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1990 J. Phys.: Condens. Matter 2 6763

(http://iopscience.iop.org/0953-8984/2/32/007)

J. Phys.: Condens. Matter 2 (1990) 6763–6770. Printed in the UK

Electronic wavefunctions in lightly doped semiconductors, in the presence of strong magnetic fields

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Received 12 March 1990

Abstract. Variable-range-hopping conduction in lightly doped semiconductors is analysed when strong magnetic and electric fields are applied in the crossed configuration. It is shown that the temperature dependence of the critical electric field above which the transport becomes activationless is a power law that depends on both the shape of the density of states spectrum and the asymptotic behaviour of the electronic wavefunction. An experimental study of transport in n-type GaAs under these conditions is in agreement with a model of hopping of exponentially localised and interacting electrons in a system where intermediate elastic scattering events are important.

1. Introduction

In lightly-doped semiconductors, the electronic wavefunctions are strongly localised around the impurities, with an envelope which decays exponentially in space [1] according to

$$\Psi(r) \sim \exp(-r/\xi) \tag{1}$$

which we will call hereafter EL (or the exponential localised wavefunction for later reference) where ξ is defined as the localisation length of the wavefunction. In these materials, at low temperatures, charge transport is by hopping [2] with a hopping rate depending on both the probability of tunnelling between sites i and j defined as

$$p_{\text{tun}} \sim |\langle \Psi_i | \Psi_j \rangle|^2 \sim \exp(-2r_{ij}/\xi)$$

and the probability of an activation caused by the absorption of a phonon of energy Δ of

$$p_{\text{act}} \sim \exp(-\Delta/kT).$$

When $T \rightarrow 0$, the impurity level distribution becomes imortant and conduction is governed by variable-range-hopping [2]. In this case, hopping occurs between impurity

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0953-8984/90/326763 + 08 $03.50

sites that lie close in energy, and the maximum of the total probability $p_{tot} = p_{tun}p_{act}$, proportional to the conductivity of the system, changes with temperature according to

$$p_{tot}(T) \sim \exp[-(T_0/T)^X] \sim \sigma(T).$$

Here $X = \frac{1}{4}$ for a non-interacting system with constant density of states at the Fermi level [2], or $X = \frac{1}{2}$ for an interacting system with a parabolic Coulomb gap in the density of states at the Fermi level [3].

In variable-range-hopping theory, the maximum probability for a hop, and so the most likely one, occurs for distance and energy equal to the optimum hopping length and optimum phonon energy respectively. For exponentially localised impurity electron wavefunctions (type EL), the optimum hopping length R decreases with temperature, as

$$R(T) \simeq \xi(T_0/T)^X \tag{2}$$

while the optimum phonon energy involved, Δ, follows $\Delta(T) = kT(T/T)^X$ (see [2]).

A strong magnetic field B compresses the wavefunctions, and the resulting reduction of the overlap between them leads to a large positive magnetoresistance. In the absence of scattering, it is suggested that $\Psi(r)$ becomes similar to the wavefunction of a free electron in a magnetic field and is of the Hasegawa–Howard type [4], which, in cylindrical polar coordinate notation, is

$$\Psi(\rho, \varphi, z) \sim \exp(-\rho^2/4\lambda^2 - |z|/\xi) \tag{3}$$

(referred to as HH) where $\lambda = (\hbar/eB)^{1/2}$ is the magnetic length. A wavefunction of the form

$$\Psi(\rho, \varphi, z) \sim \exp(-\rho^2/4\xi_\perp^2 - z^2/4\xi_\parallel^2) \tag{4}$$

where $\xi_\perp$ and $\xi_\parallel$ are the localisation length in the direction perpendicular and parallel to the magnetic field respectively, was proposed by Yafet, Keyes and Adams [5] and is referred to below as a YKA wavefunction.

Since in variable-range-hopping the optimum distance R is greater than the average distance between impurities, an electron may be scattered elastically by several impurities in the course of a single hopping event. Scattering can alter greatly the asymptotic behaviour of the EL wavefunction in strong magnetic fields, which becomes [6]

$$\Psi(\rho, \varphi, z) \sim \exp(-\rho/b - |z|/\xi) \tag{5}$$

(referred to as SE) where $b \simeq \lambda^{3/2}\xi^{1/4}\zeta^{-1/4}$ and λ, ξ, ζ are the magnetic, localisation and scattering lengths respectively.

The temperature dependence of the conductivity of the material in strong magnetic fields is expected to be expressed by a relation of the form

$$\sigma(T) \sim \exp[-(T_0/T)^X] \tag{6}$$

with a value X which depends on the asymptotic behaviour of the wavefunction. A measurement of the relation $\sigma(T)$ can therefore allow the determination of $\Psi(r)$ at large distances. In the present paper, an alternative, independent set of measurements taken under conditions of crossed strong magnetic and electric fields is shown to also enable the characterisation of the asymptotic behaviour of the wavefunction perturbed by the magnetic field. In other words, we attempt to distinguish between the EL, HH, YKA and SE forms of the impurity electron waveform from an interpretation of the experimental

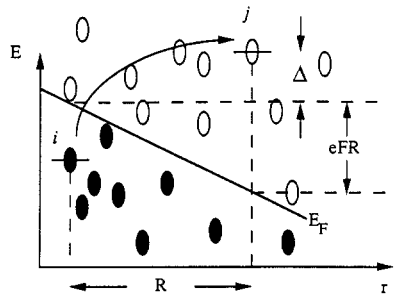

Figure 1. Electron hopping from an initial site i to a final site j a distance R away, in the presence of an electric field F. The energy involved in the transition comprises a contribution of value Δ due to phonon absorption and the energy provided by the electric field which is of magnitude eFR. A transition is activationless when $\Delta = 0$. On the figure, the full circles are occupied states and the open circles are empty states.

data. The approach is explained in section 2 and relevant experimental data are reported in section 3. The conclusion related to the present study is summarised in the last section.

2. Theory of the critical electric field

2.1. Formulation of the problem

In the presence of an electric field the optimum hopping distance $R(T, F)$ and phonon activation energy $\Delta(T, F)$ will depend on both temperature and electric field. In the limit of very low source–drain electric field F, the energy necessary for a transition to a higher energy state to occur is provided by phonon absorption. If the magnitude of the electric field is increased, a regime is first reached where the energy involved comes both from phonon absorption Δ and electrical energy eFR (see figure 1). In a field above a critical value F_c, phonon absorption is no longer necessary and the electrons may gain all their energy from the electric field only, that is $\Delta(T, F > F_c) = 0$. Conduction becomes temperature independent and transport is said to be activationless. In this case the current can be expressed in the form [7, 8]

$$I(F) = I_0 \exp[-(F_0/F)^S] \tag{7}$$

independent of the electron impurity wavefunction $\Psi(r)$ and density of states. S in (7) equals X in (6). In the absence of magnetic fields and scattering the wavefunction will be exponentially localised (i.e. an EL type wavefunction of the form of (1)) and $S = X$ with $F \simeq 1.4\, kT_0/e\xi$, where T_0 and X are defined in (6).

In crossed magnetic and electric fields, the current remains an exponential function of the electric field, expressed by (7), but with a value of S sensitive to the shape of the wavefunction at large distances, and such that $S(F > F_c) = X(F \rightarrow 0)$. Calculated values of X (or equivalently S) for various wavefunctions and for the cases of non-interacting and interacting systems are reported in the literature, and are listed in table 1 [9].

The optimum hopping length is also strictly electric-field-dependent in the high-field regime with

$$R_{EL}(F) \simeq \xi(F_0/F)^S. \tag{8}$$

The transition from thermally-assisted transport to activationless conduction occurs at a critical value of the electric field F_c such that the drop in the potential energy of an electron $eFR(T, F)$ associated with a hop of optimal length becomes comparable to

Table 1. Values of X and S defined by equations (6) and (7) respectively, and q defined by equation (28) are given, for various density of states spectra of the form of equation (12) and the wavefunctions discussed.

Wavefunction	P	XS	q
LE equation (1)	0	$\frac{1}{4}$	1
	2	$\frac{1}{2}$	1
HH equation (3)	0	$\frac{1}{3}$	$\frac{5}{6}$ $(\boldsymbol{F} \perp \boldsymbol{B}) \cdot 1$ $(\boldsymbol{F} \parallel \boldsymbol{B})$
	2	$\frac{3}{5}$	$\frac{7}{10}$ $(\boldsymbol{F} \perp \boldsymbol{B}) \cdot 1$ $(\boldsymbol{F} \parallel \boldsymbol{B})$
YKA equation (4)	0	$\frac{2}{5}$	$\frac{4}{5}$
	2	$\frac{2}{3}$	$\frac{2}{3}$
SE equation (5)	0	$\frac{1}{4}$	1
	2	$\frac{1}{2}$	1

$\Delta(T, F)$. This implies, for $\Psi \sim \exp(-r/\xi)$, that the critical field varies with temperature according to [7]

$$F_c(T) = A(kT/e\xi) \tag{9}$$

irrespective of the shape of the density of states spectrum, with A a constant of order unity. This form for the temperature dependence of the critical electrical field is in general dependent on the electron impurity wavefunction and the density of states spectrum. Below we propose a method based on percolation theory to find the critical electric field as a function of temperature given $\Psi(r)$ and the density of states spectrum. For the exponentially localised wavefunction, the derivation is done explicitly. For the other wavefunctions the results are merely stated.

2.2. *Critical electric field in the absence of* $\boldsymbol{B}$ *and scattering*

For an exponentially localised wavefunction the hopping probability is

$$p(r) \sim \exp(-L - \Delta/kT) \tag{10}$$

where $L = 2r/\xi$ is a dimensionless parameter. Percolation through the sample will occur for a value of $L = L_c$ such that [1]

$$NV(L_c) = \beta \tag{11}$$

where N is the number of states per unit volume, $V(L) = 4\pi(L\xi/2)^3/3$ is the volume within which the electron can hop, and β is the average number of sites to which an electron can go.

For motion along the electric field F the electron, initially near the Fermi energy, hops to a site with energy $E = \Delta + eFL\xi/2$ above the Fermi level, and therefore, for a density of states

$$g(E) = g_0 E^p \tag{12}$$

the number of sites an electron can hop to is

$$N = g_0(\Delta + eFL\xi/2)^{p+1}/(p+1). \tag{13}$$

In the limit $\Delta \to 0$, from (12) and (13), L_c can be determined by substituting $x = L^{-1/(p+1)}$, and by using a first-order perturbation method to solve the resulting relation

$$\beta^{1/(p+1)}x^{p+4} - \Lambda x^{p+1} - \mu = 0 \tag{14}$$

where

$$\Lambda = [\pi g_0 \xi^3/6(p+1)]^{1/(p+1)}\Delta \tag{15}$$

and

$$\mu = [\pi g_0 \xi^3/6(p+1)]^{1/(p+1)}(\xi eF/2). \tag{16}$$

This gives

$$L_c = \beta^{1/(p+4)}(\mu + \eta\Delta)^{-(p+1)/(p+4)} \tag{17}$$

with

$$\eta(F, T) = (\Lambda/\Delta)[\mu/\beta^{1/(p+1)}]^{(p+1)/(p+4)}. \tag{18}$$

Substituting L_c in (10) and maximising p with respect to Δ gives

$$\Delta(F, T) = (1/\eta)\{[\beta^{1/(p+4)}\eta(p+1)kT/(p+4)]^{(p+4)/(2p+5)} - \mu\}. \tag{19}$$

The critical field corresponds to the condition $\Delta(F, T) = 0$, which yields

$$F_c(T) = [2(p+1)/(p+4)](kT/e\xi). \tag{20}$$

2.3. *Critical electrical field with* $\boldsymbol{B}$ *in the absence of scattering*

The YKA wavefunctions (4) can be rewritten as

$$\Psi(r') \sim \exp(-\gamma r'^2) \tag{21}$$

in an appropriately chosen coordinate system, with $\gamma = \frac{1}{4}(\xi_\perp^2 \xi_\parallel)^{2/3}$. Repeating the procedure described above it is found that

$$F_c(T) = \frac{1}{e}\gamma^{1/2}\beta^{1/(2p+5)}\left(\frac{2p+2}{p+4}\right)^{(p+4)/(2p+5)}\left(\frac{3\gamma^{3/2}(p+1)}{4\pi g_0}\right)^{(p+1)/(2p+5)}(kT)^{(p+4)/(2p+5)}. \tag{22}$$

Alternatively, noting that $\Delta \sim r'^{-3/(p+1)}$, it is straightforward to show that for the YKA wavefunction the maximum of $p(r')$ occurs at a temperature-dependent value of r' such that $r'(T) \sim T^{-[(p+1)/(2p+5)]}$. Similarly, $\Delta(T) \sim T^{3/(2p+5)}$. Using $F_c(T) \simeq \Delta(T)/r'(T)$ gives the relation (22) within a factor of order unity.

For HH wavefunctions (3), $V(L) = 8\pi\lambda^2 L^2\xi/3$. When $\boldsymbol{B} \perp \boldsymbol{F}$ and for a motion along the electric field, the electron hops to a site with energy $E = \Delta + 2\lambda eF\sqrt{L}$ above the Fermi level and therefore

$$N = g_0(\Delta + 2\lambda eF\sqrt{L})^{p+1}/p + 1. \tag{23}$$

Using this new density of states per unit volume the critical electric field is obtained in an analogous way to that for the exponential wavefunctions, and has a temperature dependence

$$F_c(T) = A'(kT)^{(p+5)/(2p+6)} \tag{24}$$

where

$$A' = [\beta^{1/(2p+6)}/2e\lambda][(2p+2)/(p+5)]^{(p+5)/(2p+6)}[3(p+1)/8\pi\lambda^2\,\varepsilon g_0]^{1/(2p+6)}. \tag{25}$$

When $\boldsymbol{B} \| \boldsymbol{F}$, the potential energy change for a hop along the electric field direction is $e\xi FL/2$. A derivation similar to the above gives

$$F_c(T) = [(2p+2)/(p+3)](kT/e\xi). \tag{26}$$

2.4. Critical electric field in the presence of $\boldsymbol{B}$ *and scattering*

The SE wavefunction (5), which includes scattering events during the hop, can be treated on the same footing as the exponential localised wavefunction EL (1) by scaling the x and y coordinates. The results are the same as those in section 2.2 with the exception that the localisation length ξ has to be replaced by $\xi' = (\xi b^2/4)^{1/3}$. The critical field becomes

$$F_c(T) = [2(p+1)/(p+4)](kT/e\xi'). \tag{27}$$

2.5. Summary

The power law temperature-dependence of the critical field is listed in table 1 for the cases $p = 0$, 2 and for the wavefunctions considered. It is seen that when $\boldsymbol{B} \perp \boldsymbol{F}$, the relation

$$F_c(T) \sim T^q \tag{28}$$

depends on the asymptotic behaviour of the wavefunction. The power law is different for all wavefunctions considered, with the exception of the EL and SE wavefunctions. The latter is however the correct electron impurity wavefunction, as Ψ is compressed by the magnetic field. It follows that $\Psi(r)$ can not only be identified by the experimental evaluation of X or S from equations (6) and (7) respectively, but also from the determination of the power q from equation (28). This latter method is subsequently exploited to determine the impurity electronic wavefunction in a GaAs : Si sample, and results are discussed below.

3. Experiment

The sample used was metal–organic chemical vapour deposition (MOCVD) grown GaAs doped with silicon to $n_{Si} = 1.8 \times 10^{16}$ cm^{-3}, which is above the critical concentration for metallic conduction in this material ($n_c = 1.6 \times 10^{16}$ cm^{-3}). The structure was an etched Hall bar with evaporated Au–Ni–Ge contacts. It has been shown elsewhere [10] (sample Z in [10]) that, in the limit $F \rightarrow 0$ and $B = 0$, the conductivity of this structure has a metallic behaviour and that the critical magnetic field required to induce a metal–insulator transition is $B_c = 2.98$ T. The measurements in strong electric fields were performed using a DC two-terminal technique in a top-loading dilution refrigerator which operates in the temperature range 20–800 mK and which includes a superconducting solenoid capable of reaching $B = 13.6$ T.

Measurements in crossed strong electric and magnetic fields were performed. A representative result of the bath temperature dependence of the I–F relationship, taken at a chosen magnetic field of magnitude $B = 6$ T, is shown in figure 2. It is observed that all curves do merge at a temperature-dependent critical electric field. At temperatures below 132 mK we found that the I–F curve became temperature independent. Using a least-squares fit procedure described elsewhere [11], a best fit of the temperature-independent data (taken at $T = 132$ mK) to a law of the form of (7) gives $S = 0.53 \pm 0.08$ and $F_0 = 121\,900$ V m^{-1}. This finding is similar to that observed in lightly doped samples in zero magnetic field, where transport is suggested to be by interacting exponentially localised electrons. It is also worth noting that in strong magnetic fields, but in the limit $F \rightarrow 0$, conduction in this sample is well described within experimental error by (6) with

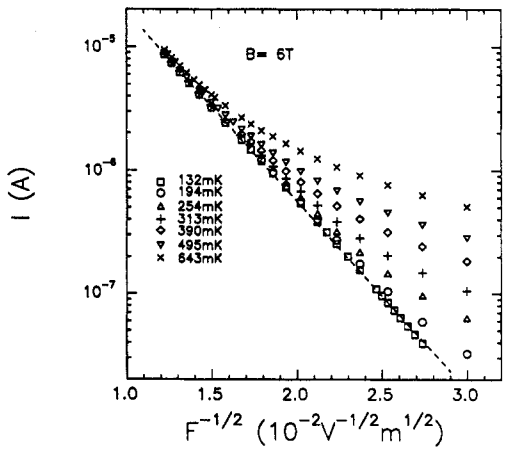

Figure 2. $I(F)$ dependence for the sample used, at various temperatures, for $B = 6$ T and $\boldsymbol{B} \perp \boldsymbol{F}$. The line is a least-squares fit to the data.

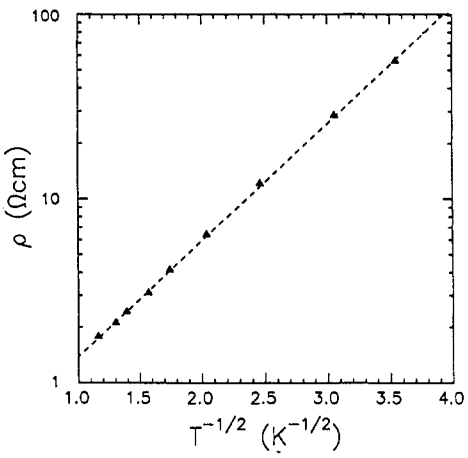

Figure 3. Temperature dependence of the resistivity of the sample used, at a fixed value of the magnetic field $B = 4.46$ T. The data are well described by (6) with $X = 0.48 \pm 0.07$, $\rho_0 = 0.32$ Ωcm and $T_0(X = \frac{1}{2}) = 2.13$ K.

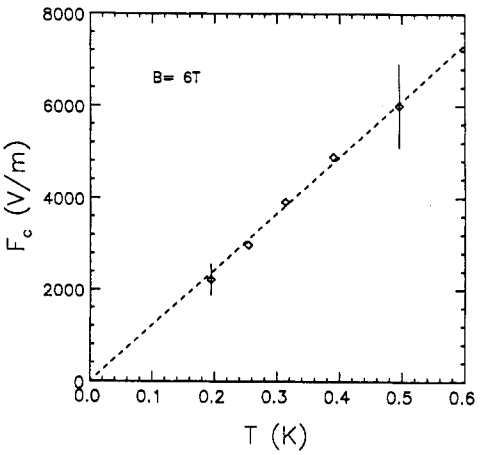

Figure 4. Temperature dependence of the critical field F_c for the sample used, at a magnetic field of magnitude $B = 6$ T and with $\boldsymbol{B} \perp \boldsymbol{F}$. The relationship between the parameters is linear within error. The line is a least-squares fit to the data.

$X = \frac{1}{2}$. This confirms the expectation that $X \simeq S$. A representative result is plotted in figure 3. This behaviour is similar to that reported for InSb [9] and for InP [12].

Within experimental error, the above result is, however, also consistent with the model of transport by HH interacting electrons. Defining $F_c(T) = F$ such that $[I(F, T_{bath}) - I(F, 132\text{ mK})]/I(F, 132\text{ mK}) \simeq 2\%$ (the result does not depend on the percentage chosen as long as it is small—less than about 10%), the relation $F_c(T)$ is found. The result is presented in figure 4. The analysis gives $q = 1.04 \pm 0.08$ for equation (28). Furthermore, from equation (27) we find for interacting electrons ($p = 2$ in (12)) a reasonable localisation length of $\xi = 119$ Å. The $p = 2$ case corresponds to the normal Coulomb gap system.

These results show unambiguously that transport in high magnetic fields for this system is better described by the theory which takes scattering into account [6] than by a system with HH ($q = 0.7$) or YKA ($q = \frac{2}{3}$) wavefunctions in the absence of scattering.

4. Conclusion

It is shown that the study of the temperature dependence of the magnitude of the critical electric field above which variable-range-hopping conduction becomes activationless is a useful tool to give information on the asymptotic behaviour of the localised wavefunctions in strong magnetic fields. Using the procedure proposed, experimental data in n-type GaAs are shown to be consistent with the existence of magnetic-field-induced hopping transport of exponentially localised carriers in the material, in agreement with recent theories which take intermediate scattering into account.

Acknowledgments

FT acknowledges partial financial support from the Natural Sciences and Engineering Research Council of Canada. R-JJ is most grateful to Trinity College, Cambridge, for their financial support. MJK is supported by a Royal Society/SERC Industrial Fellowship. This work was supported by the Science and Engineering Research Council of the United Kingdom.

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