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Effective temperature of hopping electrons in a strong electric field

S. Marianer and B. I. Shklovskii
Theoretical Physics Institute, University of Minnesota, 116 Church Street SE, Minneapolis, Minnesota 55455
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We study numerically the energy distribution of electrons and the hopping conductivity as a function of the temperature T and electric field E in the tail of the density of states of an amorphous semiconductor where states are localized with a localization length a. We find a Boltzmann distribution with an effective temperature $T_{\rm eff}(T,E)$ which in the limit of $eEa \gg k_B T$ is close to $0.67eEa/k_B$. The conductivity $\sigma(T,E)$ collapses to a single universal curve when plotted as a function of the effective temperature $T_{\rm eff}(T,E)$. This confirms the fact that $T_{\rm eff}$ determines the conductivity. The same effective temperature also determines the dependencies of the steady state and transient photoconductivities on T and E.

Transport properties of amorphous semiconductors are dominated by the disorder-induced density of localized states in the gap adjacent to the conduction and valence bands. The standard assumption about the density of states is that it decays exponentially with energy (we measure energies from the band edge *into* the gap, i.e., deeper states have higher energies)

$$g(\varepsilon)=(N/\varepsilon_0)\exp\left[-\frac{\varepsilon}{\varepsilon_0}\right], \tag{1}$$

where N is the total concentration of states in the tail. The Fermi level is thought to be deep in the gap at energies $\varepsilon_F \gg \varepsilon_0$ (Fig. 1). The main mechanisms of carrier transport vary with temperature and three temperature regimes can be observed. At high temperatures $k_B T \gtrsim \varepsilon_0$ the conductivity is determined by activation of carriers from the Fermi level into the corresponding band of extended states. At sufficiently low temperatures conduction is governed by the hopping of carriers between states in a narrow band near the Fermi level, and one obtains Mott's law for variable-range hopping conductivity. The third regime is that of intermediate temperatures where the conductivity is still determined by variable-range hopping, but the exponential growth of the density of states [Eq. (1)] plays an important role and most of the hopping transport takes place at the so-called transport energy[1]

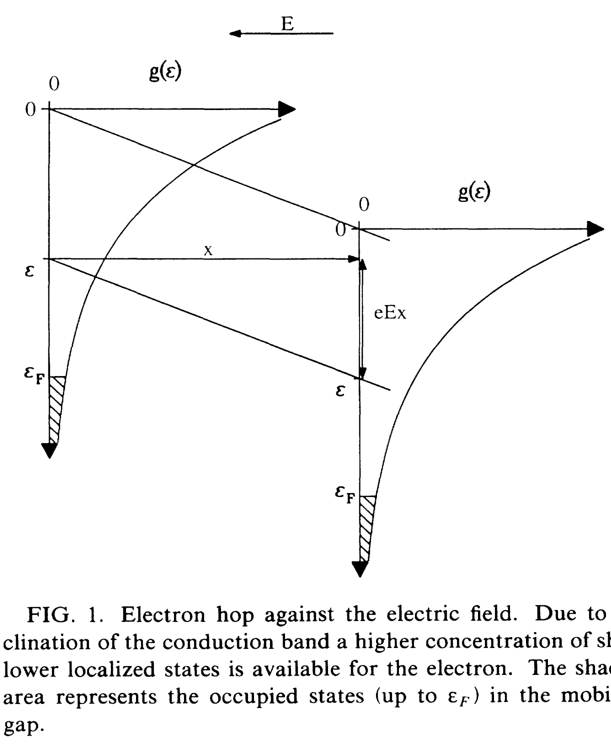

FIG. 1. Electron hop against the electric field. Due to inclination of the conduction band a higher concentration of shallower localized states is available for the electron. The shaded area represents the occupied states (up to ε_F) in the mobility gap.

$$\varepsilon_t=3\varepsilon_0 \ln\left[\frac{3\varepsilon_0}{k_B T}\frac{a}{2}N^{1/3}\right], \tag{2}$$

which gradually moves, with increasing temperature, from ε_F to ε_0. This third temperature range is the subject of our study.

The equilibrium ohmic conductivity in the intermediate temperature range was derived by Grünewald and Thomas and by Shapiro and Adler.[1] Below we follow the derivation by Shapiro and Adler. The differential conductivity of carriers with charge e at energy ε is given by

$$d\sigma(\varepsilon)=\frac{e^2}{k_B T}dn(\varepsilon)D(\varepsilon), \tag{3}$$

where the carrier concentration is

$$dn(\varepsilon)=g(\varepsilon)\exp\left[\frac{\varepsilon-\varepsilon_F}{k_B T}\right]d\varepsilon \tag{4}$$

and the diffusion constant at energy ε

$$D(\varepsilon)=\tfrac{1}{3}r^2(\varepsilon)\nu(\varepsilon), \tag{5}$$

where $r(\varepsilon)=N^{-1/3}\exp(\varepsilon/3\varepsilon_0)$ and $\nu(\varepsilon)=\nu_0\exp[-2r(\varepsilon)/a]$ (a is the localization length) are, respectively, the average hopping distance and tunneling rate at energy ε. Substituting these expressions into Eq. (3) one can see that the differential conductivity has a sharp maximum at the transport energy given by Eq. (2). The expression for

$d\sigma$ can be integrated analytically, giving

$$\sigma(T)=\frac{2\nu_0 e^2}{ak_BT}(N^{1/3}a/2)^{3\varepsilon_0/k_BT}\exp\left[-\frac{\varepsilon_F}{k_BT}\right]\times\int_{2N^{-1/3}/a}^{\infty}\exp(-y)y^{(3\varepsilon_0/k_BT)-2}dy\ , \quad (6)$$

where the last integral can be expressed in terms of the incomplete γ function $\gamma(a,x)$.

It was argued by Shklovskii *et al.*[2] that at $T=0$ a strong electric field E creates a Boltzmann-like distribution function

$$f(\varepsilon)=\exp\left[\frac{\varepsilon-\varepsilon_F}{k_BT_{\rm eff}}\right] \quad (7)$$

with an effective temperature $T_{\rm eff}=eEa/2k_B$, where a is the localization length and e is the electron charge. This is so because when an electric field is applied to the system at zero temperature an electron can increase its local energy ε by $\Delta\varepsilon=eEx$ by hopping against the field over a distance x. This is illustrated in Fig. 1. The process is similar to thermal activation with a hopping rate

$$\nu=\nu_0\exp(-2x/a)=\nu_0\exp(-2\Delta\varepsilon/eEa)=\nu_0\exp[-\Delta\varepsilon/T_{\rm eff}(E)]\ , \quad (8)$$

where $T_{\rm eff}(E)=eEa/2k_B$. The energy relaxation rate (decrease of the electron energy by $\Delta\varepsilon$) does not depend exponentially on the energy difference, and one therefore obtains Eq. (7). This means that one can find $\sigma(E)$ at $T=0$ by substituting $T=T_{\rm eff}(E)$ into Eq. (6).

The purpose of our paper is to check numerically predictions in Ref. 2 about the distribution function and the effective temperature associated with an electric field and, moreover, to obtain the effective temperature and the conductivity when both the electric field and the lattice temperature are finite. To do this we generated an array of randomly situated sites in a cube with periodic boundary conditions, and with energies distributed according to the density of states given by Eq. (1). The average distance between sites was $N^{-1/3}=3a$ since this is believed to be the value for electrons in a-Si:H ($N\simeq 3\times10^{19}$ cm^{-3}, $a\simeq 1$ nm). The transition rate from site i to site j in an electric field E in the x direction and at temperature T is given by $n_i(1-n_j)\Gamma_{ij}$, where n_i is the occupation probability of site i and

$$\Gamma_{ij}=\nu_0\exp(-2r_{ij}/a)\begin{cases}1, & \varepsilon_i+eE(x_j-x_i)<\varepsilon_j\\ \exp\{-[\varepsilon_i+eE(x_j-x_i)-\varepsilon_j]/k_BT\} & \text{otherwise}\ .\end{cases}$$

In the limit of low carrier concentration and in the temperature range we are studying ($\varepsilon_F\gg\varepsilon_0\gg k_BT$), the condition $n_i\ll 1$ holds for important sites, and we therefore neglect the term $1-n_j$ in the expression for the transition rate. This means that we can obtain the steady-state distribution n_i for a single carrier by solving the linear balance equations

$$n_i\sum_j\Gamma_{ij}=\sum_j n_j\Gamma_{ji}\ . \quad (9)$$

After we find a solution for the steady-state site occupations n_i we can calculate the energy distribution function $f(\varepsilon)$, which is given by

$$f(\varepsilon)=\sum_i n_i\delta(\varepsilon-\varepsilon_i)\ ,$$

and the conductivity

$$\sigma=\frac{1}{VE}\sum_{ij}n_i(x_j-x_i)\Gamma_{ij}\ , \quad (10)$$

where V is the volume of our system. We used a system of 1000 sites for our computation [$V=1000/N=(30a)^3$], and we have checked that the deviations between different realizations of the system were small. We therefore present below results for a single realization and do not use any averaging over different realizations.

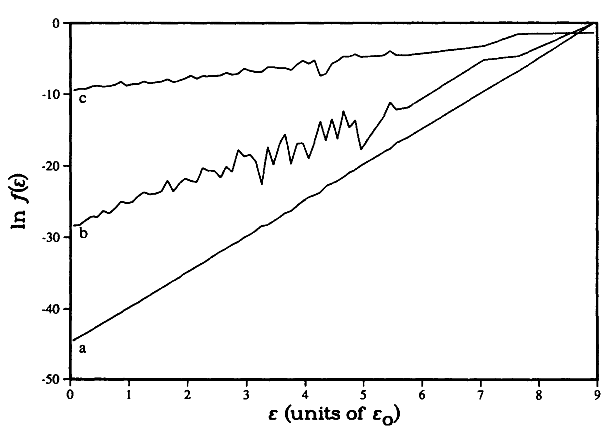

FIG. 2. The logarithm of the distribution function $f(\varepsilon)$ for various electric fields and temperature: (a) $T=0.2\varepsilon_0/k_B$, $E=0$, (b) $T=0$, $E=0.5\varepsilon_0/ea$, and (c) $T=0.8\varepsilon_0/k_B$, $E=0.8\varepsilon_0/ea$.

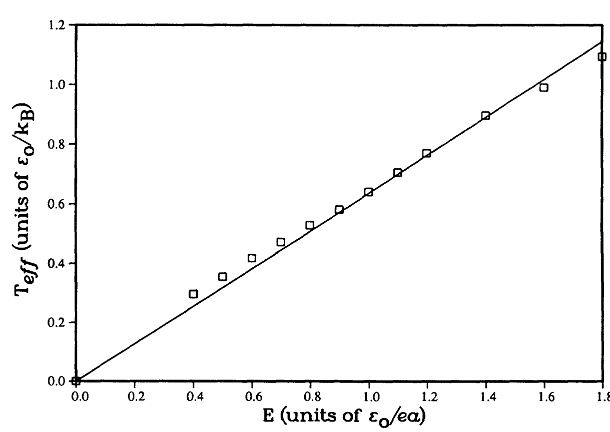

FIG. 3. The field dependence of the effective temperature.

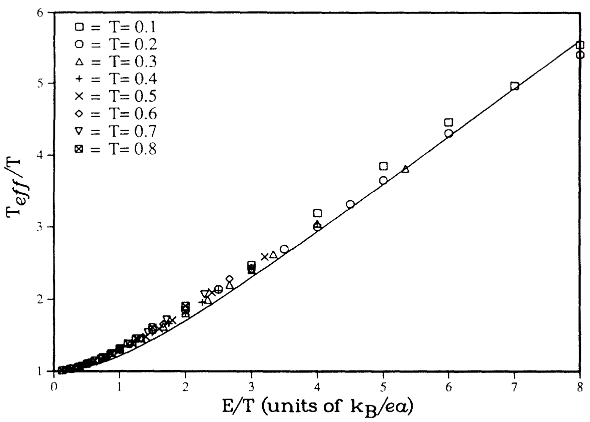

FIG. 4. T_{eff}/T vs eEa/k_BT for different temperatures. The continuous line represents our phenomenological fit $(T_{\text{eff}}/T)^2=1+(0.67eEa/k_BT)^2$.

Obviously, when the electric field is small $eEa \ll k_BT$ we have to obtain from the calculation outlined above a Boltzmann distribution function $f(\varepsilon)\propto\exp(\varepsilon/k_BT)$. To check the validity of the notion of an effective temperature for any values E and T we plotted $\ln f(\varepsilon)$ as a function of the energy ε and we indeed obtained that our calculated points lie close to a straight line for the whole range of electric fields and temperatures which we studied (we show a few examples in Fig. 2). We find the slope s of this line by a least-squares fit of our calculated $\ln f(\varepsilon)$ and the effective temperature is then given by $T_{\text{eff}}=1/k_Bs$.

First we study the case where we apply an electric field at $T=0$. We indeed obtain a Boltzmann-like distribution $f(\varepsilon)\propto\exp(\varepsilon/T_{\text{eff}})$ for this case, and we plot the field dependence of the effective temperature in Fig. 3. The effective temperature is indeed linear in the electric field,

$$T_{\text{eff}}(E)=(0.67\pm0.03)eEa/k_B\ , \tag{11}$$

as predicted by Shklovskii *et al.*,[2] but the coefficient we obtain is 30% higher than in their derivation.

For the general case when both the electric field and the temperature are finite, we show the variation of T_{eff}/T with eEa/k_BT for different temperatures (Fig. 4). One can see that all the data collapse to one line which is close to the function

$$T_{\text{eff}}^2(T,E)=T^2+(0.67eEa/k_B)^2\ . \tag{12}$$

Unfortunately we do not have a satisfactory physical interpretation of Eq. (12) and of the 30% difference between the coefficient in Eq. (11) and the prediction of Shklovskii *et al.*[2]

The conductivity we calculated using Eq. (10) is plotted as a function of the electric field for different temperatures in Fig. 5, and we observe a strong non-Ohmic behavior which resembles experimental results in many disordered systems for large electric fields E. Now we would like to test the prediction that the conductivity is determined by the effective temperature. To do this we plot in Fig. 6 the data presented in Fig. 5 as a function of the effective temperature obtained separately from the distribution function. As one can see, all the data collapse to one line. This indeed shows that the conductivity is determined only by the effective temperature rather than by the electric field and the temperature independently. We also show on the same plot the analytic dependence $\sigma(T_{\text{eff}})$ obtained from Eq. (6), and that the temperature dependence obtained numerically is the same as the theoretical one. The theory leading to Eq. (6) is of course too rough to give the exact numerical value of σ.

In order to test our predictions experimentally one needs to measure the conductivity as a function of the electric field and temperature and determine the effective temperature by comparing this conductivity to the ohmic conductivity $\sigma(T)$. We have suggested this to Nebel *et al.*, who measured the field-enhanced dark conductivity in *a*-Si:H (Ref. 3) and found good agreement with Eq. (12). Recently Soonpaa and Griffin[4] analyzed the hopping conductivity of two-dimensional crystals of $Bi_{14}Te_{11}S_{10}$ along the same lines, that is, plotting equiconductance curves in the (T,E) plain and trying to fit them to $T_{\text{eff}}(T,E)=\text{const}$, where $T_{\text{eff}}(T,E)$ is given by our phenomenological expression Eq. (12). They found a good fit for the temperature range $1<T<4.2$ K.

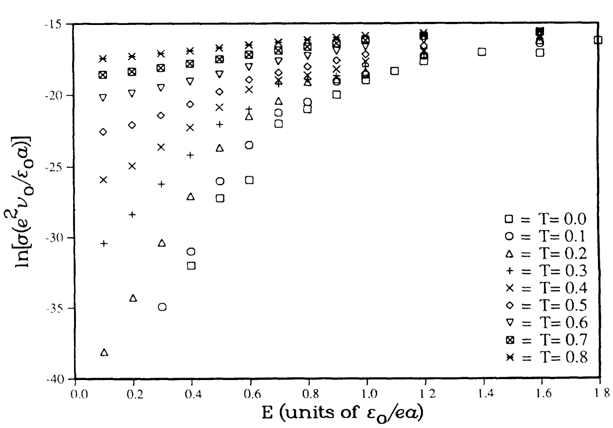

FIG. 5. The field dependence of the conductivity for different values of the temperature T.

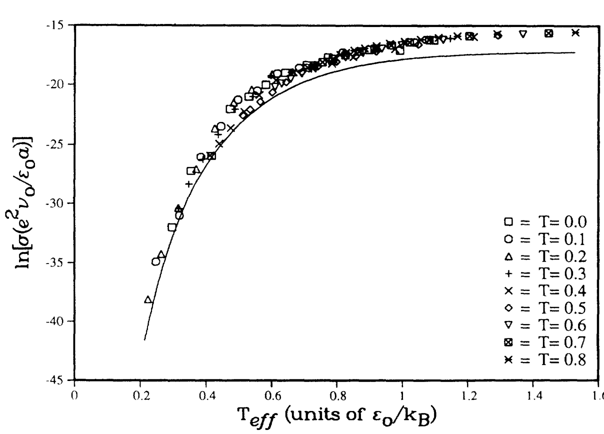

FIG. 6. The conductivity as a function of T_{eff}. The continuous line shows the analytic result obtained from Eq. (6).

To summarize, we have shown that when an electric field is applied to a semiconductor at a finite temperature one can characterize the combined effects of the field and the lattice temperature by an effective temperature which can be determined by two *independent* methods: (i) Extracting it from the energy distribution function, and (ii) defining it as the lattice temperature which gives the same conductivity. We have shown that these two methods give consistent results.

We would like to stress that the range of applicability of the concept of effective temperature and the empirical expression given by Eq. (12) is much wider than dark dc conductivity. We mention here in particular only the data on electron drift mobility[5] and on steady-state photoconductivity,[6,7] which are both in reasonable agreement with our theory.

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