Dispersive Hopping Transport from an Exponential Energy Distribution of Sites

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With use of Monte Carlo simulation techniques, it is shown that an exponential energy distribution of hopping sites gives rise to dispersive transport which is not experimentally distinguishable from multiple trapping. At low temperatures, the dispersive parameter α is equal to T/T_0. At high temperatures, the power-law approximation fails exactly as found for multiple trapping. These results show conclusively that hopping does give rise to dispersion and depending upon the hopping distribution function can be observed in a macroscopic system.

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Ever since the original proposal of Scher and Lax[1] and Scher and Montroll[2] a controversy has raged regarding whether hopping can give rise to significant anomalous dispersive transport. No such controversy exists regarding multiple trapping since Silver and Cohen[3] first showed that dispersion arises in a natural way from a multiple-trapping model where the traps are distributed exponentially with energy. Later Schmidlen[4] and Noolandi[5] formally solved the coupled rate equations for the multiple-trapping case and also found dispersive transport behavior. More recently Orenstein and Kastner[6] and Tiedje and Rose[7] using a beautifully simple quasiequilibrium argument gave a clear physical picture of the dispersive transport from multiple trapping. Thus the situation regarding the multiple-trapping case is clear and only the details regarding different distributions of traps require illucidation.

However, as stated, the situation regarding hopping remains clouded. Schmidlin,[8] Marshall and Sharp,[9] and Pollak[10] have given arguments that dispersion from hopping is not possible in macroscopic systems either from r hopping or from an energy distribution of sites. Marshall and Sharp[9] predicted little or no dispersion for a uniform distribution of hopping sites contained within an energy range of 0.4 eV. They argued that a high-energy site is hard to populate just as is a spatially isolated site. Consequently they concluded that there is no dispersion for diagonal as well as off-diagonal disorder. However, Schoenherr *et al.*[11] showed a reasonable amount of dispersion from a Gaussian distribution of hopping sites. The dispersion was primarily due to the energy relaxation of the hopping carriers which is supported by the proposal of Orenstein and Kastner[6] and Tiedje and Rose.[7] Because of the sharpness of the Gaussian trap distribution, the relaxation ceased after a short time and dispersive transport was no longer observed. This result suggested that perhaps an exponential distribution of hopping sites would yield a much longer relaxation time and hopping dispersive transport could be observed in a macroscopic system.

In the present paper, using Monte Carlo simulations, we show that dispersive transport is observed from an exponential energy distribution of hopping sites just as in the case of multiple trapping. However, these results have a profound effect upon interpretation of experimental data in that these cannot be uniquely interpreted in terms of a single transport mechanism.

The simulation techniques have been reported previously[11] and are only briefly outlined here. In the present system a cubic lattice with $30\times30\times69$ sites has been used. We also employ periodic boundary conditions thereby effectively making the transverse dimensions infinite. The assumed exponential distribution of hopping sites is $N(\epsilon_i) \propto (1/kT_0)\exp(-\epsilon_i/kT_0)$ and consequently the energy of each site is chosen by a random number R_i between 0 and 1 such that

$$\epsilon_i = -kT_0 \ln(1-R_i). \tag{1}$$

After the energies for all the 62 100 sites have been determined, we send 20 particles through each distribution of sites and then repeat for 50

different configurations. Previously we have shown that averaging of 50 configurations gives meaningful statistical results. The initial starting site for each hopping particle is chosen at random at the $x=1$ face. Hopping between two sites i and j is governed by

$$\nu_{ij}=\nu_0\exp(-\gamma|r_{ij}|)\exp\left(-\frac{(\epsilon_j-\epsilon_i)-eE(x_j-x_i)}{kT}\right) \tag{2a}$$

for $\epsilon_j-\epsilon_i-eE(x_j-x_j)>0$, and

$$\nu_{ij}=\nu_0\exp(-\gamma|r_{ij}|) \tag{2b}$$

for $\epsilon_j-\epsilon_i-eE(x_j-x_i)<0$, where r_{ij} is the distance between the sites, γ is the hopping parameter, and E is the electric field. We have taken realistic numbers and used $\nu_0=10^{13}$ s^{-1}, lattice spacing $a=10^{-7}$ cm, and $\gamma a=10$. The electric field was 10^4 V/cm so that $eEa/kT\ll 1$. Notice that this is *not* a multiple-trapping case in which the rate of depopulation of the ith state is $\nu_0\exp(-\epsilon_i/kT)$ and the population for the jth level is just ν_{tj}, where ν_0 is an escape frequency and $\nu_{tj}=b_jN_j(\epsilon)$ with b_j equal to the trapping rate constant.

The probability that a particle will jump to the site j from i is given by

$$P_{ij}=\nu_{ij}/\sum_{l\neq i}\nu_{il}. \tag{3}$$

Thus to simulate the motion, a random number is chosen, R_{ij}, which specifies to which site a particle jumps. Another random number, R_{tj}, is chosen which then specifies the time for the jump from i to j. The calculation is repeated now from the jth site. The particle is followed until it reaches the plane $x=70$. At that time the computation is terminated and a new particle is followed. We can obtain $\langle x\rangle$, $\langle \dot{x}\rangle$, the number of new sites visited (NNS), and the number of hopping particles remaining in the volume versus time.

Figure 1 shows our log$i$ vs log$t$ results for $T_0=504$ K. At four different temperatures, 200, 300, 600, and 900 K dispersive behavior is observed over the entire range of computation particularly for low temperatures. We employ as an operational definition of dispersion that $\langle \dot{x}\rangle$ is a decreasing function of time in the presence of a dc field as opposed to being a constant as in the case of normal drift. This operational definition applies for times longer than the time for a few hops, i.e., $t>(1/\nu_0)e^{\gamma a}$. Power-law behavior is

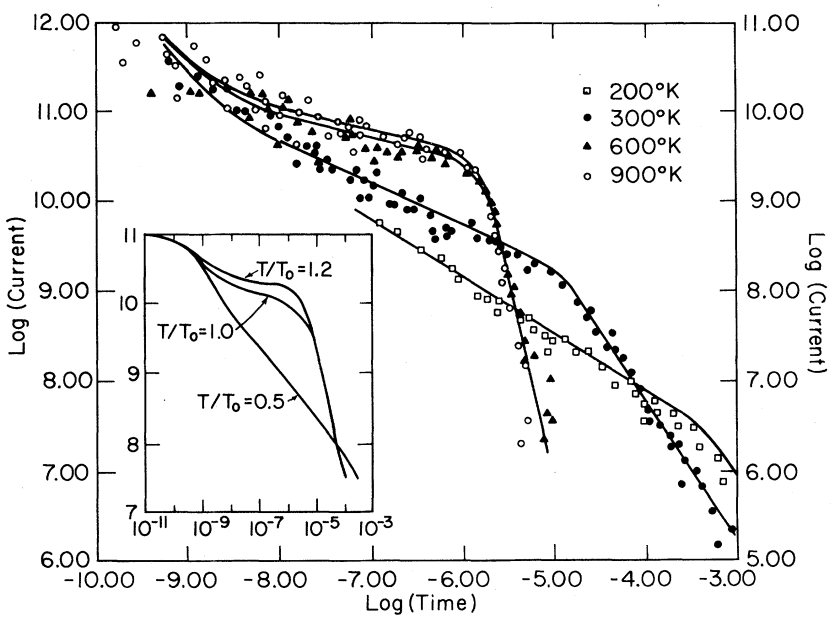

FIG. 1. Log$i$ vs log$t$ for $T=200$, 300, 600, and 900 K. For these simulations $T_0=504$ K so that the data cover a range of $T/T_0=0.4$, 0.6, 1.2, and 1.8, respectively. The scale on the right-hand side applies to the $T=200$ K results where $\alpha=T/T_0$. Notice even for $T/T_0>1$ the currents are still dispersive as evidenced by the drop in the current prior to the transit time. The inset shows comparable data for multiple trapping (Ref. 12). While the values of T/T_0 are not exactly the same as for the hopping case, the similarity between the hopping and the multiple-trapping curves is striking.

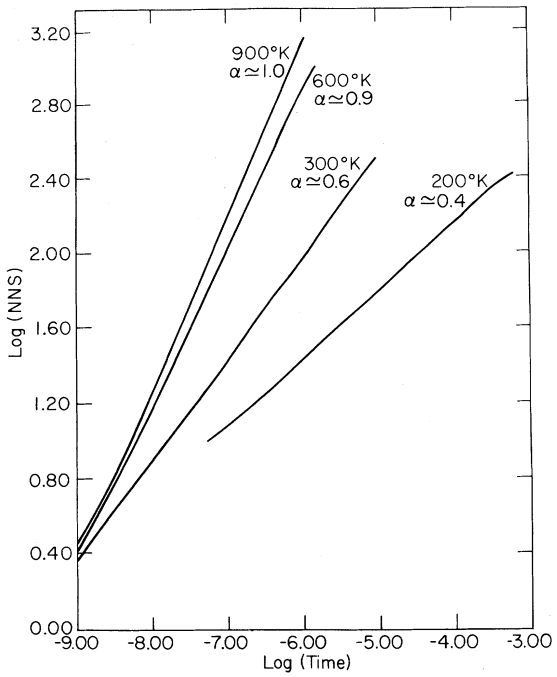

FIG. 2. Log-log plot of the number of new sites visited vs t. The number of new sites visited, NNS, is seen to be proportional to t^{α} for $T/T_0 < 1$. For $T/T_0 > 1$, the number of new sites visited approaches t only for large T/T_0. For $T/T_0 \sim 1.2$ the number of new sites visited is approximated by $t^{0.9}$. (α's displayed in the figure were obtained from the various slopes.)

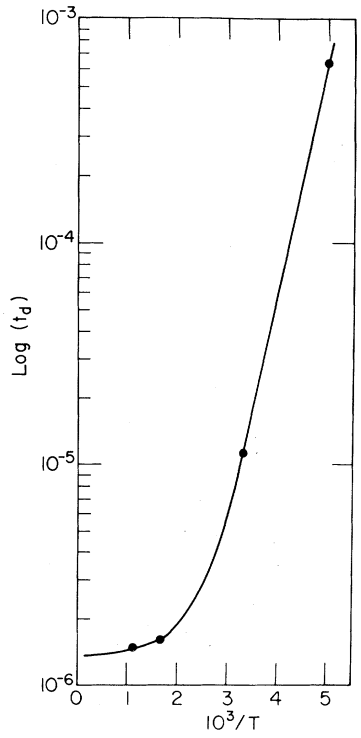

FIG. 3. Logarithm of the transit time vs $1/T$. Notice that these results yield an activation energy of -0.2 eV. This value is consistent with the predictions of Eq. (4). To obtain the activation energy we used the transit-time data at 200 and 300 K.

observed at 200 and 300 K. The slope of the log$i$ vs log$t$ curves before the transit time ($\alpha - 1$) was -0.62 and -0.37 and after the transit time ($-1 - \alpha$) was -1.4 and -1.6 for $T/T_0 = 0.4$ and 0.6, respectively. It is interesting to note that there is some dispersion at 900 K even though $T/T_0 \simeq 1.8$. Our results also show that for low temperature the transit time is proportional to $(L/E)^{1/\alpha}$ as expected from dispersion. We also show for comparison, comparable data for the multiple-trapping case. These results[12] are similar to those obtained for hopping for comparable values for T/T_0. Another interesting result is shown in Fig. 2 where we plot our data of the logarithm of the number of new sites visited versus the logarithm of time. The number of new sites visited is proportional to t^{α} as can be seen. This is expected for dispersive transport; for Gaussian transport the number of new sites visited after the first few jumps[13] is proportional to t. There is no indication of a linear behavior for the number of new sites visited versus time as would be expected from nondispersive transport except at very high temperatures.

The activation energy associated with the arrival time can be estimated from

$$\epsilon_a = -kT \ln(\nu_0 e^{-\gamma a} \tau_d). \tag{4}$$

This estimate comes from the assumption of a quasiequilibrium of hopping particles having an energy greater than ϵ_a.[6,7] The logarithm of the arrival times τ_d vs $1/T$ has been obtained and is shown in Fig. 3. In the low-temperature region, $10^3/T > 3$, the slope of the curve yields a value of $\epsilon_a = -0.2$ eV. This is in excellent agreement with our values of $\nu_0 = 10^{13}$ s^{-1} and $\gamma a = 10$ and the prediction of Eq. (4).

In conclusion we have shown for the first time that long-time dispersive transport is observed from hopping with an exponential distribution of hopping sites as predicted by the original Scher and Montroll model.[2] These results are in accord with the simple quasiequilibrium pictures of Orenstein and Kastner[6] and Rose and Tiedje[7] which were arrived at only for the case of multiple trapping. Dispersion is still observable for $T/T_0 > 1$. Finally since the α's and the arrival times as a function of temperature are the same

as in the case of multiple trapping, the mechanism for transport cannot be uniquely determined from transit-time experiments.

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Effect of Fluctuations of Magnetization on the Bound Magnetic Polaron: Comparison with Experiment

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Thermal properties of large magnetic polarons localized on donors in a magnetic semiconductor are studied theoretically with the effect of thermodynamic fluctuations of magnetization taken into account. The model quantitatively describes recent spin-flip Raman scattering data for $Cd_{0.95}Mn_{0.05}Se$.

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In order to explain strong anomalies in the electrical conductivity of magnetic semiconductors,[1] and in the optical properties[2,3] of semimagnetic semiconductors,[4] the concept of the bound magnetic polaron (BMP) has been proposed.[2,3,5] The BMP consists of an impurity electron in the localized state, which induces by the s-d interaction a space-inhomogeneous local magnetization in its neighborhood. This magnetization, in turn, leads to the spin splitting of the impurity level, even in the absence of an external magnetic field.

Existing theories[2,5,6] of BMP are based on the mean-field approach (MFA). Their starting point is usually the Ginzburg-Landau free energy functional with two variational parameters: magnetization density $\vec{\eta}(\vec{r})$ due to presence of the impurity electron, and the effective Bohr radius a of the impurity-electron wave function $\varphi(\vec{r})$. Detailed calculations predict a type of critical behavior similar to that for a bulk ferromagnet in MFA: a critical temperature T_P through a divergence of static susceptibility χ, and a square-root dependence of $\vec{\eta}(\vec{r})$ and of the electron spin splitting on $T_P - T$.

These results, as we show in the following, are in direct conflict with recent experimental results for $Cd_{0.95}Mn_{0.05}Se$. In particular, the critical behavior in χ is absent, and the zero-field spin splitting persists above the mean-field value of T_P.

In this paper we demonstrate for the first time how the thermodynamic fluctuations influence the stability of BMP. The essentially new ingredient of our model is based on the observation that a degree of spin alignment around the donor