Numerical simulations of hopping conductivity using nonflat densities of states

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We report numerical simulations of hopping conduction in lightly doped semiconductors. We model the hopping using a Miller-Abrahams resistor network. We investigate the effect of the density of states (DOS) on the temperature dependence of the hopping conductivity $\sigma(T)$ in a regime of temperature T well above the regime associated with variable-range hopping (VRH). In this "high-T" regime, we study a "peaked" DOS and a "flat-flat" DOS. The "peaked" DOS has a maximum at the $T=0$ K chemical potential μ_0 and decreases away from μ_0. The "flat-flat" DOS consists of two flat regions: an inner narrow region with density g_{inner} centered about μ_0, and an outer broad region with density $g_{\text{outer}} > g_{\text{inner}}$. For the peaked DOS, we obtain at "high T" results consistent with $\sigma(T)=\sigma_0\exp[-(T_0/T)^{1/4}]$, where T_0 is much smaller than the T_0 for VRH. This behavior agrees with certain experimental results for the conductivity in lightly doped n-type GaAs and n-type InP, and thereby provides direct support for the explanation by Shegelski and Barrie [Phys. Rev. B **36**, 7549 (1987); **36**, 7558 (1987)] that such experimental behavior results from a peaked DOS. For the flat-flat DOS, we find $\sigma(T)=\sigma_0\exp[-(T_0/T)^{1/2}]$ at "high T" if the energy width of the inner region is a fraction $\gamma \approx 0.1$ of the total width of the DOS. This result indicates that a "filling in" of the Coulomb gap (i.e., the DOS is nonzero at μ_0) is insufficient to destroy $T^{-1/2}$ behavior. We suggest that the trend toward $T^{-1/4}$ behavior evident in hopping-conduction experiments is due, not to a filling in of the Coulomb gap, but instead to a narrowing of the Coulomb gap ($\gamma \lesssim 0.02$). Such narrowing of the gap forces $T^{-1/2}$ behavior down to very low T and allows $T^{-1/4}$ behavior at high T.

I. INTRODUCTION

At low temperatures, electronic conduction in lightly doped n-type semiconductors occurs by electrons hopping between states localized about the donor impurity sites.[1] Experimental studies of hopping conductivity in lightly doped semiconductors have revealed drastic differences in the temperature dependence of the hopping conductivity $\sigma(T)$.[2-8] In these investigations, the conductivity was found to be of the form

$$\sigma(T)=\sigma_0 e^{-(T_0/T)^s}, \tag{1.1}$$

where σ_0, T_0, and s were independent of the temperature T. The drastic difference in the results is that—despite using the same materials (viz., either n-type GaAs or n-type InP), having essentially the same donor impurity concentrations n_D and compensations K, and performing the experiments *in a common range of temperatures* (1 K $\lesssim T \lesssim$ 7 K)—some of the experiments[2-5] reported $s=1$ while other, more recent, experiments[6,7] found $s \approx \frac{1}{4}$ (see Table I for details[9,10]).

Prior to the publication of these more recent experimental works,[6,7] the experimental situation for hopping conduction in lightly doped semiconductors appeared to be well understood. At extremely low temperatures ($T \lesssim 1$ K for the materials studied), Mott variable-range hopping (VRH),[11-14] for which $s=\frac{1}{4}$, was expected; at higher temperatures (but still in the hopping conductivity regime, viz., 1 K $\lesssim T \lesssim$ 5 K), activated behavior,[15,16] for which $s=1$, was expected. Experimentally, Ref. 8 reported VRH for the low-temperature range 0.1 K $\lesssim T \lesssim$ 1 K, while Refs. 2–5 reported activated behavior for the higher-temperature interval 1 K $\lesssim T \lesssim$ 5 K (see Table I). An intriguing puzzle resulted due to Refs. 6 and 7, which reported $s \approx \frac{1}{4}$, for the *higher*-temperature interval 1.4 K $\leq T \lesssim$ 5–7 K, as shown in Table I.

An important aspect of the experimental situation concerns the values of T_0 and the experimental range of T for those experiments with $s \approx \frac{1}{4}$ (Refs. 6–8). According to the theory of VRH,[11-14] the conductivity will be given by Eq. (1.1) with $s=\frac{1}{4}$ provided that the temperature is low enough. The theory also predicts the value of the quantity T_0. The experimental temperature range and values of T_0 of Ref. 8 are in good agreement with the theory of VRH. However, the values of T_0 reported in Refs. 6 and 7 were far too small, and the experimental temperature ranges were far too high, to be understood on the basis of the theory of VRH. The arguments which led to this conclusion have already been spelled out in detail[17] and will not be reported here. Instead, we illustrate the striking differences between Refs. 7 and 8 by showing in Table I the values of T_0 resulting from the two experiments, both of which used GaAs. The values of T_0 in Ref. 7 are 20 to 80 times smaller than those in Ref. 8, and

the associated $s=\frac{1}{4}$ behavior occurs in a temperature range 10 times higher than that of Ref. 8.

In summary, the essential features of the experimental results, as shown in Table I, are (1) in the higher-temperature regime (1 K $\lesssim T \lesssim$ 7 K), both $s=1$ behavior and $s=\frac{1}{4}$ behavior have been reported; (2) $s=\frac{1}{4}$ behavior has been reported for both the high-temperature regime (1 K $\lesssim T \lesssim$ 7 K) and the low-temperature regime (0.1 K $\lesssim T \lesssim$ 1 K); the values of T_0 for the high-T regime are many times smaller than the values of T_0 for the low-T regime.

An explanation for the differences in these experiments has been proposed by Shegelski and Barrie (SB).[18,19] The basic elements of the proposed explanation are as follows.

(i) The two temperature regimes evident in Table I may be categorized by the ratio of kT to the spread $\Delta\varepsilon$ in energies ε of the localized electronic states. The low-T regime corresponds to $kT \ll \Delta\varepsilon$, while the high-T regime is where kT is comparable to $\Delta\varepsilon$. For example, in lightly doped n-type GaAs, $\Delta\varepsilon$ is of order 1 meV, and 1 K $\lesssim T \lesssim$ 7 K corresponds to 0.1 meV $\lesssim kT \lesssim$ 0.6 meV, i.e., kT is *not* very much smaller than $\Delta\varepsilon$, and therefore 1 K $\lesssim T \lesssim$ 7 K is a high-T regime.[18,19]

(ii) The low-T, $s=\frac{1}{4}$, $T_0=10^4-10^5$ K results of Ref. 8 are in accord with the theoretical expectation of VRH in these materials for $T \lesssim 1$ K; the high-T, $s=\frac{1}{4}$, $T_0 \lesssim 10^3$ K results of Refs. 6 and 7 *cannot* be consistently regarded as being evidence of VRH: the temperature intervals are well above the temperature range for VRH in these materials and the values of T_0 are much too small.[17–19] Instead, in this high-T regime, the $s \approx \frac{1}{4}$ behavior may be attributed to a density of states (DOS) which has a maximum at the $T=0$ K chemical potential μ_0 and decreases away from μ_0. Such a DOS will be referred to as a "peaked" DOS.

(iii) The different values of s for the high-T conductivities, Refs. 2–5 ($s=1$) and Refs. 6 and 7 ($s \approx \frac{1}{4}$), may simply be due to the existence of fundamentally different energy dependences $g(\varepsilon)$ of the DOS in the various experimental samples.

The principal objective of the present work is to investigate the effect of the DOS on the hopping conductivity at temperatures which are well above the temperature regime of VRH. In so doing, we test the explanation proposed by SB. In particular, we test the explanation that the high-T, $s \approx \frac{1}{4}$, small-T_0 experimental results may be accounted for if a peaked DOS is used.

As in the work by SB, our study is based on the resistor-network model of Miller and Abrahams.[20] In this approach, a doped semiconductor is modeled by a set of resistors. Each pair i,j of donor impurities is associated with a resistance R_{ij} which depends on the distance r_{ij} separating the two donor sites and the ground-state energies ε_i and ε_j of the electronic states localized around the

TABLE I. Essential features of experimental results for the hopping conductivity $\sigma(T)$ in lightly doped semiconductors. Two types of behavior were reported, one with $s=1$ in $\sigma(T)=\sigma_0\exp[-(T_0/T)^s]$, the other with $s=\frac{1}{4}$. Indicated are the values of the donor impurity concentration n_D, the compensation K, and the range of temperatures T ($T_{\min} \lesssim T \lesssim T_{\max}$) for which the behavior was found. For Refs. 7 and 8, the values of T_0 are also given. For Ref. 7 the T_0 values are as reported in that paper; for Ref. 8, we estimated T_0 from their Fig. 2. The temperature intervals fall into two categories: "high T" (1 K $\lesssim T \lesssim$ 7 K) and "low T" (0.1 K $\lesssim T \lesssim$ 1 K). The two principal features of the table are (1) at high T, the same material with essentially the same n_D and K exhibits either $s=1$ or $s=\frac{1}{4}$ behavior, and (2) $s=\frac{1}{4}$ behavior occurs at both high T and low T, and the values of T_0 at high T are 1 to 2 orders of magnitude smaller than those for low T.

	Ref.	Material	Sample	n_D (10^{15} cm^{-3})	K	$T_{\min}$ (K)	$T_{\max}$ (K)	T_0 (K)
$s=1$, high T	2	InP	several	1–5	0.35–0.75	2	4.2	
	3	GaAs	several	2.1–7.2	0.1–0.67	2	5	
	4	GaAs	1	7.62	0.19	1.5	3	
			2	3.03	0.62	1.5	3	
			3	8.81	0.78	1.5	4	
	5	GaAs	1	1.35	0.70	1.7	5.0	
			2	1.90	0.62	1.6	5.3	
			3	2.10	0.53	1.6	4.2	
$s=\frac{1}{4}$, high T	6	InP	1	2.1	0.62	1.4	4.4	
			2	3.0	0.47	1.4	3.2	
			3	8.4	0.32	1.4	2.6	
	7	GaAs	1	6.4	0.64	1.4	7	1072.9
			2	8.7	0.43	1.4	6	915.1
			3	9	0.31	1.4	5	764.4
$s=\frac{1}{4}$, low T	8	GaAs	1	2	0.024	0.4	1.2	6×10^4
			2	2.5	0.67	0.2	1	4×10^4
			3	5.2	0.2	0.2	1	4×10^4
			4	7.2	0.3	0.1	1	2×10^4

donor sites. The conductivity of the semiconductor is given by the conductivity of the resulting resistor network.

For doped semiconductors such as n-type GaAs or n-type InP, which have isotropic, parabolic bands, the resistance R_{ij} is given by[21]

$$R_{ij}=R_0 f_{ij} X_{ij}^{-2} e^{X_{ij}} , \tag{1.2}$$

$$f_{ij}=\frac{kT}{\varepsilon_j-\varepsilon_i}(1+\tfrac{1}{2}e^{(\varepsilon_i-\mu)/kT})(1+2e^{-(\varepsilon_j-\mu)/kT}) \times(e^{(\varepsilon_j-\varepsilon_i)/kT}-1) , \tag{1.3}$$

where $X_{ij}=2r_{ij}/a$, a is the electronic localization length, μ is the electronic chemical potential, $\varepsilon_j>\varepsilon_i$, and R_0 is a constant which depends on various properties of the material.

Many investigations have been done using the $T\to 0$ K asymptotic form for R_{ij}; this is valid only when $kT\ll\Delta\varepsilon$.[18,19] The $T\to 0$ K form for the resistor network can be used to derive the well-known Mott law of VRH.[11–14] As noted above, the results of Ref. 8 may be understood as VRH in the $T\to 0$ K limit.

The other experimental results, Refs. 2–7, occur in a higher-temperature range, where kT may be of order $\Delta\varepsilon$, in which case the $T\to 0$ K form of the resistor network is not valid. Shegelski and Barrie developed an analytic theory[18,19] which was based on the *full* resistor network of Eqs. (1.2) and (1.3), and not the $T\to 0$ K simplified form. They used their analytic theory to calculate the hopping conductivity $\sigma(T)$ in the high-T regime. They found that the experimental results for $s=1$ (Refs. 2–5) could be understood using the full resistor network in the high-T regime and taking the DOS to be flat.[22] They also proposed that the high-T, $s\approx\frac{1}{4}$ results, with small values of T_0 (Refs. 6 and 7) could be accounted for by using the full resistor network in the high-T regime and using a peaked DOS. (An example of a peaked DOS is given in Sec. II.)

In this paper, we report numerical simulations which determine $\sigma(T)$ for the full resistor network of Eqs. (1.2) and (1.3). We examine three fundamentally different DOS. We compare our numerical results to the analytical results obtained by SB. In a previous publication[23] we verified SB's results for high T and a flat DOS. In this paper, we pay particular attention to the conductivity which results from a peaked DOS. Furthermore, we examine the $\sigma(T)$ resulting from a DOS which is fundamentally different from both a flat DOS and a peaked DOS. This third DOS differs from the other two in that its *minimum* value occurs at $\varepsilon=\mu_0$. By examining these three DOS, we explore the extent to which the DOS can affect $\sigma(T)$ when T is well above the VRH regime.[24]

We find that the DOS can drastically affect the form of $\sigma(T)$. In particular, we establish that a peaked DOS gives $\sigma(T)$ which is consistent with those high-T experimental results where $s\approx\frac{1}{4}$ and T_0 is small, thereby providing direct support for SB's explanation of these experimental results.

II. METHOD

Since the method that we use to calculate $\sigma(T)$ has been described in our previous paper,[23] we state only its main features. We perform a numerical simulation based on the full resistor network of Eqs. (1.2) and (1.3). We model a lightly doped semiconductor by distributing sites randomly in a three-dimensional unit cube. The sites i are assigned energies ε_i randomly but in accordance with a chosen DOS.[25] We refer to a particular set of positions and energies of the sites as a "sample."

Prior to being reduced to the Miller-Abrahams resistor-network form, the problem of calculating the conductivity involves stochastic variables which include the electron occupation numbers of the sites and stochastic processes which include transitions of electrons between sites. However, once the problem has been cast in the form of the Miller-Abrahams resistor-network model, only the average occupation numbers and average transition rates are involved—as represented by the resistors of Eq. (1.2)–and the only stochastic variables that remain are the positions and energies of the sites, or, equivalently, a "sample." We take into account the randomness in the positions and energies of the sites by producing several samples.

For each sample, we construct a resistor network using Eqs. (1.2) and (1.3). Then, for various temperatures T, we calculate the current I which flows in the resistor network when a potential difference of one unit is applied across the sample. We repeat this process for each sample, and average over the samples to obtain the average current $\langle I(T)\rangle$. For convenience, we work with the dimensionless temperature $t\equiv kT/\Delta\varepsilon$, where $\Delta\varepsilon$ is the band width of the DOS, and we make $\langle I(t)\rangle$ dimensionless by choosing R_0 as the unit of resistance.

The choice $R_0=1$ means that, for each sample, the numerical values of the *conductance* and of the current are equal. As we show below, the standard deviations in our values of $\langle I(t)\rangle$, which result from averaging over different random samples, are small. In consequence, we may proceed in the usual manner[26] and identify the dominant temperature dependence of $\langle I(t)\rangle$ with the dominant temperature dependence of the *conductivity* $\sigma(t)$ of the model. Specifically, we write $\langle I(t)\rangle=I_0(t)\exp[-(t_0/t)^s]$ and $\sigma(t)=\sigma_0(t)\exp[-(t_0/t)^s]$, where $I_0(t)$ and $\sigma_0(t)$ depend weakly on t, and we identify the exponential parts of $\langle I(t)\rangle$ and $\sigma(T)$ as being equal.[27]

For a chosen DOS, we obtain a particular result for $\langle I(t)\rangle$ and extract the dominant temperature dependence by plotting $\ln\langle I(t)\rangle$ versus t^{-s} for expected values of s. In this manner, we establish a correspondence between the DOS, the value of s, and the range of t. For example, in our previous investigation,[23] we studied the case of a flat DOS with band width $\Delta\varepsilon$. We verified the well-known results that $s=\frac{1}{4}$ at low t ($t\equiv kT/\Delta\varepsilon\lesssim 0.05$) while $s=1$ at high t ($0.07\lesssim t\lesssim 0.2$).

In our present investigation, we examine DOS which are not flat. We choose the peaked DOS to have the following form:

$$g(\tilde{\varepsilon})=\begin{cases} g_F & \text{if } 0\le|\tilde{\varepsilon}|\le\dfrac{\eta}{2}\ , \qquad (2.1a)\\ g_F\left[1-\left[\dfrac{2|\tilde{\varepsilon}|-\eta}{1-\eta}\right]^{\lambda}\right] & \text{if } \dfrac{\eta}{2}\le|\tilde{\varepsilon}|\le\dfrac{1}{2}\ , \qquad (2.1b)\end{cases}$$

where $\tilde{\varepsilon}\equiv\varepsilon/\Delta\varepsilon$, η is the fraction of the band width for which the DOS is flat, $0<\eta<1$, and $0<\lambda<1$; see Fig. 1. Based on some preliminary runs with trial values of η and λ, we choose $\eta=\frac{1}{20}$ and $\lambda=\frac{1}{2}$. For convenience, we choose $\mu_0=0$, work with symmetrical DOS, and take the band to be half filled. These choices yield a simple temperature dependence for μ, $\mu=-kT\ln 2$, which leads to a convenient expression for R_{ij}. It is clear on physical grounds that the choice $K=\frac{1}{2}$ for the compensation does not give fundamentally different results than for other values of K, as long as K is not extremely small or extremely close to unity. The value of g_F in Eq. (2.1) is readily expressed in terms of the number of impurity sites per unit volume, N, and is given by $g_F=[(\lambda+1)/(\lambda+\eta)]N$.

In order to examine the effect of the DOS on the conductivity, we consider a third DOS which differs fundamentally from both the flat DOS and the peaked DOS. We consider the following DOS:

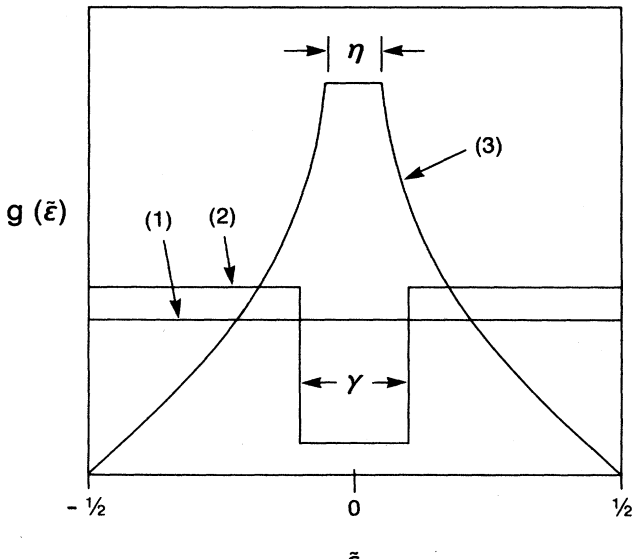

FIG. 1. The densities of states (DOS) investigated numerically: (1) the "flat" DOS, (2) the "flat-flat" DOS, (3) the "peaked" DOS. The value of $g(\tilde{\varepsilon})$ is plotted against the ratio $\tilde{\varepsilon}$ of the energy ε to the band width $\Delta\varepsilon$ of the DOS. Each DOS is symmetrical about $\tilde{\varepsilon}=0$; $\varepsilon=0$ corresponds to the $T=0$ chemical potential μ_0. The mathematical forms for these DOS, and the values of η and γ, are given in the text.

$$g(\tilde{\varepsilon})=\begin{cases} g_{\text{inner}} & \text{if } 0\le|\tilde{\varepsilon}|<\dfrac{\gamma}{2}\ , \qquad (2.2a)\\ g_{\text{outer}} & \text{if } \dfrac{\gamma}{2}<|\tilde{\varepsilon}|\le\dfrac{1}{2}\ , \qquad (2.2b)\end{cases}$$

which is also shown in Fig. 1. We will find that this DOS, which we call the "flat-flat" DOS, results in a fundamentally different form for $\sigma(T)$ than either the flat or the peaked DOS.

One of the reasons we choose to study the DOS of Eq. (2.2) is due to a recent paper by Summerfield, McInnes, and Butcher,[28] who showed that the Coulomb gap described by Efros and Shklovskii (ES) (Ref. 29) begins to "fill in" at finite temperatures. The DOS of Eq. (2.2) is the simplest nontrivial DOS which models such filling in of the Coulomb gap. We choose $\gamma=\frac{1}{10}$ and $g_{\text{outer}}/g_{\text{inner}}=5$. The choice $\gamma=\frac{1}{10}$ may be interpreted as choosing $\gamma=\Delta_{\text{ES}}/\Delta\varepsilon$ and $\Delta\varepsilon\approx 4.6\varepsilon_c$, where $\Delta_{\text{ES}}=e^3 g_F^{1/2}/(4\pi\varepsilon_0\kappa)^{3/2}$ is a measure of the energy width of the Efros-Shklovskii Coulomb gap (Ref. 14, p. 237), κ is the dielectric constant, and $\varepsilon_c=e^2/(4\pi\varepsilon_0\kappa N^{-1/3})$ is a measure of the Coulomb energy between electrons localized around neighboring donor sites.

III. RESULTS AND DISCUSSION

For each of the values of t, and for each of the DOS, we average 6 samples of 1000 sites each ($N=1000$) in calculating $\langle I(t)\rangle$. We choose the localization length a such that $N^{-1/3}a^{-1}=5$, a choice motivated by the experimental values $4.8\lesssim N^{-1/3}a^{-1}\lesssim 5.4$ reported in Ref. 7.

Figure 2 shows $\ln\langle I(t)\rangle$ versus $t^{-1/4}$ for the peaked DOS. The solid line is a least-squares fit to the curve $\ln\langle I(t)\rangle=\ln I_0^p-(t_0^p/t)^{1/4}$ over the interval $0.006\le t\le 0.045$. We obtain $\chi^2=0.03$, which indicates an excellent fit. Since a finite number of samples provides our results, we take into account the standard deviations in the average values $\langle I(t)\rangle$ when we determine the slope. Our result is $(t_0^p)^{1/4}=4.24(16)$, which leads to $t_0^p=325(50)$.

Since $\langle I(t)\rangle$ varies exponentially with t^{-s}, an appropriate measure of the scatter in our numerical results is the standard deviation $\Delta\ln I(t)$ in the values of $\ln I(t)$. For our samples, $\Delta\ln I(t)$ satisfies, for all DOS and for all values of t, $\Delta\ln I(t)/\ln\langle I(t)\rangle\lesssim 0.1$. This shows that we have enough samples to account for the random fluctuations in the values of the current.

In Fig. 3 we plot $\ln\langle I(t)\rangle$ versus $t^{-1/2}$ for the flat-flat DOS. The numerical values fit very well to $\ln\langle I(t)\rangle=\ln I_0^{f\text{-}f}-(t_0^{f\text{-}f}/t)^{1/2}$ for $0.013\le t\le 0.06$ ($\chi^2=0.04$), with $(t_0^{f\text{-}f})^{1/2}=1.83(6)$, which gives $t_0^{f\text{-}f}=3.35(22)$. An attempt to fit the flat-flat DOS numerical results to a curve with $s=\frac{1}{4}$ results in a completely unsatisfactory fit; similarly, the peaked-DOS results are unequivocally better fit to $s=\frac{1}{4}$ than to $s=\frac{1}{2}$.

In our previous paper,[23] we found two types of behavior for the flat DOS: for $0.015\le t\le 0.07$ we fit to $\ln\langle I(t)\rangle=\ln I_0^f-(t_0^f/t)^{1/4}$ ($\chi^2=0.07$), with $(t_0^f)^{1/4}=6.4(3)$, or $t_0^f=1700(300)$; for $0.07\le t\le 0.2$ we fit to $\ln\langle I(t)\rangle=\ln I_0^{f2}-(\tilde{\varepsilon}_a^f/t)$ with $\tilde{\varepsilon}_a^f=0.217(8)$ for the dimensionless activation energy. (When $s=1$, we will often

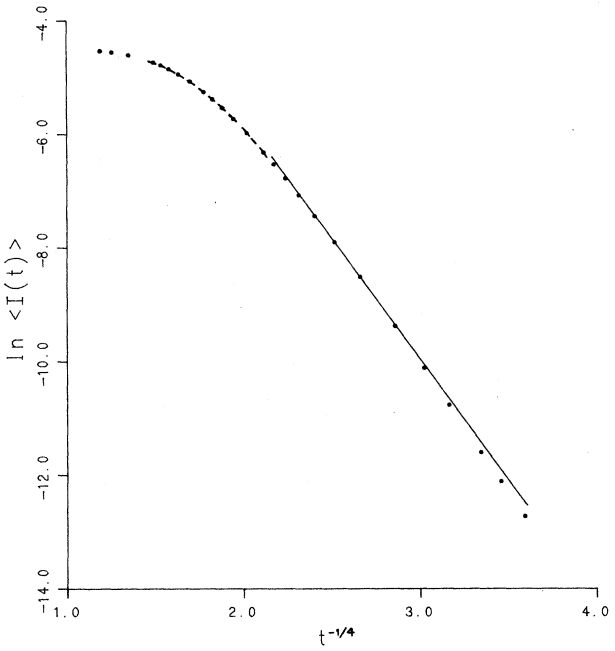

FIG. 2. The average current $\langle I(t)\rangle$ vs $t^{-1/4}$ for the peaked DOS. For the interval $0.006 \le t \le 0.045$, the solid line represents the best χ^2 fit to the numerical values and indicates a slope of $-4.24(16)$. The dashed curve indicates the best fit to activated behavior for $0.05 \le t \le 0.2$. See also Fig. 1 and Table II.

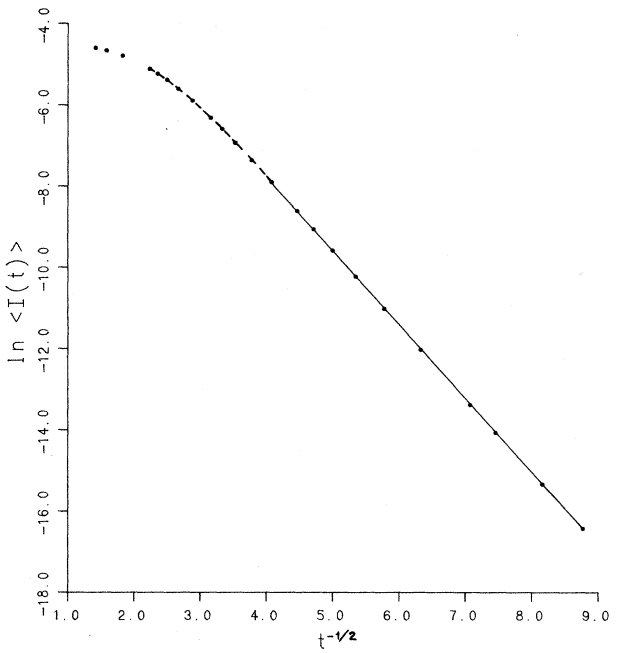

FIG. 3. The average current $\langle I(t)\rangle$ vs $t^{-1/2}$ for the flat-flat DOS. For the interval $0.013 \le t \le 0.06$, the solid line is the best χ^2 fit and gives a slope of $-1.83(6)$. The dashed curve indicates the best fit to activated behavior for $0.06 \le t \le 0.2$. See also Fig. 1 and Table II.

write $\tilde{\varepsilon}_a$ instead of t_0.)

We have also examined our numerical results for the peaked and flat-flat DOS in a higher range of t. For both DOS we find excellent fits using $s=1$. Specifically, we obtain $\tilde{\varepsilon}_a^p = 0.108(5)$ for $0.05 \le t \le 0.2$ for the peaked DOS, and $\tilde{\varepsilon}_a^{f\text{-}f} 0.243(8)$ for $0.06 \le t \le 0.2$ for the flat-flat DOS. See Figs. 2 and 3.

Our results for the three distinct DOS are summarized in Table II. The table reveals that the DOS drastically affects the temperature dependence of the resultant conductivity. In the "lower range of t," we find $s = \frac{1}{4}$ for the flat and the peaked DOS, but $s = \frac{1}{2}$ for the flat-flat DOS. Moreover, though they have a common value of s, the values of t_0 for the flat and peaked DOS differ considerably. In the "higher range of t," $s=1$ for all three DOS, but the values of $t_0 \equiv \tilde{\varepsilon}_a$ show marked difference. That $s=1$ for all three DOS in the upper range of t is not surprising: the temperature is so high that essentially all the sites participate in the hopping process, and the hops are predominantly nearest neighbor.

To ensure clarity, we state explicitly that it has long been known that the DOS affects the value of s *in the* $T \to 0$ *K limit.*[13,30] In this context, "$T \to 0$ K" means that kT is much smaller than the scale of energy over which the form of the DOS changes in any appreciable way. In this sense, it is only the result for the lower range of t for the flat DOS which falls into the "$T \to 0$ K" category; the remaining entries in Table II all correspond to ranges of t

TABLE II. Numerical results for the three DOS of Fig. 1. The results were obtained by fitting the average current to the expression $\ln\langle I(t)\rangle = \ln I_0 - (t_0/t)^s$ over a t interval $t_{\min} \le t \le t_{\max}$. In the "lower range of t" ($t \le 0.045$–0.07), the three DOS show drastically different behavior: $s = \frac{1}{4}$, but with very different t_0 values, for the flat and peaked DOS, whereas $s = \frac{1}{2}$ for the flat-flat DOS. In the "higher range of t" (0.05–$0.07 \le t \le 0.2$), all three DOS have $s=1$, but each has a different value of t_0. See also Figs. 2 and 3.

	DOS	$t_{\min}$	$t_{\max}$	s	t_0^s	t_0
lower	flat	0.015	0.07	$\frac{1}{4}$	6.4(3)	1700(300)
range	peaked	0.006	0.045	$\frac{1}{4}$	4.24(16)	325(50)
of t	flat-flat	0.013	0.06	$\frac{1}{2}$	1.83(6)	3.35(22)
higher	flat	0.07	0.2	1		0.217(8)
range	peaked	0.05	0.2	1		0.108(5)
of t	flat-flat	0.06	0.2	1		0.243(8)

TABLE III. A comparison of the theoretical quantities t_c and $t_0^{\rm VRH}$ to the numerical values $t_{\rm max}$ and $t_0^{\rm num}$ obtained for the flat DOS and the peaked DOS. For $t \lesssim 2t_c$, variable range hopping (VRH), viz., $\ln\langle I(t)\rangle = \ln I_0 - (t_0/t)^{1/4}$, is expected, with $t_0 = t_0^{\rm VRH}$. Whereas the theoretical and numerical ranges of t agree for the flat DOS, the upper limit $t_{\rm max}$ of the numerical range of t well exceeds $2t_c$ for the peaked DOS. As discussed fully in the text, the table reveals that while the flat DOS result indicates VRH, the peaked DOS result does not.

DOS	t_c	$t_{\rm max}$	$t_0^{\rm VRH}$	$t_0^{\rm num}$
flat	0.03	0.07	2650(150)	1700(300)
peaked	0.007	0.045	972(55)	325(50)

for which kT is comparable to the scale of energy over which the DOS changes significantly. As such, we are presenting evidence that the DOS also affects the form of $\sigma(T)$ at temperatures which are well above the $T \to 0$ K limit.

Our results indicate that the peaked and the flat-flat DOS exhibit three temperature regimes. As the temperature is lowered, there occurs first a regime where $s=1$ for both DOS (the "higher range of t" in Table II), then a regime where $s = \frac{1}{4}$ for the peaked DOS while $s = \frac{1}{2}$ for the flat-flat DOS (the "lower range of t" in Table II), and finally there occurs for both DOS the $T \to 0$ K VRH regime.

In Table III we compare the $s = \frac{1}{4}$ results for the peaked DOS with the $s = \frac{1}{4}$ results for the flat DOS. Theoretically, VRH is expected to exist for $t < \alpha t_c$, where $\alpha \lesssim 2$.[18,31] We see that, whereas the numerical and theoretical ranges of t agree for the flat DOS, the numerical range for the peaked DOS is well above the theoretical range. As such, the $s = \frac{1}{4}$ behavior for the peaked DOS is *not* low-t VRH. Moreover, the numerical value of t_0 for the peaked DOS is considerably smaller than the low-t VRH value. We note that the t_0 for the flat DOS is also smaller than its corresponding theoretical value; however, the difference is not nearly so much as for the peaked DOS, and some difference between the theoretical and numerical values is expected even for a flat DOS.[32] The important point is that the numerical range of t for $s = \frac{1}{4}$ behavior for the peaked DOS is far too high, and the value of t_0 far too small, to be explained as low-t VRH. This is precisely the experimental behavior reported in Refs. 6 and 7, viz., high-T, small-T_0, $s \approx \frac{1}{4}$ behavior. We conclude that the $s = \frac{1}{4}$ behavior for the flat DOS is in good agreement with theoretical VRH, but that, just as for the experimental results, the $s = \frac{1}{4}$ behavior for $0.006 \le t \le 0.045$ for the peaked DOS is *not*.

Next, we present a *quantitative* comparison between the high-T, small-T_0, $s \approx \frac{1}{4}$ experimental results of Refs. 6 and 7 and the high-t, small-t_0, $s = \frac{1}{4}$ numerical results of this work. Specifically, in Table IV we compare the range of the experimental quantity $\xi^{\rm expt} \equiv (T_0/T)^{1/4}$ to the range of the numerical quantity $\xi^{\rm num} \equiv (t_0/t)^{1/4}$; in the table we list both quantities under the same heading, $\xi^{\rm obs}$. The reason we compare $\xi^{\rm expt}$ and $\xi^{\rm num}$ is that, if the experimental and numerical temperature ranges overlap, and if the values of T_0 and t_0 agree, then the ranges of $\xi^{\rm expt}$ and $\xi^{\rm num}$ will overlap. Since $t \equiv kT/\Delta\varepsilon$, the parameter which connects experimental and numerical results is $\Delta\varepsilon$.

We see from the table that, while the range of $\xi^{\rm num}$ does not match any of the ranges of $\xi^{\rm expt}$ for Ref. 7, the range of $\xi^{\rm num}$ is in agreement with all three ranges of $\xi^{\rm expt}$ for Ref. 6, though the numerical value $N^{-1/3}a^{-1} = 5$ is less than the experimental values of $n_D^{-1/3}a^{-1}$. We can easily calculate the value of $\Delta\varepsilon$ required to bring the numerical value of t_0 and range of t into agreement with the experimental value of T_0 and range of T. For example, $\Delta\varepsilon = 8$ meV means that $t_0 = 325$ and $0.015 \le t \le 0.034$ correspond to $T_0 = 3 \times 10^4$ K and 1.4 K $\le T \le$ 3.2 K, which are the experimental values for sample 2 of Ref. 6. The value 8 meV for $\Delta\varepsilon$ is quite reasonable in view of the value $\varepsilon_d = 8.6$ meV for the bare donor binding energy in InP. Similar results are obtained for samples 1 and 3. The only differences between the experimental results of Ref. 6 and the numerical results of this work are differences between $n_D^{-1/3}a^{-1}$ and $N^{-1/3}a^{-1}$ as well as slight differences in the values of K.

We interpret the results of the above quantitative comparison as follows. A DOS having a peaked nature, such as the one given by Eq. (2.1), *qualitatively* accounts for the high-T, small-T_0, $s \approx \frac{1}{4}$ behavior of Refs. 6 and 7. Moreover, a DOS which has a form close to that of Eq. (2.1) (with $\eta \approx \frac{1}{20}$ and $\lambda \approx \frac{1}{2}$) will also account *quantita-*

TABLE IV. Quantitative comparison between experimental and numerical results. The range of the experimental quantity $\xi^{\rm expt} \equiv (T_0/T)^{1/4}$ is compared to the range of the numerical quantity $\xi^{\rm num} \equiv (t_0/t)^{1/4}$ in the column "Range of $\xi^{\rm obs}$." The range of $\xi^{\rm num}$ (this work) agrees with the three ranges for $\xi^{\rm expt}$ for Ref. 6. Also given in the table are the values of $n_D^{-1/3}a^{-1}$ and K.

Ref.	Sample	$n_D^{-1/3}a^{-1}$	K	Range of $\xi^{\rm obs}$
6	1	10	0.62	8.7 – 11.5
	2	9.0	0.47	9.9 – 12.2
	3	6.4	0.32	13.3 – 15.5
7	1	5.4	0.64	3.52 – 5.26
	2	4.9	0.43	3.51 – 5.06
	3	4.8	0.31	3.51 – 4.83
This work		5	$\frac{1}{2}$	9.2(4) – 15.2(6)

tively for the experimental results of Ref. 6. Since the values of ξ^{expt} for Ref. 7 are quite small, the DOS which quantitatively reproduces the results of Ref. 7 will differ somewhat from Eq. (2.1), but will nevertheless have a peaked character. In short, our numerical results show that the high-T, small-T_0, $s \approx \frac{1}{4}$ experimental results can be *fully* explained within the context of the resistor-network model of hopping conduction, using a peaked DOS.

Since $t \ll 1$ for the $s = \frac{1}{4}$ numerical results for the peaked DOS, it is tempting to try to reproduce these results analytically using the $T \to 0$ K simplified form for the resistor network. Proceeding in the standard manner,[30] we obtain $\sigma(t) = \sigma_0 e^{-\xi_c(t)}$, where $\xi_c(t)$ is given analytically by an implicit equation involving a quantity $n_c(\lambda, \eta, t)$ which is a critical parameter in the associated percolation problem (see Refs. 12–14 and 30), and which depends on λ, η, and t. Since $n_c(\lambda, \eta, t)$ is an unknown function of t for the temperatures of interest, $\xi_c(t)$ may not be obtained by such a simple analytic approach, and a numerical solution, such as the one we have obtained, is required instead.

We turn next to a discussion of the numerical results for the flat-flat DOS. As noted earlier, this DOS models the finite temperature filling in of the Efros-Shklovskii Coulomb gap. In the Efros-Shklovskii theory of the Coulomb gap, the DOS has the form

$$g(\varepsilon) \sim \begin{cases} g_F \dfrac{|\varepsilon - \mu_0|^2}{\Delta^2} & \text{for } |\varepsilon - \mu_0| \lesssim \Delta \ , \quad (3.1a) \\ g_F & \text{for } |\varepsilon - \mu_0| \gtrsim \Delta \ , \quad (3.1b) \end{cases}$$

where Δ is the energy spread of the Coulomb gap (see Ref. 14, Chap. 10). This DOS implies a conductivity of the form

$$\sigma(t) = \sigma_0 e^{-(t_0^C/t)^{1/2}} \ , \quad (3.2a)$$

$$t_0^C = \beta_1 \left[\frac{\tilde{\Delta}^2}{g_F \Delta \varepsilon a^3} \right]^{1/3} \approx \beta_1 N^{-1/3} a^{-1} \tilde{\Delta}^{2/3} \ , \quad (3.2b)$$

where $\tilde{\Delta} \equiv \Delta / \Delta\varepsilon$, $\Delta\varepsilon$ is again the width of the DOS, and $\beta_1 \approx 2.8$ (Ref. 14, p. 240). Once again, the conductivity given by Eq. (3.2) holds only for low-enough t. According to a recent paper by Summerfield, McInnes, and Butcher,[28] the Coulomb gap fills in at finite temperature, so the DOS does not vanish at $\varepsilon = \mu_0$. In consequence of this filling in, the low-temperature form of the conductivity will have $s = \frac{1}{4}$ instead of $s = \frac{1}{2}$. For the flat-flat DOS of Eq. (2.2), with $\gamma = \frac{1}{10}$ and $g_{\text{outer}}/g_{\text{inner}} = 5$, the t_c associated with this $s = \frac{1}{4}$ VRH is $t_c = 0.0008$.[31] Thus, for $t \lesssim 0.002$, $\sigma(t)$ will be given by Eq. (1.1) with $s = \frac{1}{4}$. We have found that, for $0.013 \le t \le 0.06$ (viz., t well above the range for VRH), $\sigma(t)$ obeys Eq. (1.1) with $s = \frac{1}{2}$ and $t_0 = 3.35(22)$. Our result indicates that, even if the Coulomb gap does fill in, provided the DOS has a dip near μ_0, the conductivity can still display $s = \frac{1}{2}$ behavior in a temperature range above that for which VRH occurs; it is only at the very lowest of temperatures that the DOS of Eq. (2.2) will lead to $s = \frac{1}{4}$ behavior.

If Δ is chosen so that the areas under the DOS of Eqs. (2.2) and (3.1) are equal, then $t_0^C \approx 2.2$: the DOS of Eq. (3.1) leads to $s = \frac{1}{2}$ behavior with $t_0 \approx 2.2$ in the limit $t \to 0$, while the DOS of Eq. (2.2) gives $s = \frac{1}{2}$ behavior with $t_0 \approx 3.3$ in a much higher temperature range. Our numerical work shows that $s = \frac{1}{2}$ behavior with t_0 of order unity can occur when the DOS is nonzero at μ_0.

IV. SUMMARY AND CONCLUSIONS

In this paper, we have reported numerical simulations of hopping conduction in lightly doped semiconductors. We have modeled such hopping conduction using a Miller-Abrahams resistor network. We have used the full expression for the resistances instead of the simplified $T \to 0$ K asymptotic form usually employed.

Our study centered on how the temperature dependence of the hopping conductivity $\sigma(T)$ depended on the DOS. It is well known that the DOS is important in determining $\sigma(T)$ as $T \to 0$ K; our results show that the DOS also plays a crucial role at higher temperatures. We found two distinct temperature regimes above the $T \to 0$ K regime. In the lower of these two regimes, we found that the parameter s in Eq. (1.1) for $\sigma(T)$ was unity for a flat DOS, whereas $s = \frac{1}{4}$ for the peaked DOS of Eq. (2.1), while $s = \frac{1}{2}$ for the flat-flat DOS of Eq. (2.2). In the higher of these two regimes, we found $s = 1$ for all three DOS, but with the activation energy depending on the DOS in a nontrivial way.

The numerical results for the peaked DOS indicate that, in addition to VRH behavior, which is expected to occur as $T \to 0$ K and for which $s = \frac{1}{4}$, $s = \frac{1}{4}$ behavior can also occur in a temperature range well above the range for VRH, and with a value of T_0 much smaller than the value associated with VRH. Our work thereby validates the claim by SB, viz., that the high-T, $s \approx \frac{1}{4}$, small-T_0 experimental results of Refs. 6 and 7 can be explained in the context of the Miller-Abrahams full resistor-network model using a peaked DOS.

One important difference between our numerical results and the analytical results of SB is that SB's results embodied having kT of order $\Delta\varepsilon$, while we find that this is not crucial, i.e., that our numerical results can explain the experimental results while having $kT \ll \Delta\varepsilon$. We emphasize that, even though $kT \ll \Delta\varepsilon$, our results do not simply reduce to low-T VRH. Like SB, we find that the form of the DOS plays a crucial role in explaining the experimental results.

Our numerical results also reveal that activated behavior ($s = 1$) can occur at temperatures above the VRH regime for a variety of DOS, not just for a flat DOS. Also, depending on the band width $\Delta\varepsilon$, a peaked DOS could give either $s = 1$ or $s = \frac{1}{4}$ in the temperature range 1 K $\lesssim T \lesssim$ 5–7 K. A large value of $\Delta\varepsilon$ will give $s = \frac{1}{4}$, while a small $\Delta\varepsilon$ will give $s = 1$. However, $s = 1$ behavior in this range of T could also occur for a flat DOS or a flat-flat DOS. It appears that activated hopping conductivity results whenever kT is of order $\Delta\varepsilon$ (viz., $0.05 \lesssim kT/\Delta\varepsilon$

$\lesssim 0.2$). As such, it would seem that the experimental results of Refs. 2–5 could be associated with any DOS. On the other hand, the experimental results of Refs. 6 and 7 are almost certainly due to a *peaked* DOS, for it is only in this case that our numerical results reproduce small-T_0, $s=\frac{1}{4}$ behavior in the temperature range $1\ \mathrm{K} \lesssim T \lesssim 5$–$7$ K. We note that, in the event of such high-T, small-T_0, $s \approx \frac{1}{4}$ behavior, one might expect $s=1$ behavior at even higher T. However, if $\Delta\varepsilon$ is large enough, say of order 10 meV in InP, which is essentially the value we found in Sec. III, then activation of electrons to the conduction band would dominate activated hopping for $T \gtrsim 5$–7 K; this is precisely the behavior reported in Refs. 6 and 7.

The filling in of the Coulomb gap at finite temperature, as reported by Summerfield, McInnes, and Butcher,[28] implies VRH at low-enough T. Our numerical simulations give $s=\frac{1}{2}$ at high T for the flat-flat DOS. As such, our work indicates that a Coulomb gap, even if filled in, gives rise to $s=\frac{1}{2}$ behavior, except at the very lowest of temperatures. In light of our numerical results, the lack of reported $s=\frac{1}{2}$ behavior in lightly doped semiconductors suggests that the Coulomb gap is either much wider or much narrower than originally predicted by Efros and Shklovskii. A much wider, filled-in Coulomb gap would result in VRH occurring at higher temperatures. However, since a filled-in Coulomb gap implies a smaller value of g_F, and hence a larger value of T_0 than the T_0 for a flat DOS, this could not account for those experimental results where T_0 is smaller than the T_0 for a flat DOS. On the other hand, a narrower gap not only shifts the $s=\frac{1}{2}$ behavior to lower temperatures, but also restores a regime of temperature, above that for $s=\frac{1}{2}$ behavior, wherein the temperature dependence of $\sigma(T)$ is determined by the form of the DOS. As a final point concerning the Coulomb gap, we note that, for doped semiconductors where the doping is heavier than has been considered in this paper, the experimental trend has also been toward $s=\frac{1}{4}$ behavior and not $s=\frac{1}{2}$ behavior. Our work suggests that this trend is due, not to the filling in of the Coulomb gap, but more plausibly to a narrowing of the gap.

In closing, we emphasize the need for further experimental and theoretical work. More experimental work in lightly doped semiconductors at high T ($T \gtrsim 1$ K) is required in order to establish in which cases $s=1$ behavior occurs, and in which $s=\frac{1}{4}$ occurs. Further work at low T ($T \lesssim 1$ K) will tell whether VRH always results, as it does in Ref. 8, or if the Coulomb gap will reveal itself in some cases. Further theoretical investigations can help understand why $s=\frac{1}{4}$ behavior results for the peaked DOS, whereas $s=\frac{1}{2}$ results for the flat-flat DOS, or, more generally, what the connection is between the DOS and the associated value of s at high T.

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