx 16.5\), at \(J' = 0\), to \(\Delta \approx 27\) at \(J' \approx 8\), before dropping to \(\Delta \approx 12\) for \(J' \rightarrow \infty\) (see Fig.3.(a)). The optical conductivity data, Fig.3.(b) illustrates how the low frequency conductivity increases as \(J'\) grows from 0.2 to 2.0, at \(\Delta = 16\), and drastically reduces again for \(J' = 20\). There is an **insulator-metal-insulator transition with increasing \(J'\)** for \(26 > \Delta > 16.5\).

While the IMT driven by ‘small \(J'\)’ may be motivated as the ‘extrapolation’ of the antilocalising effect of spin flip scattering, new physical effects emerge rapidly as \(J'\) is increased, staying in the large \(\Delta\) regime. The reducing resistivity, Fig.1.(a), and Fig.2.(a), exhibits a minima, and then **rises** again with increasing \(J'\). Such behaviour can be viewed as an extension of the \(J'^2\) term seen at weak disorder, but it is probably more fruitful to approach the problem from the strong coupling, double-exchange, end.

(iv) **Double exchange with disorder:** This regime corresponds to \(J'/W \rightarrow \infty\), in the presence of arbitrary structural disorder, i.e., the right edge of panel 1.(b). The form of the resistivity \(\rho(J)\) arising from ‘magnetic disorder’ at large \(J\) is very different from what one observes in \(\rho(\Delta)\) at large \(\Delta\). This is because \(J'\) contributes to both ‘band splitting’ and effective disorder, and the effective disorder saturates as \(J'/W \rightarrow \infty\) with \(J'\) controlling only the band splitting.

A standard transformation \([20]\) and projection maps on the \(t-J'\) problem to a spinless fermion model with hopping amplitudes \(t_{ij}\) dependent on nearest neighbour spin orientation:
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Fig. 3. – (a). The insulator-metal phase diagram in $\Delta - J'$, (b) the optical conductivity illustrating the 'I-M-I' feature, (c) Combining the weak coupling and strong coupling expansions, Fig.2.(a) and Fig.2.(e), for a 'global' description of the resistivity.

$$H = \sum_{ij} t_{ij}(\theta, \phi) \gamma_i^\dagger \gamma_j + \sum_i \epsilon_i \gamma_i^\dagger \gamma_i \equiv \sum_{ij} t_{ij} \gamma_i^\dagger \gamma_j + \sum_{ij} \delta t_{ij} \gamma_i^\dagger \gamma_j + \sum_i \epsilon_i \gamma_i^\dagger \gamma_i$$ with the hopping amplitude specified by $t_{ij} = -t(\cos \theta_i \cos \theta_j + \sin \theta_i \sin \theta_j e^{i(\phi_i - \phi_j)})$. We have split this into the 'mean hopping', $t_0 = \langle |t_{ij}| \rangle$, and the fluctuation $\delta t$.

The localisation properties of this model have been studied by Li et al. [4], although they did not calculate the resistivity. The 'hopping disorder' by itself localises less than 0.5% of the states in the band, and, as we observe, the resistivity at band center remains finite, $\sim 0.2 \rho_{\text{Mott}}$. On adding structural disorder the mobility edge moves inward, with localisation of the full band occurring at $\Delta/t \sim 11.5$. The critical disorder, visible approximately at large $J'$ in Fig.3.(a), can be motivated by the band narrowing in $t_0$ compared to $t$. In the fully spin disordered phase $t_0/t \sim 2/3$, and a crude scaling of $\Delta_c(J'$) would suggest, $\Delta_c(\infty)/\Delta_c(0) \sim 2/3$, so that the double exchange model in the paramagnetic phase would localise at $\Delta \sim 11$. The small deviation from this value arises from the presence of $\delta t_{ij}$ and the Berry phase involved in it. Apart from the mobility edge calculation [4] we do not know of any exact results on transport in the strongly disordered double exchange model.

The growth in resistivity with $\Delta$, remaining at large $J'$, is visible in the right edge of Fig.1.(b). Within our calculation the MIT at large $J'$ occurs slightly above $\Delta = 12$.

(v) Strongly disordered, intermediate coupling metal: This is the most complicated regime in the problem and also the most relevant for real disordered magnetic systems. The regime corresponds to $\Delta/W \sim 1$ and $J'/W \sim 1$, and, as obvious from Fig.1, $\rho/\rho_{\text{Mott}} > 1$. This is a nominally 'metallic' but diffusive, highly resistive regime. There are no analytical tools for directly estimating transport properties in this regime, but much of the physics can be motivated by an expansion about the double exchange limit.

When $J'$ is finite, both the electron spin states, polarised parallel and anti-parallel to the core spin, need to be retained. In terms of these states the Hamiltonian assumes the form:

$$H = \sum_{i\alpha} t_{ij}^{\alpha} \gamma_i^{\dagger \alpha} \gamma_j^{\alpha} + \sum_i \epsilon_i n_i - \frac{J'}{2} \sum_i (n_{i\alpha} - n_{i\beta})$$. At large $J'$ the chemical potential will be in the lower band, if we want $n < 1$. We can split the $t_{ij}^{\alpha \beta}$ as we did for the single band model, into mean amplitudes and fluctuations. The major source of disorder is still $\epsilon_i$, with additional contribution from the $\delta t_{ij}^{\alpha \beta}$. The orbital mixing effect of 'off diagonal' couplings, either in terms of mean amplitude or fluctuations, is regulated by the large energy denominator $J'$. Although
the ‘reference’ problem, \( J' \to \infty \), is not analytically tractable in the presence of structural disorder, we expect orbital mixing to generate corrections to conductivity \( \sim O(1/J') \). Fig.2.(e) fits the data, for \( \Delta \) up to 8 and \( J' \) down to 6, to the form \( \sigma(J', \Delta) \mid_{J' \to \infty} \approx \sigma(\infty, \Delta) + d_1/J' \). Fig.2.(f) show \( \rho(\infty, \Delta) = 1/\sigma(\infty, \Delta) \) and Fig.2.(g) is the coefficient \( f_1 \).

Fig.3.(a) puts together the phase diagram that emerges from tracking the conductivity across the full \( \Delta - J' \) range. While the \( \Delta \) dependence seems intuitive, in that increasing structural disorder always leads to a MIT, the effect of \( J' \), at fixed large \( \Delta \), is nontrivial. We can identify a clear I-M-I transition which, we believe, is a new result. As discussed before, the \( \sigma(\omega) \) in panel 3(b) confirms the I-M-I transition seen in the resistivity.

Fig.3.(c) puts together the weak coupling and strong coupling fits to \( \rho(J', \Delta) \), for \( \Delta < 8 \), comparing with the full numerical data. The quality of the fit indicates that the dominant transport regimes in this problem can be classified as we had suggested earlier and some of the physics can be motivated by extending concepts that are already available in the transport literature. The regions of MIT cannot be described by these expansions and should probably be accessed via a complementary scaling approach.

**Conclusions.** – We have presented exact results on electron transport in the background of arbitrary structural and spin disorder and provided a framework within which the data can be analysed. We have identified the distinct transport regimes in the model, explored the Anderson transition in the presence of weak spin disorder, and located a novel insulator-metal-insulator transition driven by increasing magnetic coupling. In addition to the intrinsic interest as a non trivial disorder problem, our results should be useful in understanding transport in the paramagnetic phase in several currently interesting magnetic materials.

**Acknowledgement** We acknowledge use of the Beowulf cluster at H.R.I.

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