MONTE CARLO SIMULATION OF VARIABLE RANGE HOPPING AT THE FERMI LEVEL

G. Schönherr, H. Bässler, M. Silver

To cite this version:
G. Schönherr, H. Bässler, M. Silver. MONTE CARLO SIMULATION OF VARIABLE RANGE HOPPING AT THE FERMI LEVEL. Journal de Physique Colloques, 1981, 42 (C4), pp.C4-111-C4-114. <10.1051/jphyscol:1981420>. <jpa-00220827>

HAL Id: jpa-00220827
https://hal.archives-ouvertes.fr/jpa-00220827
Submitted on 1 Jan 1981

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
MONTE CARLO SIMULATION OF VARIABLE RANGE HOPPING AT THE FERMI LEVEL

G. Schönherr, H. Bässler and M. Silver

Fachbereich Physikalische Chemie, Philipp-Universität, Hans-Meerwein-Straße, D-3550 Marburg, F.R.G.
*Department of Physics and Astronomy, University of North Carolina, Chapel Hill, N.C. 27514, U.S.A.

Abstract.- Employing the Monte Carlo technique hopping at the Fermi level in a cubic lattice has been simulated as a function of temperature, electric field, hopping parameter 2a, and time. It has been found that the predictions of the simple theories agree remarkably well with our computer experiments. In our work we find a true d.c. conductivity proportional to \( \exp \left(-\frac{T}{T_0}\right)^{1/4}\) at low temperatures. The time dependence shows dispersion at short times due to energy relaxation and later equilibrium to the average hopping distance.

Introduction.- Perhaps the most simple, yet elegant approach to hopping at the Fermi level was the optimization approach by Mott (1) where the famous \( \ln \sigma \propto T^{1/4}\) law was found. This law has since been verified (see for examples G.G. Robert et al. (2)) and now put on firm theoretical grounds by Movaghar and Schirmacher (3). While experiments (2) have shown the \( T^{1/4}\) law the experimental data gave a conductivity which was too large by a factor of more than \( 10^4\). Because of this discrepancy we have decided to perform a computer simulation to test these simple theoretical ideas and approximations. We have found excellent agreement between our Monte Carlo simulations and theory regarding temperature, hopping parameter, and electric field. At high temperature an activated conductivity is found and simple arguments are presented for the magnitude of the activation energy.

Computational Methods.- Because of its simplicity the Monte Carlo Method has frequently been applied to treat transport properties of disordered solids (see e.g. (4,5)). In the present computation a volume of 30x30x69 sites with cubic symmetry (lattice parameter \( a = 10^{-7}\) cm) was used employing periodic boundary conditions along y and z rendering the effective sample dimensions in transverse directions practically infinite. To mimic hopping at the Fermi level the distribution of the energy of the hopping sites was approximated by a half-Gaussian, \( N(\epsilon) = \frac{2 \exp(-\epsilon^2/\sigma^2)}{(2\pi)^{1/2}\sigma}\) for \( \epsilon \geq 0\), the Fermi level being located at \( \epsilon = 0\). We chose \( \sigma = 0.3\) eV which is \( \gg kT\) at all temperatures studied. Hopping between two sites \( j \) and \( k \) is governed by:

\[
\begin{align*}
\nu_0 \exp(-2a|\epsilon_{ij}|) \exp\left(-\frac{|\epsilon_{ij}| - \epsilon(x_j - x_i)}{kT}\right) & \text{ for } \epsilon_{ij} - \epsilon(x_j - x_i) > 0, \\
\nu_{ij} \exp(-2a|\epsilon_{ij}|) & \text{ for } \epsilon_{ij} - \epsilon(x_j - x_i) < 0.
\end{align*}
\]

To simulate real systems we assumed \( \nu_0 = 10^{13} \text{s}^{-1}\). For details of the simulation method see refs. (5,6).
In order to study the energy relaxation we initially create a hopping particle at random on an arbitrary site located within the $x = 1$ plane. This gives us an initial energetic non-equilibrium. However, since the particle thermalizes in only a few jumps, this does not distort our d.c. conductivity results. We study 20 particles per lattice configuration and average over 50 different configurations. We store $n(x,t,s)$, where $n$ is the number of jumping particles. We thus can calculate $\langle x(t) \rangle$ and $\langle \varepsilon(t) \rangle$ from which we obtain the conductivity and the average energy. These average values are studies as a function of temperature and electric field for $2\alpha a$ ranging from 3 to 10.

Results and Discussion. Figure 1 summarizes our results for $\log i_0$ vs $T^{-1/4}$ for various values of $2\alpha a$ in the long time limit (thermodynamic equilibrium). At high temperatures the current is activated while at low temperature $\log i_0 \approx (T_0/T)_{1/4}$. Our $T_0$ data are best fitted by $T_0 = 24\alpha^3/\pi k N_F(2,3)$ where $N_F$ is the density of states at the Fermi level, in the present case $N_F = 2/(2\pi)^1/2a^3$. Using the simple relationship derived by Mott (1) we also can derive a value of the most probable hopping distance $<R>$. Data for $T = 250 K$ are listed in Table 1.

![Figure 1: log $i_0$ vs $T^{-1/4}$](image)

**Table 1**: Simulation results for hopping at the Fermi level. Data for $<R>/a$ refer to $T = 25 K$.

<table>
<thead>
<tr>
<th>$2\alpha a$</th>
<th>$T_0 (K)$</th>
<th>$&lt;R&gt;/a$</th>
<th>$p (T=\infty)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>$1.1 \times 10^5$</td>
<td>2.4</td>
<td>35</td>
</tr>
<tr>
<td>5</td>
<td>$5.2 \times 10^5$</td>
<td>2.1</td>
<td>16.2</td>
</tr>
<tr>
<td>7</td>
<td>$12 \times 10^5$</td>
<td>2.0</td>
<td>10.9</td>
</tr>
<tr>
<td>10</td>
<td>$42 \times 10^5$</td>
<td>1.8</td>
<td>6.5</td>
</tr>
</tbody>
</table>

The fact that $<R>$ considerably exceeds the lattice parameter $a$, explains why we can recover the analytic results, which have originally been worked out for a much more complicated spatial array of hopping sites (3), by confining the simulations to a simple cubic lattice.

Also shown in the insert in figure 1 is the high temperature activation energy $E_a$ vs the hopping parameter $2\alpha a$. It is easily verified that it should be given by $E_a = (N_F a^3 p)^{-1}$ where $p$ is the number of sites which on average a particle located a given site can jump to. Since $\lim_{T \to \infty} \log i(T) \approx p \exp(-2\alpha a)$, $p (T=\infty)$ is obtained by extrapolating the $\log i_0 T^{-1}$ region to $T=\infty$. Notice that our data for $E_a$ can very well be fitted by using the $p$ values from Table 1.

Apsley and Hughes (7) have predicted the conductivity behavior as a function of electric field in the low temperature regime. The results of our simulations shown in figure 2 demonstrate excellent agreement with their predictions. Consequently, the entire simplified analytic model for hopping at the Fermi level agrees with our computer experiment. Even the magnitude of the current is in accord with theory when we normalize it to our empirical jump frequency.
One final point is of interest. The simulations allow us to examine the dynamics of relaxation to the quasi equilibrium hopping at the Fermi level. In figure 3 we show the log i vs log t, log 〈ε〉 vs log t and finally log N_{NS} vs log t where 〈ε〉 is the average energy of the hopping particles, and N_{NS} is the number of new sites a particle has visited after a given time t. As stated earlier, we start our particles off with a population proportional to the density of states. One sees that the energy relaxation to the equilibrium value is very fast, occurring after approximately 10 jumps. Within this time regime the current decays in a power-law fashion yielding a straight line with slope α_2^{-1} when plotted on a log t vs log t scale indicating that transport is dispersive (8). However, even after 〈ε(t)〉 has become constant, i(t) continues to decrease as i(t) \propto t^{α_2^{-1}} with α_2>α_1. This signals existence of a second dispersive regime at low temperature. It is also seen the log N_{NS} vs log t-plot which shows two linear segments with slopes α_1<α_2<1. The magnitude of α_2 decreases with decreasing T. The second dispersion obviously is not due to the energy relaxation term but is a result of the inherent disorder arising from the inclusion of all possible hops. At low temperature more than 100 new sites visited are needed even in this simple system before the true d.c. conductivity is achieved. For the parameters used to calculate the data of fig.3 this figure even exceeds the total number of new sites a particle visits before being collected at the absorbing boundary which terminates the simulation volume. Only for T>50 K true thermodynamic equilibrium is attained within a time less than the carrier transit time through the sample. This suggests that perhaps one should study the a.c. conductivity for Fermi level hopping as well as the d.c. conductivity. Perhaps some of the discrepancies between the experimental results and simple theory may be revealed.

In conclusion, we have simulated hopping at the Fermi level in a cubic lattice and show remarkably good agreement with simple theories. We show the high temperature saturation predicted by Movaghar and Schirmacher (3) including an activation energy which has a particularly simple interpretation.

Supported in part by the National Science Foundation under grant DMR 790023 and NATO grant (SA-2-05B(1953)/870(80)AG).
References


5 SCHÖNHERR G., BÄSSLER H. and SILVER M., Phil.Mag.B, in press


7 APSLEY N. and HUGHES H.P., Phil.Mag.B 31 (1975) 1327