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Low Temperature Hopping Diffusion in Doped Semi-coinductors

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Mott's law for the low temperature hopping conductivity is reconsidered to take account of the fact that the site wave functions are more localized than the hidrogenic-like wave functions. With Gaussian-like functions a $T^{-2/5}$ law for the logarithm of the conductivity is obtained, in good agreement with experimental data. The low temperature difusion coefficient, of n-CdS, which can be measured through the Spin Flip Raman Scattering in doped semiconductors, is shown to have the same temperature behavior, in the temperature range from 10K to 50K.

A lei Mott para a condutividade por "hopping" em baixas temperaturas é reanalisada, levando em conta que as funções de onda dos sítios são mais localizadas do que funções de onda hidrogênicas. Obtém-se que o logarítmo da condutividade é proporcional a $T^{-2/5}$, com a hipótese da função de onda ser Gaussiana. Este comportamento da condutividade está de acordo com os resultados experimentais. Mostra-se também que o coeficiente de difusão, que pode ser medido através do espalhamento Raman com "Spin-Flip" em semicondutores dopados, tem o mesmo comportamento com a temperatura, no intervalo de 10 a 50K.

1. INTRODUCTION

Since Mott[1] has proposed phenomenologically his famous $\exp\left[-(T_0/T)^{1/4}\right]$ law for the low-temperature conductivity of the disordered semiconductors, based upon the hopping formalism of Miller and Abrahams[2], there have been many experimental evidence of such low temperature behavior of the conductivity of those materials[3,4]. Several theoretical efforts had been made to derive Mott's law within semi-classical and quantum-mechanical approaches[5].

The derivation of Mott's law is based upon the following two hypothesis: i) the probability that an electron jumps from one site to another decreases exponentially with the distance between sites; this factor represents the overlap of wave functions of neighboring sites. ii) The mean activation energy for hopping is equal to the average energy difference between two levels of the localized electrons inside a sphere of radius R.

Ba'nyai and Aldea[5] analysed the hopping both semi-classically and quantum mechanically. In both approaches they calculated the electric current density. In the semi-classical approach the electric current density was assumed to be function of the occupation number of the states of a site and of the transition probability from one site to another due to emission or absorption of phonons in thermal equilibrium. In the quantum mechanical approach the conductivity was derived through Kubo's formula, i.e. within the framework of the linear response theory. They showed that in both approaches identical results are obtained. In their treatment the overlap of wave functions of neighboring sites was not explicitely considered. With the same hypothesis used by Mott[1] to derive the transition probability through phonon absorption or emission, they obtained $T^{-1/4}$ law. The Einstein's relationship between diffusion and conductivity was not used in their treatment.

Redfield[4] pointed out that his conductivity data of n-GaAs had a better fit for a law $\ln\sigma \sim T^{-1/2}$ than for $\ln\sigma \sim T^{-1/4}$. If one assumes that the site wave functions are more localized than the hydrogenic-like wave functions there would be less overlap between wave functions of neighbouring sites and the temperature dependence would change in the right cirection.

Gaussian wave functions have been used in crystal and amorphous semiconductors. With this type of wave functions and the tight binding approximation, the electronic density of states and charge density are in good agreement with those obtained by other methods[6]. Also, the Gaussian wave functions yield, through chemical-bond approach, good results for the dielectric constant of the elemental semiconductors[7].

This suggests us to reconsider the derivation of Mott's law by changing hypothesis (i), assuming that the hopping probability decreases with the mean distance between sites as a Gaussian. This is done in the section 2. In the section 3 we present the results and conclusions.

2. MODIFIIED MOTT PROCEDURE

According to Mott procedure[1], the diffusion coefficient is first determined and the conductivity is next obtained through Einstein relation. This rneans that the temperature dependence of the conduçtivity is dictated by the temperature behavior of the diffusion coefficient. Following the derivation of Mott[1], the diffusion coefficient is proportional to $pR^2\rho(\varepsilon_F)k_BT$, where p is the hopping probability, of the electron between two localized states, R is the radius, $\rho(\varepsilon_F)$ is the density of states by unit volume at the Fermi level and k_B is the Boltzman constant.

The hopping probability p contains the following factors :

a) The Boltzman factor, exp $(-W/k_BT)$, where W is the difference between the energies of the two states. This is the mean activation energy for hopping.

b) a factor depending on the overlap of the wave functions of the two states.

c) a factor ν_{ph} depending on the phonon spectrum. ν_{ph} is of the order of the maximum phonon frequency.

Now supposing that the localized wave functions are Gaussians, instead of hydrogenic-like wave functions[1], the overlapping factor is proportional to $\exp(-2\alpha^2R^2)$, where a is the rate at which the Gaussian function falls off with the distance.

Like Mott[1] we consider the mean activation energy for hopping given by

$$W = \frac{3}{4\pi R^3\rho(\varepsilon_F)} \tag{1}$$

Then the hopping probability *p*, with the new assumption reads,

$$p - \nu_{ph} \exp\left[-2\alpha^2R^2-(3/4\pi R^3\rho(\varepsilon_F)k_BT)\right] \tag{2}$$

The extremal value of the argument of the exponential in Eq.(2) comes from a values of R such that

$$2\alpha^2 = 9/8\pi R^5\rho(\varepsilon_F)k_BT \quad . \tag{3}$$

Hence the modified Mott procedure yields for the diffusion coefficient

$$D \sim \left(\frac{T}{T_0}\right)^{3/5} \exp\left[-1.68 \left(\frac{T_0}{T}\right)^{2/5}\right] \qquad (4$$

where $T_0 = \alpha^2/k_B\rho(\varepsilon_F)$.

3. RESULTS AND CONCLUSIONS

Following the same procedure of Mott[1] we obtain for the conductivity a temperature dependence of the type $\ell n\sigma - T^{-2/5}$. Although this does not agree with the $T^{-1/2}$ law proposed by Redfield[4] to fit his experimental data, the $T^{-1/2}$ and $T^{-2/5}$ behaviors cannot be distinguished within the experimental error in the temperature range measured by Redfield, as it is shown in figure 1. We should mention that the same result was obtained for the low temperature conductivity of heavily doped semiconductors in the presence of high magnetic fields[8]. The Redfield[4] experiments were performed at zero magnetic field.

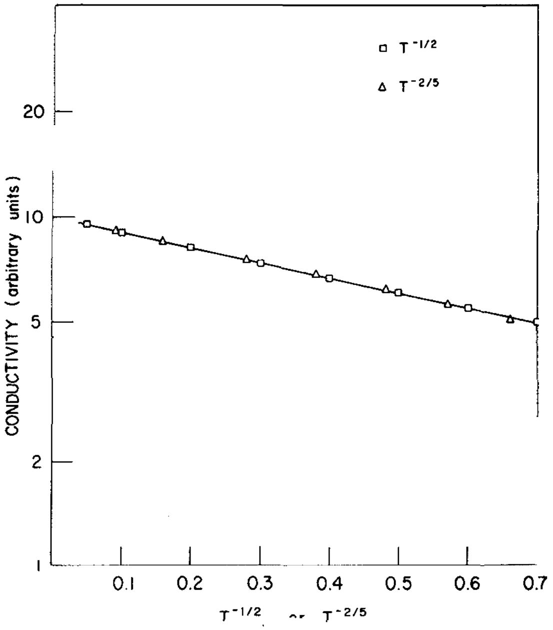

Fig.1 - Temperature dependence of the conductivity in the low temperature range O $\ell n\sigma - T^{-1/2}$ and A $\ell n\sigma \sim T^{-2/5}$.

The temperature behavior of the spin Flip Raman Scattering (SFRS) line width in n-CdS, to which the spin diffusion is related[9], was explained based upon hopping effects[10] in the temperature range from 10K to 50K. This suggest to reconsidere the temperature behavior of the SFRS line width within the modified Mott procedure. The figure 2 shows that the experimental data for the SFRS line width in n-CdS, with $n = 5\times10^{17}$ cm^{-3}, obtained by Scott *et al.*[11] have the temperature behavior given by Eq. (4), in the temperature range from 10K to 50K. Recently, Geschwind *et al.*[12] measured the resistivity and the line width of the SFRS from 1.6K to 10K for the n-CdS with $n = 2.3\times10^{17}$cm^{-3}. The resistivity changed by more than three decades in that temperature range, whereas the line width of SFRS remained pratically constant. They suggested that the spin diffusion mechanics responsible for the linewidth of SFRS should be exchange between bound donors[13].

In conclusion we may say that comparing the present result with the previous one[10], we cannot decide, within the experimental er-

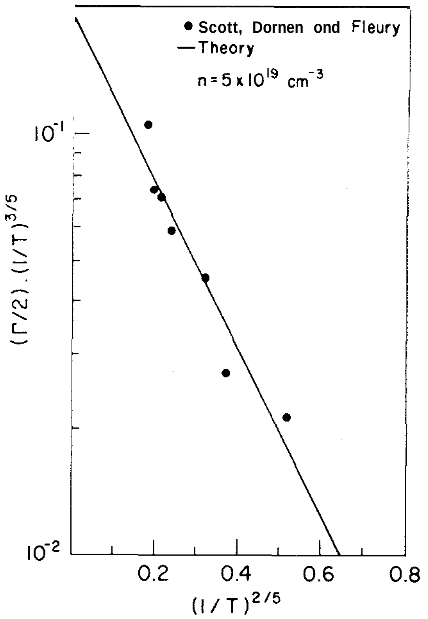

Fig.2 - Temperature dependence of the Spin Flip Raman Scattering line width for *n*-CdS.

ror, which temperature behavior the SFRS linewidth in n-CdS fits better in temperatures from 10K to 50K. But it seems that, in this temperature range, hopping should be responsible for the spin diffusion. Although, for temperature less than 10K exchange effects should be considered[12,13] . However, our results allow us to conclude that the experimental behavior of the low temperature conductivity[4] can be understood within Mott's model, assuming the site wave functions are more localized than the hydrogenic-like functions, thus reducing the overlap between the wave functions of neighboring sites. Finally, we should mention that the $T^{-1/2}$behavior of Rnain Redfield[4] experiments was verified in the temperature range from 2K to 30K.

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