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# Magnetoresistance of an insulating quasicrystalline AlPdRe film in large magnetic fields

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**Abstract**

A metal–insulator transition in a quasicrystalline icosahedral AlPdRe film series was recently observed. The resistance of one of the films follows an activated Mott variable-range hopping law, thus indicating insulating behaviour. The magnetoresistance (MR) ratios $r = R(B, T)/R(0, T)$ of this insulating film exhibited large positive values at low temperatures of 93 mK and magnetic fields up to l7 T. The data are fitted using the wave function shrinkage model for insulating films, and the fits to the data above 1 K are acceptable. The low temperature MR data exhibit anomalous behaviour at high fields above 12 T, characterized by a saturation of the ratio data and followed by a turnover to smaller values. A possible explanation for the saturation of the $R(B, T)/R(0, T)$ ratio is proposed involving a field dependence of the localization length and of the density of states, which both appear in the wave function shrinkage theory. In contrast, the weak localization theory and electron–electron interaction theory, used to describe electronic transport in *metallic* films, failed badly to describe the transport data of this *insulating* film.

## 1. Introduction

The most anomalous property of quasicrystals (QCs) is their very high resistivity values observed in the liquid helium region [1]. The physical origin for the highly resistive behaviour is currently not well understood for a system composed only of metals. This behaviour has challenged experimentalists to determine whether a metal–insulator transition (MIT) exists in some of the QC systems. Ever since Tsai *et al* fabricated the icosohedral (i) i-AlPdRe quasicrystals [2], much experimental effort has been spent on demonstrating the existence of the MIT on this system through measurements of zero field resistance versus temperature and through magnetoresistance (MR) measurements in the liquid helium temperature range. There is yet no clear consensus amongst the experimentalists on the definite existence of the MIT in the QC i-AlPdRe structure, as summarized in [3].

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## 2. Experimental background

There have been published a great number of good magnetoresistance (MR) data on the quasicrystalline (QC) i-AlPdRe system [4–11]. However, in many publications, the magnetoresistance data have been analysed using the weak localization (WL) theory together with the electron–electron interaction (EEI) theory, which describe electronic transport in *metallic* films. However, most of the films studied *appear* to be on the *insulating* side of the metal–insulator transition where these theories are no longer valid. Often the reported fitting parameters, appearing in these WL and EEI fits to the data, appear unphysical. For example, values for the diffusion constant $D_{\mathrm{dif}}$ were set to magnitudes considerably greater than 1 $\mathrm{cm}^2\ \mathrm{s}^{-1}$, values that are characteristic of metallic films. Magnitudes for the electron screening or interaction parameter $F_\sigma$ exceeded the theoretical maximum value of 0.93. Moreover, Lin's group has recently observed experimentally that $F_\sigma$ *decreases* from 0.31 to 0.01 as the spin orbit scattering time $\tau_{\mathrm{so}}$ is increased from $1.4 \times 10^{-11}$ s to $4 \times 10^{-12}$ s in disordered TiAlSn alloys [12]. Thus, it is most unlikely that values for $F_\sigma$ will exceed 0.3 in the strong spin–orbit scattering material of the QC AlPdRe. Also large variations in the spin–orbit scattering time $\tau_{\mathrm{so}}$, a fitting parameter appearing in the WL theory, have been reported between different QC samples. It is hard to justify magnitude changes of the order of $10^3$ in $\tau_{\mathrm{so}}$ since the chemical contents of the heavy nuclei elements (Pd and Re) determine the scattering strength, and these two chemical components change only by a few atomic per cent when crossing the MIT. Thus, we believe that the WL and EEI theories have been incorrectly applied to the majority of MR data on the QC AlPdRe system.

We now summarize the experimental MR results on QCs [4–11]. A good review paper of the experimental MR data is reference [11]. The published data are represented either by plots of the ratio $r = R(B,T)/R(0,T)$ or $\Delta\rho/\rho = [\rho(B) - \rho(0)]/\rho(0)$ or $\Delta\sigma = \sigma(B) - \sigma(0)$, leading to difficulties when trying to compare results between different groups. However, there are some common features shared between all the published MR data. Provided that the samples are *sufficiently insulating*, that is, samples having temperature ratios $R(4.2K)/R(300\ \mathrm{K}) > 10$, then the MR ratio $r = R(B,T)/R(0,T)$ is *always slightly less* than 1 (negative MR) in *small* fields. Only in *intermediate* to *strong* fields and at *low temperatures* do the MR ratios become *significantly larger* than 1 (positive MR) and often take on magnitudes as large as 2 to 5. If the sample is *weakly* insulating with the temperature ratios $R(4.2\ \mathrm{K})/R(300\ \mathrm{K})$ ranging only between 5 and 10, then the *negative* MR is *extremely small* or *absent* and only the positive MR process dominates over the entire field range. For example, Wang *et al* demonstrated that as the QC samples are made more insulating, then the orbital magnetoconductance process (forward interference model) becomes more and more dominating at *low* fields, resulting in $R(B,T)/R(0,T)$ ratios that are *smaller* than 1 [5, 6]. Refer to figure 3 in [5] of Wang *et al* for this beautiful result. The absence of the negative MR contribution was also reported by Sarachik's group in doped Si samples, a semiconductor system [13]. However, the general behaviour of a *negative* MR at low fields and a *positive* MR at high fields is also observed in *highly insulating* amorphous $\mathrm{Ni}_x\mathrm{Si}_{1-x}$ films and in other systems [14–19].

## 3. MR theories for *insulating* samples

This paper describes attempts to explain the MR data of insulating QC films using theories valid for *strongly insulating* films. A simple phenomenological model of two hopping processes acting simultaneously—the wave function shrinkage process and the orbital magnetoconductance (forward interference) process—can nicely explain the MR ratio data

observed in *insulating* amorphous $Ni_xSi_{1-x}$ films [14]. We extend this same model to our QC MR data taken on an *insulating* film exhibiting a Mott variable-range hopping (VRH) law in its resistance behaviour.

We are not aware of a *satisfactory* 3D theory to explain the magnetoconductance (MC) or magnetoresistance (MR) data of samples located *just below* the MIT. Our current position on MR data taken on these *weakly insulating* samples is simply to present the data without interpretation. Eventually, there will appear satisfactory theoretical descriptions to describe such results.

### *3.1. The wave function shrinkage model for positive MR ratios*

Up to *moderately high temperatures*, many *highly insulating* 3D samples exhibit resistances that follow the Mott VRH law in zero magnetic field [20, 21]:

$$R(0, T) = R_{\mathrm{Mott},0} \exp(T_{\mathrm{Mott}}/T)^{1/4} \tag{1}$$

where $R_{\mathrm{Mott},0}$ is the prefactor. $T_{\mathrm{Mott}}$ is the characteristic Mott temperature that can be determined from the zero field resistance data using the $w = -\mathrm{d}\ln R/\mathrm{d}\ln T = y(T_{\mathrm{Mott}}/T)^y$ method of Zabrodskii and Zinov'eva [22]; this method also yields a value for the hopping exponent $y \approx \frac{1}{4}$. According to theory, $T_{\mathrm{Mott}} \approx 18.1/(k_{\mathrm{B}} g_0 a_0^3)$ where $g_0$ is the constant Mott density of states (DOS) and $a_0$ is the Bohr radius or localization length [23]. Note that this localization length is expected to diverge to infinity as the MIT is approached from below. Thus, $T_{\mathrm{Mott}} \to 0$ K just below the MIT. For the Mott model to be valid, the optimum hopping distance $r_{\mathrm{opt}}$ should be greater than the localization length $a_0$ (or Bohr radius). This implies that the measurement temperatures must satisfy the relation $T < T_{\mathrm{Mott}}$ since $r_{\mathrm{opt}} \approx (3/8)a_0(T_{\mathrm{Mott}}/T)^{1/4}$ [23].

Strong positive increases of the resistance with application of a magnetic field had been predicted originally by Tokumoto *et al* [24], and by Shklovskii [25, 26] and elaborated by Shklovskii and Efros [27] using the wave function shrinkage model. Numerical calculations for predicting the $R(B, T)/R(0, T)$ ratios in *small* and *modest* magnetic fields for the case of the *Efros–Shklovskii* (ES) VRH law had been made by Schoepe [28]. The application of a magnetic field decreases the overlap probability between two sites, thus resulting in an increase of the resistance with field.

We now summarize the positive MR ratio predictions of the wave function shrinkage model for the case when the resistance exhibits a *Mott VRH* law.

(a) For *very small* magnetic fields, Shklovskii and Efros found this expression for the MR ratio [27]:

$$R(B, T)/R(0, T) \approx \exp[t_1(\mathrm{e}^2 a_0^4/\hbar^2)(T_{\mathrm{Mott}}/T)^{3/4} B^2]. \tag{2}$$

Here, $t_1$ is predicted to be $t_1 \approx 5/2016 = 0.002\,48$ and $a_0$ is the Bohr radius, approximately equal to the localization length. $R(0, T)$ is the resistance in zero field at temperature $T$, given by equation (1).

(b) For *high fields*, Shklovskii and Efros suggest this expression [27]:

$$R(B, T) \approx R_{\mathrm{Mott},B} \exp[(e a_0^2/6\hbar)^{1/3}(T_{\mathrm{Mott}}/T)^{1/3} B^{1/3}]. \tag{3}$$

Here, $R_{\mathrm{Mott},B}$ is the prefactor, different from the zero field prefactor.

(c) For the interval of *intermediate* and *large* fields, there are no analytical predictions for the $R(B, T)/R(0, T)$ ratio. Here we strongly rely on a procedure described by Schoepe in reference [28] where values for the percolation parameter (optimum hopping probability parameter) in moderately strong fields are calculated for the *Efros–Shklovskii* (ES) VRH

case. The difficult problem is to estimate the corresponding hopping volume $V_\xi$ around a donor site, which gradually changes from an isotropic sphere at small fields to a double paraboloid in large fields. Schoepe uses the volume expression suggested by Ioselevich [29, 28]. Recently, numerical calculations have been summarized in tables also for the *Mott VRH* case [30]. Values for the normalized percolation parameter $\xi_c(B)/\xi_c(0)$ can be read off from figure 1 of this paper as a function of the normalized magnetic field $B/B_c$ and inserted into equation (4) below to estimate values for $R(B, T)/R(0, T)$:

$$R(B, T)/R(0, T) = \exp\{(T_{\text{Mott}}/T)^{1/4}[\xi_c(B)/\xi_c(0) - 1]\} \tag{4}$$

where $R(0, T)$, the resistance in zero field, is given by equation (1). $\xi_c(0)$ is defined as $\xi_c(0) = (T_{\text{Mott}}/T)^{1/4}$. There is one free fitting parameter, $B_c(T)$—the normalizing characteristic field, that must be extracted from each set of MR ratio data points. But since $B_c(T)$ has the temperature dependence [28]

$$B_c(T) = 6\hbar/[ea_0^2\xi_c(0)] = (6\hbar)/(ea_0^2)(T/T_{\text{Mott}})^{1/4} \tag{5}$$

$B_c(T)$ can also be estimated at all other temperature measurement points once it is determined at one temperature. However, we have treated $B_c$ as a free fitting parameter and have determined its value at each fixed temperature where MR data were taken.

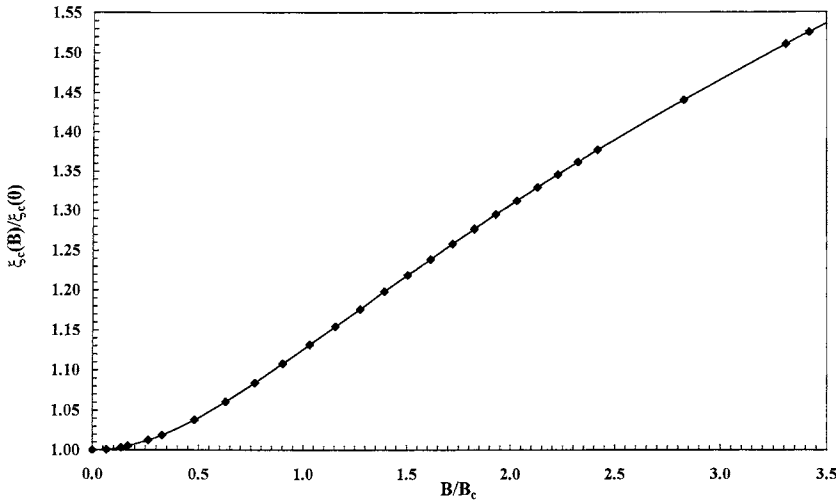


**Figure 1.** Normalized percolation parameter (the optimum hopping probability parameter) $\xi_c(B)/\xi_c(0)$ as a function of normalized magnetic fields $B/B_c$, where $\xi_c(0) = (T_{\text{Mott}}/T)^{1/4}$ and $B_c = (6\hbar/ea_0^2)(T/T_{\text{Mott}})^{1/4}$. Note the different dependences of the hopping probability upon magnetic field, with a quadratic $B^2$ dependence at very small fields and a small linear $B$ region at modest fields. Magnitudes for the resistance ratios $r = R(B, T)/R(0, T)$ upon magnetic field are obtained by using equation (4) together with values from this figure.

In the limit of small fields, the numerical calculations yield a quadratic $B^2$ dependence for the $r = R(B, T)/R(0, T)$ ratio; and in the very high field limit, the ratio has the weak field dependence going as $\ln(r) \propto B^{1/3}$.

### *3.2. The orbital magnetoconductivity theory for negative MR ratios*

Although our sample does not exhibit any negative MR and this orbital contribution is not needed in our special case, we include this section for completeness for investigators who might wish to analyse their data on *more insulating* samples.

The orbital magnetoconductivity (MC) theory or forward interference theory predicts small *negative* magnetoresistances. This model takes into account the *forward* interference among random paths in the hopping process. Nguyen, Spivak and Shklovskii (NSS) [31, 32] considered the effect of interference among the various paths associated with the hopping between two sites spaced at a distance equal to the optimum hopping distance $r_{\rm opt}$. NSS found that the interference between all possible paths within a cigar-shaped area of length $r_{\rm opt}$ and width $(a_0 r_{\rm opt})^{1/2}$ will change the hopping probability between two sites. Averaging numerically the logarithm of the conductivity over many random impurity realizations, they obtained under most conditions a *negative* MR (positive MC) which is linear in magnetic field.

Sivan, Entin-Wohlman and Imry (SE-WI) expanded the NSS model by using a critical percolating resistor method rather than the logarithmic averaging method [33]. Their calculated MC is always positive for strong fields and is predicted to *saturate* at sufficiently large fields. The field at which saturation starts to occur, $B_{\rm sat}$, is given by this approximate formula:

$$B_{\rm sat} \approx 0.7(h/e)(8/3)^{3/2}(1/a_0^2)(T/T_{\rm Mott})^{3/8}. \tag{6}$$

For this case, the saturation field $B_{\rm sat} \propto T^{3/8}$, and thus the MC saturates at smaller fields as the temperature is lowered.

For small magnetic fields, the SE-WI model predicts a quadratic magnetic field dependence of the MC; but the magnitudes are extremely small and difficult to observe experimentally in most cases.

We approximate the orbital MC contribution by the following expression:

$$\sigma(B,T)/\sigma(0,T) \approx 1 + c_{\rm sat}[B/B_{\rm sat}(T)]/[1 + B/B_{\rm sat}(T)]. \tag{7}$$

Equation (7) saturates at high fields to a value of $(1 + c_{\rm sat})$ and yields a linear dependence upon $B$ at intermediate fields. Here $c_{\rm sat}$ is a temperature *independent* fitting parameter. Inverting equation (7), we obtain for the orbital contribution to $R(B,T)/R(0,T)$:

$$R(B,T)/R(0,T) = 1/\{1 + c_{\rm sat}[B/B_{\rm sat}(T)]/[1 + B/B_{\rm sat}(T)]\}. \tag{8}$$

For the case of a small $B/B_{\rm sat}$ ratio and a small prefactor $c_{\rm sat}$,

$$R(B,T)/R(0,T) \approx 1 - c_{\rm sat} B/B_{\rm sat}. \tag{9}$$

### *3.3. Combining the wave function shrinkage theory with the orbital magnetoconductivity theory*

We now make the assumption that the resistive contributions from both the wave function shrinkage theory and the orbital magnetoconductance theory can be *added*, based upon the behaviour of our MR data. Many experimental groups have used this assumption, since 'acceptable' fits to the low field data can be obtained [15, 16]. A more rigorous theory is certainly needed, which would probably consider a hopping probability that is composed of these two processes acting simultaneously [34]. Thus, in our phenomenological empirical model, the final expression for the magnetoresistance ratio $R(B,T)/R(0,T)$ takes this form:

$$R(B,T)/R(0,T) \approx \exp\{\xi_{\rm c}(0)[\xi_{\rm c}(B)/\xi_{\rm c}(0) - 1]\} + 1/\{1 + c_{\rm sat}[B/B_{\rm sat}(T)]/[1 + B/B_{\rm sat}(T)]\} - 1 \tag{10}$$

where $c_{\rm sat}$, $B_{\rm sat}(T)$ and $B_{\rm c}(T)$ are three fitting parameters. The last term, $-1$, is needed to assure that the ratio has the correct limit when $B = 0$, namely that $R(B \to 0, T)/R(0,T) = 1$. Recall that $B_{\rm sat}(T) \propto T^{3/8}$, $B_{\rm c}(T) \propto T^{1/4}$, and $c_{\rm sat}$ should be independent of temperature.

We have recently observed that *weakly insulating* films do not exhibit this *negative* MR contribution. These weakly insulating films generally have Mott characteristic temperatures

smaller than 100 K or $R(4.2\ \mathrm{K})/R(300\ \mathrm{K})$ temperature ratios less than 10. We speculate on the absence of the negative MR in reference [35]. The film studied in this paper with $T_{\mathrm{Mott}} = 3.425$ K also does not exhibit ratios smaller than 1 (that is, no negative MR present); hence $c_{\mathrm{sat}} = 0$ and equation (10) reduces to the simple form of equation (4), where the wave function shrinkage theory dominates at all fields.

## 4. The weak localization theory and electron–electron interaction theory for *metallic* samples

The weak localization (WL) theory and the electron–electron interaction (EEI) theory have been very successful in describing the low temperature magnetoconductance (MC) data and zero field conductivity data of *metallic* films. Unfortunately, these theories have often been applied incorrectly to *insulating* quasicrystalline films, resulting in unphysical fitting parameters. When these theories are used to describe the electronic transport properties of *metallic* quasicrystalline films, the resulting fitting parameters take on reasonable physical values [36]. We will try to fit these two *metallic* theories to our transport data on the '*insulating*' A2 film.

Electron–electron interactions (EEI) produce a dip in the density of states close to $E_{\mathrm{F}}$. This dip results in a small correction to the zero field conductivity that reduces the conductivity with decreasing temperatures. According to the 3D prediction of Altshuler and Aronov [37], the particle–hole contribution arising from EEI to the zero field conductivity is

$$\sigma_{\mathrm{EEI}}(T) = \frac{1.294}{\sqrt{2}}\frac{e^2}{4\pi^2\hbar}\left(\frac{4}{3} - \frac{3}{2}\tilde{F}_\sigma\right)\left(\frac{k_{\mathrm{B}}T}{\hbar D_{\mathrm{dif}}}\right)^{1/2} \tag{11}$$

where the electron screening or interaction parameter $\tilde{F}_\sigma$ ranges between 0.2 and 0.4 for many thin metallic films. According to theory, the electron screening parameter cannot exceed the value of 0.93 [38, 39]; this parameter has an extremely weak dependence upon the free carrier concentration $n$ going as $\tilde{F}_\sigma \propto 1/(n)^{1/6}$. In addition, the diffusion constant $D_{\mathrm{dif}}$ is predicted to vanish as the metal–insulator transition is approached from above [40]. The small diffusion constant associated with a *barely insulating* film makes the prefactor of the $T^{1/2}$ term large, and this causes problems when fitting to the conductivity of films located close to the MIT. Also, a conversion factor of 1/100 must be used if the conductivity is expressed in units of $(\Omega\ \mathrm{cm})^{-1}$.

Lee and Ramakrishnan have calculated the 3D magnetoconductivity (MC) contribution, $\Delta\sigma = \sigma(B) - \sigma(0)$, arising from EEI in the particle-hole channel [39]:

$$\Delta\sigma_{\mathrm{EEI}}(B,T) = \frac{-e^2}{4\pi^2\hbar}\tilde{F}_\sigma\left(\frac{k_{\mathrm{B}}T}{2\hbar D_{\mathrm{dif}}}\right)^{1/2} g_3\left(\frac{g_{\mathrm{e}}\mu_{\mathrm{B}}B}{k_{\mathrm{B}}T}\right) \tag{12}$$

where $g_{\mathrm{e}}$ is the Lande factor. Ousset *et al* have suggested suitable approximations for the function $g_3(x)$ [41]. Note that the low field behaviour of $\Delta\sigma_{\mathrm{EEI}}$ has a $B^2$ dependence and the high field behaviour goes as $B^{1/2}$. It is useful to note that $g_{\mathrm{e}}\mu_{\mathrm{B}}/k_{\mathrm{B}} \approx 4/3$ in units of $K/T$ if $g_{\mathrm{e}} = 2$. The MC from the EEI process is always negative. Again the $(D_{\mathrm{dif}})^{-1/2}$ dependence will cause problems for highly resistive films.

The weak localization (WL) theory generally applies to very metallic films, but it appears to work successfully for *barely metallic* films too. Kawabata first derived the 3D WL correction to the *zero field* conductivity for the case of no spin–orbit scattering [42]. Fukuyama and Hoshino extended the Kawabata zero field results to include the spin–orbit scattering $\tau_{\mathrm{so}}$ and obtained a zero field correction to the conductivity [43]. Hickey *et al* have suggested the

following zero field expression that includes magnetic spin scattering [44]:

$$\sigma_{\mathrm{WL}}(T) = \frac{e^2}{2\pi^2\hbar}\frac{1}{\sqrt{D_{\mathrm{dif}}}}\left[3\left(\frac{1}{4\tau_{\mathrm{in}}(T)}+\frac{1}{3\tau_{\mathrm{so}}}+\frac{1}{\tau_{\mathrm{s}}}\right)^{1/2}-\left(\frac{1}{4\tau_{\mathrm{in}}(T)}+\frac{1}{4\tau_{\mathrm{s}}}\right)^{1/2}\right] \tag{13}$$

where $\tau_{\mathrm{so}}$ is the temperature independent spin-orbit scattering time, $\tau_{\mathrm{s}}$ is the temperature independent magnetic spin scattering time and $\tau_{\mathrm{in}}(T)$ is the temperature dependent inelastic scattering time. The characteristic fields are related to the scattering times through the expression $B_x = \hbar/(4eD_{\mathrm{dif}}\tau_x)$. A magnitude for the spin-orbit scattering time [45, 46] can be estimated from the expression $\tau_{\mathrm{so}} \approx \tau_{\mathrm{o}}(l37/Z)^4$ where $Z$ is the atomic number ($Z = 75$ for Re and $Z = 46$ for Pd) and where $\tau_{\mathrm{o}} \approx 10^{-15}$ s is the elastic scattering time. For our case of strong spin-orbit scattering and hence a small magnitude for $\tau_{\mathrm{so}}$, equation (13) predicts weak *anti*-localization where $\sigma_{\mathrm{WL}} \propto (-1/2)[\tau_{\mathrm{in}}(T)]^{-1/2}$; in this case, the WL contribution produces an *increase* in the conductivity with decreasing temperatures, in opposition to the EEI contribution. However, the EEI contribution of equation (11) seems always to dominate, resulting in an overall major decrease of the zero field conductivity with decreasing temperatures. For films located just above the MIT, $\tau_{\mathrm{in}}(T)$ takes on the simple temperature dependence of $\tau_{\mathrm{in}}(T) = a/T^1$ [47–49].

Thus, the zero field conductivity can be represented by this expression:

$$\sigma(T) = \sigma_0 + \Delta\sigma_{\mathrm{EEI}}(T) + \Delta\sigma_{\mathrm{WL}}(T) \tag{14}$$

where $\Delta\sigma_{\mathrm{EEI}}(T)$ and $\Delta\sigma_{\mathrm{WL}}(T)$ each have a simple temperature power law dependence and $\sigma_0$ is a *positive* offset constant.

For the 3D weak localization magnetoconductivity (MC) theory, Baxter *et al* extended the results of Fukuyama and Hoshino to include weak magnetic scattering for the case where $\tau_{\mathrm{s}}^{-1} \ll \tau_{\mathrm{so}}^{-1}$ [50]; the Zeeman splitting correction at high fields has been neglected in this expression [50]:

$$\Delta\sigma_{\mathrm{WL}}(B,T) = \frac{e^2}{2\pi\hbar^2}\sqrt{\frac{eB}{\hbar}}\left[\frac{3}{2}f_3\left(\frac{B}{B_{\mathrm{in}}(T)+\frac{4}{3}B_{\mathrm{so}}+\frac{2}{3}B_{\mathrm{s}}}\right)-\frac{1}{2}f_3\left(\frac{B}{B_{\mathrm{in}}(T)+2B_{\mathrm{s}}}\right)\right]. \tag{15}$$

Baxter *et al* gave a numerically convenient approximation for the function $f_3(x)$, which is accurate over the entire range of $x$, and retains the correct asymptotic limits [50].

Note that at low fields $\Delta\sigma_{\mathrm{WL}}$ exhibits a $B^2$ dependence, and at high fields a $B^{1/2}$ dependence since $f_3(x)$ saturates at 0.605.

## 5. Data analysis techniques

Films may be classified electronically as being either insulating or metallic. *Insulating* 3D films exhibit *infinite* resistivities or *zero* conductivities at absolute zero in temperature. In contrast, *metallic* 3D films always display finite resistivities or positive conductivities at absolute zero. Note that films that exhibit decreasing conductivities with decreasing temperatures still can be *metallic*.

*Strongly insulating* samples (perhaps also including *insulating* quasicrystal films) exhibit an activated hopping conductivities which can be described by the variable-range hopping (VRH) expression in zero magnetic field:

$$\sigma(T) = \sigma_0/[\exp(T_0/T)^y] \tag{16}$$

where $\sigma_0$ is the prefactor, $T_0$ is a characteristic temperature and $y$ is the hopping exponent.

In contrast, the conductivity of a 3D *metallic* sample (most likely including *metallic* quasicrystal films) at sufficiently low temperatures can be described by the power law expression

$$\sigma(T) = \sigma(0) + CT^z \tag{17}$$

where $\sigma(0)$ is the positive zero temperature conductivity, $C$ is the prefactor and $z$ is the exponent of the temperature power law. Equation (17) might approximate the conductivity contribution from the 3D electron–electron interaction (EEI) theory and/or from the 3D weak localization (WL) theory. Note that in the above procedures the exponents $y$ and $z$ are free fitting parameters.

An useful and sensitive technique to identify the metal–insulator transition was previously introduced [51, 52]. The mathematical function $w(T)$ exhibits distinctively different temperature behaviours for insulating and metallic films:

$$w(T) = \mathrm{d}\ln\sigma/\mathrm{d}\ln T = (T/\sigma)\,\mathrm{d}\sigma/\mathrm{d}T = -(T/R)\,\mathrm{d}R/\mathrm{d}T. \tag{18}$$

For *strongly insulating* films exhibiting variable-range hopping conductivity, inserting equation (16) into equation (18) yields

$$w(T) = y(T_0/T)^y; \tag{19}$$

notice that $w(T)$ increases to *infinity* as the temperature approaches absolute zero. A least regression fit through the $\log(w)$ versus $\log(T)$ data will determine the hopping exponent $y$ and the characteristic temperature $T_0$ that appears in the VRH law.

For 3D *metallic* films exhibiting slowly decreasing conductivities with decreasing temperatures at low temperatures, equation (17) can be substituted into equation (18) to yield

$$w(T) = zCT^z/[\sigma(0) + CT^z] = zCT^z/\sigma(T). \tag{20}$$

Observe that if the film is indeed *metallic* and exhibits a finite positive conductivity $\sigma(0)$ at absolute zero, then $w(T)$ should extrapolate to *zero* as $T \to 0$ K. Thus, if one fits MR data using the WL and EEI theories, then the zero field conductivity data better exhibit $w \to 0$ as the $T \to 0$ K, indicating self-consistency between the zero field conductivity expressions and the finite field MC expressions. Unfortunately, this important test has been ignored or neglected in the quasicrystalline transport field.

For the special *insulating* case of the conductivity following a simple power law with $\sigma(0) = 0$ in equation (17), that is

$$\sigma(T) = CT^z \tag{21}$$

then equations (21) and (18) predict that the $w$ are independent of temperature and that $w = z$.

## 6. Comparison between experimental and numerical results

### *6.1. Analysis of a metallic quasicrystalline AlPdRe film*

We have previously studied a *metallic* 2200 Å AlPdRe film, C5, having a temperature ratio $R(4.2\text{ K})/R(300\text{ K})$ of 2.9 [36]. Both the MC data and zero field conductivity data could be nicely fitted using the WL and EEI theories summarized above. The fitting parameters used were $D_{\mathrm{dif}} = 0.75\ \mathrm{cm}^2\ \mathrm{s}^{-1}$, $F_\sigma = 0.2$, $\tau_{\mathrm{so}} = 1.5 \times 10^{-13}$ s, $\tau_{\mathrm{in}} = 1.6 \times 10^{-11}/T^{1.03}$ s and $\sigma_0 = +18.7\ (\Omega\ \mathrm{cm})^{-1}$; these magnitudes are reasonable and physical. In addition, the $w = -\,\mathrm{d}\ln R/\mathrm{d}\ln T$ data extrapolated to zero as $T \to 0$ K, suggesting that this film is *metallic*. This film C5 has a geometric factor $f_{\mathrm{g}} = 4.4 \times 10^{-6}$ cm, needed to convert resistances to resistivities. Refer to reference [36] for additional details.

*6.2. Analysis of an insulating quasicrystalline AlPdRe film.*

We now compare the numerical calculations to MR ratio data taken on an *insulating* 2000 Å quasicrystalline AlPdRe film A2. This film has an $R(4.2\ \mathrm{K})/R(300\ \mathrm{K})$ ratio of 8.7 and a geometric conversion factor $f_g = 2.9 \times 10^{-6}$ cm. For details on film preparation, refer to reference [3]. Values for the hopping exponent $y = 0.244$ and for the Mott characteristic temperature $T_{\mathrm{Mott}} = 3.425$ K were obtained using the method described by Zabrodskii and Zinov'eva [22] by fitting a least regression fit of equation (19) through the $w$ data ($w = -\mathrm{d}\ln R/\mathrm{d}\ln T$) as shown in figure 2. The zero field resistivity data and the Mott VRH fit are shown in figure 3, and agreement is excellent below 1.5 K. Above 4 K, the resistance no longer follows a Mott VRH law. However, we note that for the Mott VRH model to be valid, the optimum hopping distance $r_{\mathrm{opt}}(T)$ must satisfy the criterion that $r_{\mathrm{opt}}(T)/a_0 \approx 0.375(T_{\mathrm{Mott}}/T)^{1/4} \geqslant 1$. This criterion is barely satisfied in the 0.07 K to 2 K temperature region of interest, owing to the small value of the Mott temperature, $T_{\mathrm{Mott}} = 3.425$ K.

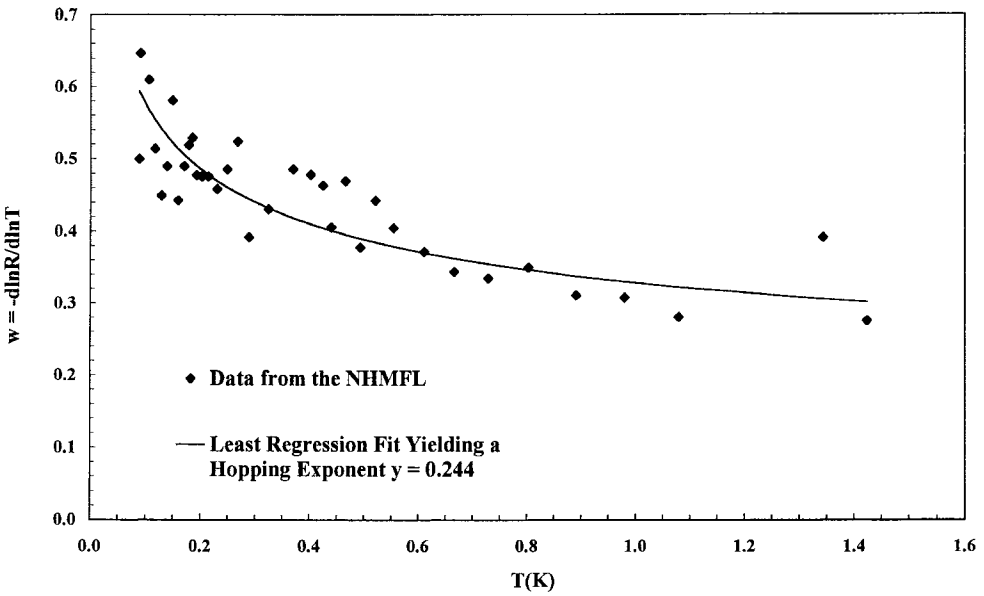


**Figure 2.** The increasing behaviour of $w = -\mathrm{d}\ln R/\mathrm{d}\ln T$ with decreasing temperatures strongly suggests that the resistivity of this QC film A2 is characterized by a VRH law. A least regression fit through the $w$ data yields a hopping exponent of $y \approx 0.244$ and a characteristic temperature $T_{\mathrm{Mott}} \approx 3.425$ K.

In figure 4, the MR ratio data are compared between an *insulating* and a *metallic* QC film, A2 and C5, at $T \approx 1.6$ K. The difference in magnitudes between the two ratio sets is striking. Note that the $R(B, T)/R(0, T)$ ratios in *metallic* films *rarely exceed* values greater than 1.05.

We first try to fit the WL and EEI theories, valid for metallic films, to the MC data at $T = 1.77$ K of the '*insulating*' QC film A2, using equations (12) and (15). We set $F_\sigma = 0.25$, $\tau_{\mathrm{so}} = 10^{-13}$ s, $\tau_{\mathrm{in}}(T = 1.77\ \mathrm{K}) = 10^{-11}$ s and $D_{\mathrm{dif}} = 0.1\ \mathrm{cm}^2\ \mathrm{s}^{-1}$. A value for $D_{\mathrm{dif}}$ can also be estimated using the relation $D_{\mathrm{dif}} = 1/[\mathrm{e}^2\rho\mathrm{DOS}(E_{\mathrm{F}})]$. Using a specific heat $\gamma$ of 0.17 mJ $\mathrm{mol}^{-1}$ and the relation that DOS $\approx 0.422\gamma$ [1, 11], one estimates that the $\mathrm{DOS}(E_{\mathrm{F}}) \approx 3 \times 10^{46}$ states $\mathrm{J}^{-1}\ \mathrm{m}^{-3}$. To obtain this result, we have assumed that 1 mole = 56 g for the $Al_{70}Pd_{21}Re_9$ material and that its density is about 4.6 g $\mathrm{cm}^{-3}$. Using a room temperature

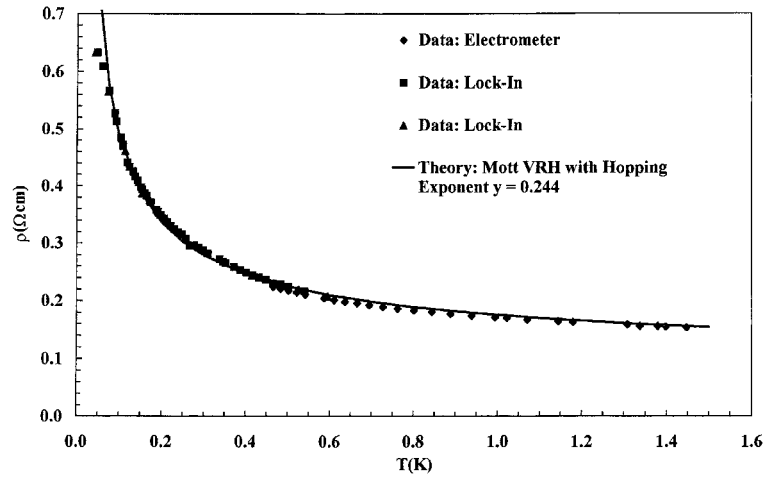


**Figure 3.** Fit of the Mott VRH law, $\rho(0, T) = \rho_{\mathrm{Mott},0} \exp(T_{\mathrm{Mott}}/T)^{0.244}$, to the low temperature resistivity data of the quasicrystalline AlPdRe film A2 with $T_{\mathrm{Mott}} \approx 3.425$ K.

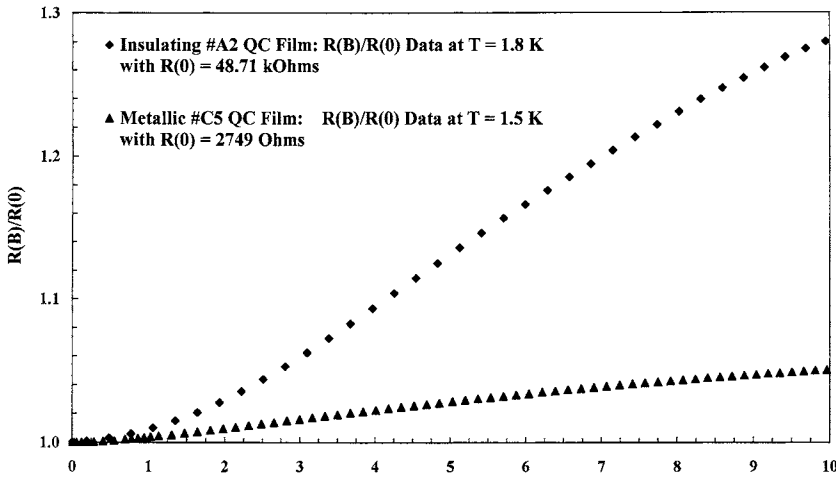


**Figure 4.** Comparison between the MR magnitudes of an *insulating* and a *metallic* quasicrystalline AlPdRe film, A2 and C5, at similar temperatures. Notice the much larger magnitudes of the MR ratios for the *insulating* film, A2.

resistance of 4000 Ω or an equivalent resistivity of 0.000 116 Ω m, the estimated value for $D_{\mathrm{dif}}$ is about 0.11 $\mathrm{cm}^2\ \mathrm{s}^{-1}$.

The raw resistance data at $T = 1.77$ K was converted to conductivities and then values for the MC, $\Delta\sigma = \sigma(B) - \sigma(0)$, were calculated. The first striking observation is the small magnitudes for the MC data, resulting from the high film resistances of 48 700 Ω at 1.77 K, as illustrated in figure 5. These small magnitudes are in conflict with the large predicted values of the theories, arising mainly from the small magnitude of the diffusion constant that appears inversely in the prefactors. In figure 5, the predicted fit from the EEI theory exceeds the MC data values; an additional smaller contribution from the WL theory makes the final theoretical predictions of the combined theories a factor of two greater than the measured values; this poor agreement in figure 5 suggests that these metallic theories fail to explain the data.

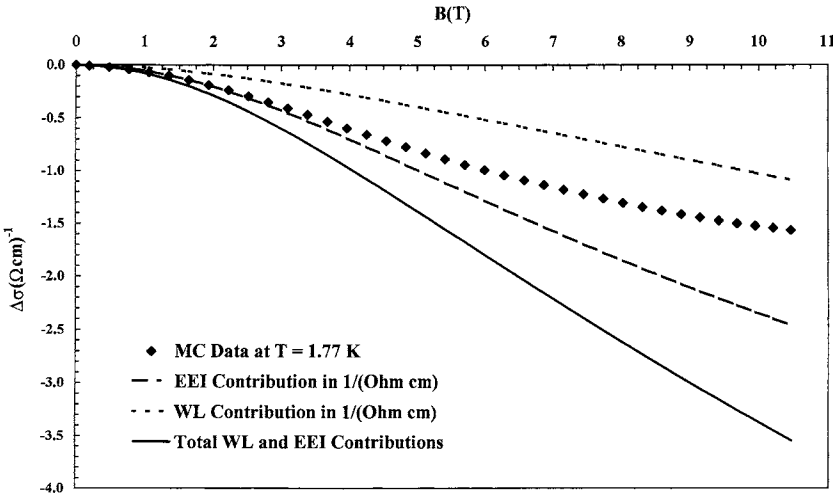


**Figure 5.** An attempt using the *metallic* quantum correction theories to fit the MC data of film A2 at $T = 1.77$ K. Note that values of $r = R(B, T)/R(0, T)$ of film A2 from figure 4 have been converted to MC values appearing in this figure, where $\Delta\sigma = \sigma(B) - \sigma(0)$. The weak localization (WL) and electron–electron interaction (EEI) theories give unacceptable fits to the MC data of this 'insulating' film.

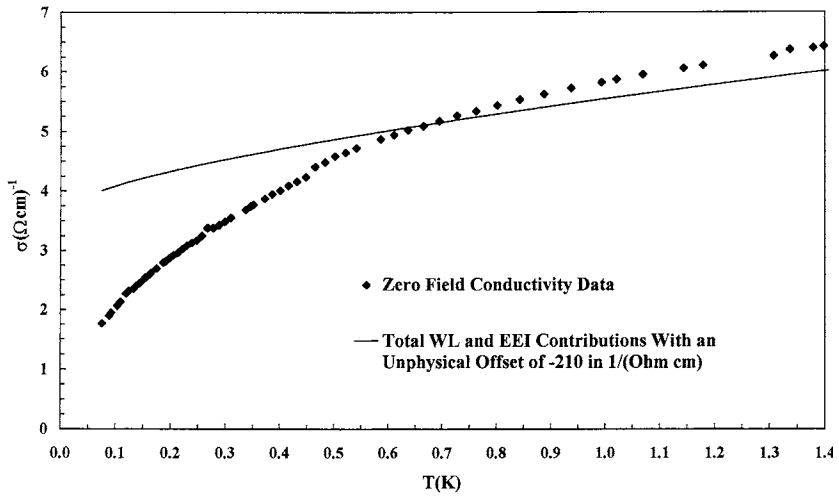


**Figure 6.** An attempt using the *metallic* quantum correction theories to fit the zero field conductivity data. Note that values of the resistivity from figure 3 have been converted to conductivities appearing in this figure. Not only is the predicted temperature dependence of the conductivity unacceptable using the WL and EEI theories, but an unphysical *negative* conductivity offset constant, $\sigma_0 = -210\ (\Omega\ \mathrm{cm})^{-1}$, had to be included. Thus, the WL and EEI theories fail badly to describe the zero field conductivity data of this insulating film.

But the most convincing evidence for the fitting failure comes when trying to fit the above parameters to the zero conductivity data, as shown in figure 6. Equations (11), (13) and (14) were used. First, the temperature dependence is incorrect in that the conductivity data actually follows an activated Mott VRH law and not simple temperature power laws; but much more important, a *negative* offset value of $-210(\Omega\ \mathrm{cm})^{-1}$ was required to pass the solid theoretical

line through the data in this figure. Negative conductivities are not physical. Thus, these two metallic theories fail badly to describe the 'insulating' data, and it is unfortunate that such consistency tests were neglected in earlier MC analyses.

The large values for the MR ratios at $T = 1.77$ K clearly suggest that film A2 is an *insulator*. We now try fitting the MR ratio data at $T = 1.77$ K using the wave function shrinkage theory. The line in figure 7 is a fit using equation (4) and the numerical values from figure 1. $B_c$ was the only free fitting parameter, since $c_{sat} = 0$ owing to the absence of any negative MR. $T_{Mott}$ was set to the value of 3.425 K, which was extracted from the zero field resistance data. Note the deviations between theory and ratio data at fields higher than 6 T. Overall, the fit is acceptable. Using the value $B_c = 6.25$ T at $T = 1.77$ K and equation (5), the Bohr radius (localization length) was estimated to be $a_0 \approx 230$ Å.

## 7. Saturation behaviour of the magnetoresistance ratio

The discrepancies between the wave function shrinkage predictions and the ratio data become much worse for temperatures below 1 K, as illustrated in figure 8. The behaviour of the ratio data is anomalous and surprising with the ratios tending to *saturate* around 13 T and then slightly decrease at higher fields. Both the theory and numerical calculations predict a slow *increase* of the ratio data going as $\ln(r) \propto B^{1/3}$. There has been reported a similar saturation behaviour in QC AlPdRe melt-spun annealed ribbons by the French group [8]. Only one fitting parameter, $B_c$, was used in figure 8: $B_c(T = 0.093\ \text{K}) = 0.725$ T, $B_c(T = 0.295\ \text{K}) = 1.37$ T and $B_c(T = 0.54\ \text{K}) = 2.23$ T.

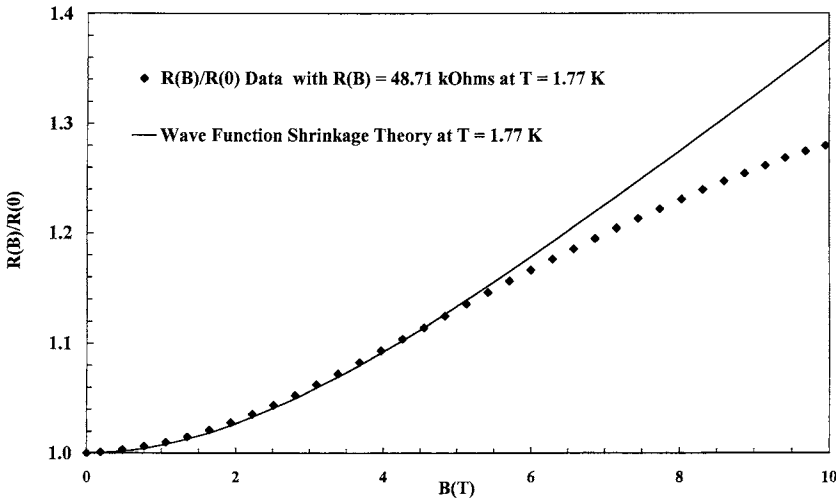


**Figure 7.** Magnetoresistance (MR) ratio data at $T = 1.77$ K for the *insulating* crystalline AlPdRe film A2. The solid line is a fit obtained by using the wave function shrinkage equation (4) along with the numerical calculated values of the percolation parameter appearing figure 1. One free fitting parameter was used: $B_c = 6.25$ T. Observe that there are *no* MR ratios *smaller than* 1 at low fields, probably owing to the fact that this film is not sufficiently insulating with its small Mott temperature of $T_{Mott} = 3.425$ K.

Moreover, the dependence of $B_c$ did not scale as $T^{1/4}$ according to the theory but exhibited a strong $T^{0.7}$ dependence. Thus, either the wave function shrinkage model needs to be modified or perhaps it simply does not apply to these *weakly insulating* Mott VRH films.

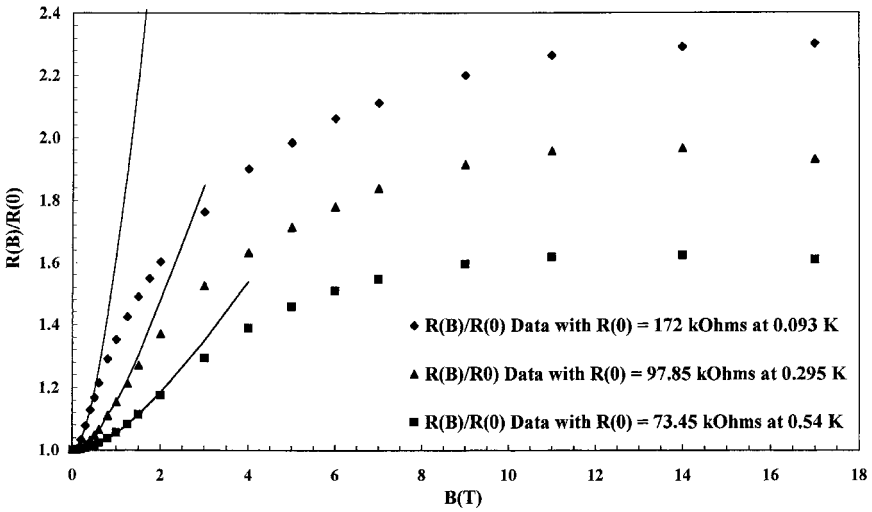


**Figure 8.** The magnetoresistance ratio data at low temperatures for the *insulating* quasicrystalline AlPdRe film A2. The three lines are fits obtained by using equation (4) along with the numerical calculated values of the percolation parameter appearing in figure 1. The anomalous saturation behaviour and turnover of the $r$ values for $B > 12$ T are not well understood.

The saturation behaviour of the ratio data suggests that either additional mechanisms within the wave function shrinkage process become important or that a new conduction process dominates over the wave functions shrinkage process at high fields. Raikh's group has suggested that the density of states (DOS), $g_B$, in a 2D electron gas has a magnetic field dependence and increases with application of a field [53]. Perhaps a similar behaviour occurs in 3D films, but the 3D behaviour of $g_B$ is not currently known. In addition, Pichard's group suggests that the localization length or Bohr radius, $a_B$, has a magnetic field dependence that is influenced by spin-orbit scattering [54]. A prediction that the Bohr radius is field dependent was also made by Lea's group [24]. Medina *et al* suggest that the localization length increases as $B^{1/2}$, that is $a_B \approx a_0(1+mB^{1/2})$ [55]; here $m$ is a fitting parameter. Hence both parameters, $g_B$ and $a_B$, might influence the magnitude of the normalized percolation parameter $\xi_c^*$ in large magnetic fields.

According to Schoepe [28], the normalized percolation parameter $\xi_c^* = \xi_c(B)/\xi_c(0)$ can be expressed as a function of both the density of states (DOS) $g_B$ and of the localization length $a_B$ in any field. Recall that the MR ratio $r = R(B)/R(0)$ is given by $r = \exp\{\xi_c(0)[\xi_c^* - 1]\}$ with $\xi_c^* = \xi_c(B)/\xi_c(0)$ and $\xi_c(0) = (T_0/T)^v$. Here $T_0$ is the characteristic VRH temperature and $v = y$ is the VRH exponent extracted from the zero field resistance versus temperature data. There is a relation between the hopping exponent $v$ in the VRH resistance law and the exponent of the power law dependence of the DOS near the Fermi energy $E_F$, namely $\mathrm{DOS} = g_0|E - E_F|^n$ with $v = y = (n+1)/(n+4)$ according to Hamilton [56]. Recall that $R(T) = R_0 \exp(T_0/T)^v$ in zero field. For example, in the Mott VRH case of a constant DOS, then $n = 0$ and $v = y = \frac{1}{4}$; for the case of the Coulomb gap where $n = 2$, then $v = y = \frac{1}{2}$. We often observe a hopping exponent of $v = y \approx 0.62$ in very strongly insulating 'soft-gap' films, which corresponds to a DOS exponent $n \approx 4$ [14].

Following Schoepe's procedure [28], we find

$$\xi_c^* = \xi_c(B)/\xi_c(0) = (g_0/g_B)^{1/(n+4)}(E_B/E_0)^{3/[2(n+4)]}s^{3/(n+4)}/\{[F(s)]^{1/(n+4)}6^{1/(n+4)}\} \qquad (22)$$

$$B^* = B/B_c = [F(s)]^{1/(n+4)} s^{(n+1)/(n+4)} 2^{1/(n+4)} / \{(g_0/g_B)^{1/(n+4)} (E_0/E_B)^{(n+5/2)/(n+4)} 3^{(n+3)/(n+4)}\}. \tag{23}$$

Here $E_0$ and $E_B$ are the binding energies in zero and finite field defined as $E_0 = \hbar^2/(2ma_0^2)$ and $E_B = \hbar^2/(2ma_B^2)$. Tabulated values of $F(s)$ versus $s$ are listed in table 1 [28–30]. Thus, if one has theoretical expressions for the behaviour of the DOS $g_B$ and for the localization length $a_B$ in large finite fields, one should be able to calculate the normalized percolation parameter and hence the MR ratio $r$ for any field.

Moreover, to inquire whether saturation is possible either in a Mott or ES VRH film, let us consider two special cases. For the Mott case when $n = 0$ with $v = \frac{1}{4}$, then equations (22) and (23) simplify to

$$\xi_c^*(\text{Mott}) = \xi_c(B)/\xi_c(0) = (g_0/g_B)^{1/4} (a_0/a_B)^{3/4} s^{3/4} / \{[F(s)]^{1/4} 6^{1/4}\} \tag{24}$$

$$B^*(\text{Mott}) = B/B_c = [F(s)]^{1/4} s^{1/4} 2^{1/4} / \{(g_0/g_B)^{1/4} (a_B/a_0)^{5/4} 27^{1/4}\} \tag{25}$$

with $B_c = 6\hbar/[ea_0^2 (T_{\text{Mott}}/T)^{1/4}]$ and $\xi_c(0) = (T_{\text{Mott}}/T)^{1/4}$.

For the ES case where $n = 2$ with $v = \frac{1}{2}$, then equations (22) and (23) yield

$$\xi_c^*(\text{ES}) = \xi_c(B)/\xi_c(0) = (g_0/g_B)^{1/6} (a_0/a_B)^{1/2} s^{1/2} / \{[F(s)]^{1/6} 6^{1/6}\} \tag{26}$$

$$B^*(\text{ES}) = B/B_c = [F(s)]^{1/6} s^{1/2} 2^{1/6} / \{(g_0/g_B)^{1/6} (a_B/a_0)^{3/2} 3^{5/6}\} \tag{27}$$

with $B_c = 6\hbar/[ea_0^2 (T_{\text{ES}}/T)^{1/2}]$ and $\xi_c(0) = (T_{\text{ES}}/T)^{1/2}$.

Values for $B_c$ and hence for $a_0$ can be extracted from the MR ratio data in the small to intermediate field regime where the saturation effect is negligible or small. In this case, one sets $g_B = g_0$ and $a_B = a_0$ in all four equations (24)–(27).

For saturation of the MR ratio $r$ to occur, the normalized percolation parameter $\xi_c^* = \xi_c(B)/\xi_c(0)$ must become field independent at high fields. This might happen if the DOS $g_B$ and/or the localization length $a_B$ both increase in magnitude with increasing field. But inspection of equations (24) and (26) suggests that the influence of the density of states upon $\xi_c^*$ will be small in both cases owing to the small power law exponents of $\frac{1}{4}$ and $\frac{1}{6}$ appearing in equations (24) and (26). In contrast, the saturation in the *Mott* VRH case could result in a rather strong dependence of $\xi_c^*$ upon the localization length, namely $\xi_c^* \propto (a_0/a_B)^{3/4}$ according to equation (24). In contrast, a *weaker* saturation effect would be predicted for the $ES$ case owing to the smaller power law exponent of $\frac{1}{2}$ where $\xi_c^* \propto (a_0/a_B)^{1/2}$, and for a *very strongly* insulating a:$Ni_xSi_{1-x}$ film where $y = v \approx 0.62$ and hence $n \approx 4$, the predicted saturation effect becomes even weaker since $\xi_c^* \propto (a_0/a_B)^{3/8}$; experimentally, a very *small* tendency towards saturation in the MR data was observed in fields up to 12 T for this 'soft-gap' film [14].

In order to compare MR data to theory, one must generate a table of $\xi_c^*$ values versus the normalized field $B^*$ values. This is a straightforward procedure at small and intermediate fields using $F(s)$ versus $s$ values listed in table 1, when setting $g_B = g_0$ and $a_B = a_0$, thus ignoring their field dependences. This approximation was made for the numerical values appearing in figure 1.

However, at high fields where the localization length $a_B$ might be much larger than the zero field value $a_0$, the calculations are more complicated. Note that the normalized field parameter $B^* = B/B_c$ appears both on the left side of equation (25) as well as in the denominator on the right side through $a_B$. Thus, a theoretical expression for $a_B$ is badly needed in order to solve for $B^*$ in a self-consistent way for any given value of $s$ and $F(s)$. Once a value for $B^*$ has been determined for a particular value of $s$ and hence $F(s)$, then a unique value for $\xi_c^*$ can be found using these same parameters along with the magnitude of $a_B(B^*)$.

As a fitting example, we generate $r$ ratio values using equations (24) and (25) where $a_B = a_0[1 + m(B^*)^2]$. Here $B^* = B/B_c$ and $g_B = g_0$. The three fitting parameters

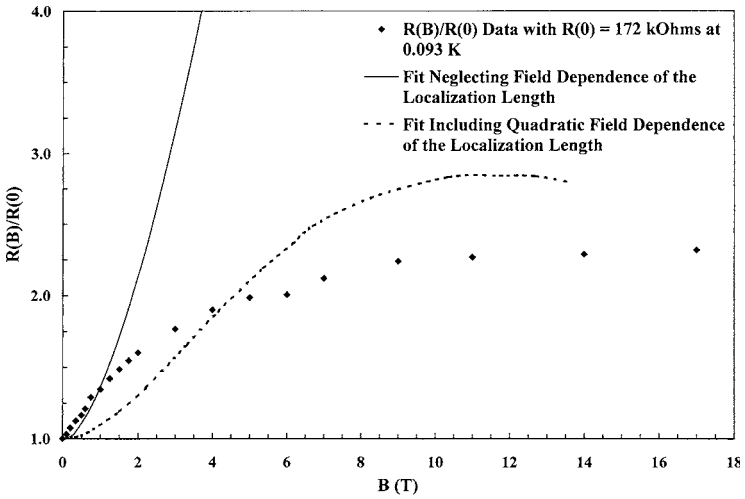


**Figure 9.** MR ratio data taken at $T = 0.093$ K compared to the predictions of Schoepe's expressions, equations (24) and (25). The upper solid curve neglects the field dependence of the localization length while the lower dashed curve includes a quadratic field dependence. Three fitting parameters were used. The density of states (DOS), the fourth fitting parameter, was assumed to be field independent and thus $g_B/g_0 = 1$.

**Table 1.** Tabulated values for the Ioselevich integral $F(s)$ versus $s$ [29].

| $F(s)$ | $s$ | $F(s)$ | $s$ | $F(s)$ | $s$ |
|---|---|---|---|---|---|
| 0 | 0 | 15.24 | 6.000 | 380.8 | 27.81 |
| 0.001 329 | 0.2000 | 18.21 | 6.500 | 482.7 | 31.27 |
| 0.010 53 | 0.4000 | 21.44 | 7.000 | 612.4 | 35.18 |
| 0.020 42 | 0.5000 | 24.93 | 7.500 | 777.5 | 39.60 |
| 0.034 98 | 0.6000 | 28.68 | 8.000 | 987.8 | 44.61 |
| 0.081 21 | 0.8000 | 32.68 | 8.500 | 1256 | 50.27 |
| 0.1547 | 1.000 | 36.94 | 9.000 | 1598 | 56.67 |
| 0.4841 | 1.500 | 41.46 | 9.500 | 2035 | 63.92 |
| 1.054 | 2.000 | 46.23 | 10.00 | 2593 | 72.13 |
| 1.884 | 2.500 | 55.92 | 10.94 | 3306 | 81.42 |
| 2.984 | 3.000 | 70.54 | 12.22 | 4218 | 91.94 |
| 4.355 | 3.500 | 89.00 | 13.67 | 5384 | 103.8 |
| 5.997 | 4.000 | 117.7 | 15.65 | 6876 | 117.4 |
| 7.908 | 4.500 | 155.8 | 17.93 | 8765 | 132.6 |
| 10.09 | 5.000 | 206.3 | 20.57 | 11 230 | 149.9 |
| 12.53 | 5.500 | 300.7 | 24.75 | 14 360 | 169.5 |

are $m = 0.03$, $B_c = 2$ T and an assumed *quadratic* field dependence of $a_B$, along with $T_{\text{Mott}} = 3.425$ K and $\upsilon = 0.25$. We plot the MR ratio data taken at $T = 0.093$ K in figure 9 along with two fitting curves. The upper solid curve has $a_B = a_0$ ($m = 0$) where the field dependence of $a_B$ has been neglected. The lower dashed curve includes the quadratic field dependence of $a_B$; saturation and a turnover to lower $r$ values are observed. No field dependence was assumed for the DOS. The crucial point now is the physical justification of this strong field dependence of $a_B$ and and a prediction of a possible field dependence for the DOS, $g_B$. Weaker field dependences for $a_B$ yielded unacceptable fits. For example the

suggested $B^{1/2}$ dependence gave ratio values much too high at high fields and ratio values much too low at small fields [55].

In conclusion, if we assume that the localization length as well as the 3D DOS increase in large magnetic fields, then the above arguments suggest possible saturation of the resistance in Mott VRH films and a much smaller tendency for saturation effects in the more resistive ES and 'soft-gap' VRH films.

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