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TEMPERATURE DEPENDENCE OF THE HOPPING HALL MOBILITY IN SPATIALLY AND ENERGETICALLY DISORDERED SYSTEMS

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Abstract.- We present an averaging procedure for the calculation of the Hall mobility for spatial and energetical disordered hopping systems in the framework of percolation theory. For a constant density of states function the temperature dependence of the Hall mobility follows a $T^{-1/4}$ law with a slope which is by a factor of about 8/3 smaller than that of the conductivity. The comparison with the self consistent Random Walk Theory of transport yields qualitatively the same results.

Introduction.- We consider hopping transport in model systems where sites are randomly distributed in space and site energies are distributed according to a given density of states function $N(E)$. The elementary process governing the Hall Effect is assumed to be the three site interference process due to Holstein. The model we consider for the calculation of the DC-Hall-mobility $\mu_H$ was introduced by Böttger and Bryskin (BB) and Friedman and Pollak (FP). The problem of R-hopping conduction (no energy fluctuations), they tackle, was transformed into the calculation of the average transverse current which develops in the equivalent random resistor network with extrinsic currents. In the spirit of percolation theory the average has then been performed in different ways over the percolation path and the results for $\mu_H$ of BB and FP were quite different. On the other hand, Movaghar et al. derived an expression for the conductivity in disordered systems starting from a completely different point of view, namely the microscopic description of a random walk. Movaghar, Pohlmann and Würtz extended this theory to yield the transverse conductivity. They showed that the random walk expression for $\mu_H$ in the low density regime is quite close to that one found by BB. They have the same dependence on the site density and differ only by a constant prefactor of about 30. But one should remember that in percolation theory it is somewhat difficult to calculate prefactors. The different approaches and results are discussed in detail in ref. 5.

The models so far considered deal with the so called R-hopping problem where only spatial disorder is present. In this paper we follow the work of BB but we allow for fluctuations in the site energies as well. In the framework of percolation theory we present an averaging procedure to calculate the Hall mobility for a given density of states function. The basic formalism for calculating the Hall mobility is given, in more detail in ref. 6. As an example for systems including energy fluctuations we consider a constant density of states, yielding Mott's law for the conductivity $\sigma_{xx} = -(T_0^2/T)^{1/4}$. For $\mu_H$ we find $\mu_H/\mu_{DC} = -(T_0^2/T)^{1/4}$ with $T_0 \approx 1. T_0$. The magnitude of $\mu_H$ is rather small ($\approx 10^{-10}$ cm²/Vs) if parameters characteristic for hopping near the Fermi level in amorphous semiconductors are chosen.

The conductivity $\sigma_{xx}$.- As shown by Miller and Abrahams, the problem of DC-hopping conduction is equivalent to the calculation of the conductivity of a resistor network. The impedances of this network $Z_{ij}$ are determined by the two site thermal equilibrium jump rate $\Gamma_{ij}$ between sites i and j.

$$Z_{ij}^{-1} = e^2 F \Gamma_{ij} = e^2 F v_{20} e^{-2ar_{ij}} \Delta_{ij} \quad (1)$$

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where $v_{20}$ is a frequency prefactor and $a^{-1}$ the decay length of the localized states. Percolation theory is based on the concept that nearly all of the current is carried by a critical path (or a system of critical paths), the conductivity of which is determined essentially by the largest impedance on this path (or on a section of it). This critical impedance will be written in terms of a critical exponent $\xi/kT$ as

$$\frac{1}{Z_c} = \frac{2}{2\theta} \cdot v_{20} \cdot e^{-\xi/kT}. \quad (3)$$

The conductivity of the whole system is then approximately

$$\sigma_{xx} \approx g^{-1} \cdot \frac{1}{L}, \quad (4)$$

where the characteristic length $L$ cannot be determined by percolation theory alone. It can roughly be taken as the separation of sites where critical paths intersect. The critical path is formed by impedances all smaller than $Z_c$. The number $n(E_i, \xi)$ of such impedances linked to a given site $i$ with energy $E_i$ is obtained by integrating over the volume of the "cone capped cylinders",

$$n(E_i, \xi) = \frac{4\pi}{3} \int dE_j \ N(E_j) \ x^3(E_i, E_j) \quad (5)$$

with

$$x(E_i, E_j) = \frac{\theta}{2\theta} (\xi - \frac{1}{2} (|E_i| + |E_j| + |E_i - E_j|)). \quad (6)$$

Percolation sets in if the average number of bonds per site is equal to

$$\nu_c = <n(E_i, \xi)>_c \quad (7)$$

with percolation number $\nu_c = 2.7^{11}$. $<...>_c$ means averaging over the path which is done by multiplying with

$$n(E_i, \xi) \cdot N(E_i) / \int dE \ n(E, \xi) \ N(E) \quad (8)$$

and integrating over $E_i^{9,10}$. For constant $N(E) = N_o$ we obtain via eqs. (5), (7), (3), and (4) the famous Mott law

$$\ln \sigma_{xx} \sim \xi \beta = \frac{\tau_0}{T}^{1/4} \quad (9)$$

with

$$\tau_0^{1/4} = 2 \cdot (\frac{3}{kN_o})^{1/4}. \quad (10)$$

The Hall conductivity, $\sigma_{xy}$ and Hall mobility $\mu_H$ result if higher order jump-processes are considered where one or more intermediate sites are involved. So the Hall effect is due to at least three-site hops at triads within the system of percolation paths. On the basis of this model (BB) obtain for the transverse conductivity $\sigma_{xy}$ (with the magnetic field $H$ being in z-direction)

$$\sigma_{xy} = e^2 \beta \sigma_{xx} L \left( <\Delta W_{ijp}^H \ Z_{pi}^Z \ Z_{pj}^Z \ Z_{ji}^Z>^c \right) \quad (11)$$

The brackets $<...>_c$ denote the average over all possible spatial and energetical paths. $\Delta W_{ijp}^H$ is the magnetic field dependent part of the three site transition rate.
with the intermediate site $p$, given by Holstein. For small electron-phonon coupling

$$
\Delta W_{ipj}^H = v_{30} e^\frac{\hbar}{\hbar} |A_{ipj}^Z| \cdot e^{-a(r_ip+r_pj+r_{ji})} \cdot \Delta_{ipj},
$$

(12)

\[ \Delta_{ipj} = \frac{1}{3} \left[ e^3|E_1| \Delta_j A_{ipj}^p + e^3|E_p| \Delta_i A_{pjp}^p + e^3|E_j| \Delta_p A_{jip}^p \right] \]

where $v_{30}$ is a frequency prefactor and $A_{ipj}^Z$ is the projection in the $Z$-plane of the vector area spanned by the triad $(ipj)$. Inserting eqs. (12), (4), and (1) with (2) into eq. (11) and dividing by $E_{ixx}H$ we obtain the Hall mobility $\mu_H$

$$
\mu_H = \sigma_{xy} \frac{\sigma_{xx} H}{\sigma_{xx}} = \frac{v_{30} e^{-\alpha(r_ip+r_pj+r_{ji})}}{v_{20} \hbar^2 Z} \left( e^{-2a(r_{ij}+r_{ip}+r_{ji})} \Delta_{ipj} + e^{-2a(r_ip+r_pj)} \Delta_{ipj}^p + e^{-2a(r_{pi}+r_{ji})} \Delta_{pjp} \right)
$$

(13)

The configurational average $\langle \ldots \rangle_c$ is performed as

$$
\langle f(r_i, r_p, r_j ; E_i, E_p, E_j) \rangle_c = \frac{\int dE_n(E_i, E_p, E_j) f(r_i, r_p, r_j ; E_i, E_p, E_j) dE_n(E_i, E_p, E_j) dE_n(E_j, E_p, E_j) dE_n(E_i, E_p, E_j) dE_n(E_j, E_p, E_j) dE_n(E_i, E_p, E_j) dE_n(E_j, E_p, E_j) \Delta_i \Delta_j \Delta_p}{\int dE_n(E_i, E_p, E_j) dE_n(E_i, E_p, E_j) dE_n(E_j, E_p, E_j) dE_n(E_i, E_p, E_j) dE_n(E_j, E_p, E_j) dE_n(E_i, E_p, E_j) dE_n(E_j, E_p, E_j) \Delta_i \Delta_j \Delta_p}
$$

(14)

with the restrictions $E_m \leq \xi$ and $r_{mn} \leq \frac{\sqrt{2}a}{2\alpha} (\xi - \frac{1}{2} (|E_m| + |E_n| + |E_m - E_n|))$.

The temperature dependence of $\mu_H$ may be deduced approximately by the following argument. The main contribution to $\mu_H$ is due to equilateral triangles with sides of length $<R>$ and site energies $<E>_c$ related to the critical exponent $\xi$ by

$$
\xi = 2a <R> + 8 <R> = 15
$$

(15)

The mean critical quantities $<R>_c$ and $<E>_c$ are obtained from the averaging procedure as prescribed by eq. (8) but taking care that always eq. (15) is fulfilled. We obtain for $<R>_c$

$$
\alpha <R>_c = \frac{3}{8} \left( \frac{T_0}{T} \right)^{1/4}
$$

(16)

which is identical to the average hopping distance obtained from the simple "Mott-optimization". Thus the Hall mobility $\mu_H$ from eq. (13) results in

$$
\mu_H \approx e^{-\frac{\xi}{8}} \cdot e^{\alpha <R>_c + \beta <E>_c} = e^{-\frac{\xi}{8}} \cdot e^{\alpha <R>_c + \beta <E>_c} = e^{-\frac{3}{8} \left( \frac{T_0}{T} \right)^{1/4}} = e^{-\frac{\xi}{8} \left( \frac{T_0}{T} \right)^{1/4}}
$$

(17)

$\mu_H$ follows a $(T_0/T)^{1/4}$-law where $T_0$ is the $T_0$ appearing in the conductivity eq. (9) reduced by a factor of $\approx 50$. This result is confirmed by a direct numerical calculation of eq. (14) using Monte Carlo integration techniques. Fig. 1 shows the numerical results for log $\mu_H$ vs. $(T_0/T)^{1/4}$ for a constant density of states $N(E) = N_0$. The slope in this plot is indeed $= 3/8$ and the value of $\mu_H$ is very small. For the following parameters $v_{30}/v_{20} = 0.1$ (FP), $a^{-1} = 10$, $N = 10^{15}$ cm$^{-3}$ eV, we obtain for the prefactor $v_0 = \frac{v_{30}}{v_{20}} \cdot \frac{e^{\alpha}}{\hbar^2} = 2$ cm$^2$/Vs. Setting $T = 300 K$ we compute via eq. (16) $(T_0/T)^{1/4} = 16$ and with Fig. 1 the Hall mobility $\mu_H$ to

$$
\mu_H = 10^{-4} \text{ cm}^2/\text{Vs}
$$

(18)

We remark in agreement with (BB) that there is an uncertainty in the preexponential factors of the conductivity $\sigma_{xx}$ and Hall conductivity $\sigma_{xy}$ because in percolation theory there exists no unambiguous scheme for calculating prefactors. If one is interested in the correct prefactors one should use the more sophisticated
random walk theory\textsuperscript{4,5}. The Random Walk Theory formulated for the Hall effect in the R-hopping problem\textsuperscript{3} can also easily be extended to the case of variable range hopping. The averaging procedure over all spatial and energetical coordinates of the system is somewhat more difficult from the numerical point of view. First numerical results show in the low temperature and low density regime the same qualitative behaviour (\(T^{-1/4}\)-law) as obtained by the percolation theory described in this paper.

We have presented an averaging procedure for the Hall mobility for spatial and energetical disordered hopping systems in the framework of percolation theory. The treatment applied in this paper is based on a model of the Hall effect where three site processes dominate and where the transition rates are describable by eq. (1), e.g. due to s-like wavefunctions. For a constant density of states model the absolute value of the Hall mobility \(\mu_h\) is quite sensitive to the value of \(T_0/T\). The temperature dependence of \(\mu_h\) follows a \(T^{-1/4}\)-law with a slope which is approximately by a factor 8/3 smaller than that of the conductivity.

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