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Effects of Donor Size and Heavy Doping on Optical, Electrical and Thermoelectric Properties of Various Degenerate Donor-Silicon Systems at Low Temperatures

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Abstract: In various degenerate donor-silicon systems, taking into account the effects of donor size and heavy doping and using an effective autocorrelation function for the potential fluctuations expressed in terms of the Heisenberg uncertainty relation and also an expression for the Gaussian average of $\frac{\hbar^2}{2m}$, $a \geq 1$ $E_k$ being the kinetic energy of the electron, calculated by the Kane integration method (KIM), we investigated the density of states, the optical absorption coefficient and the electrical conductivity, noting that this average expression calculated by the KIM was found to be equivalent to that obtained by the Feynman path-integral method. Then, those results were expressed in terms of $E^{\alpha-1(1/2)}$ for total electron energy $E \geq 0$, vanished at the conduction-band edge: $E = 0$, and for $E \leq 0$ exhibited their exponential tails, going to zero as $E \to -\infty$ and $\infty$, and presenting the maxima, in good accordance with an asymptotic form for exponential conduction-band tail obtained by Halperin and Lax, using the minimum counting methods. Further, in degenerate d-Si systems at low temperatures, using an expression for the average of $E^p$, $p \geq 3/2$, calculated using the Fermi-Dirac distribution function, we determined the mobility, electrical conductivity, resistivity, Hall factor, Hall coefficient, Hall mobility, thermal conductivity, diffusion coefficient, absolute thermoelectric power, Thomson coefficient, Peltier coefficient, Seebeck thermoelectric potential, and finally dimensionless figure of merit, which were also compared with experimental and theoretical results, suggesting a satisfactory description given for our obtained results.

Keywords: Donor Size, Heavy Doping, Electrical Conductivity, Hall Effect, Diffusion Coefficient

1. Introduction

Donor (acceptor)-silicon d (a)-Si system at a given temperature $T$, doped with a given d (a)-density $N$, assuming that all the impurities are ionized, is the base material of modern semiconductor devices [1-6]. Then, due to the Fermi-Dirac statistics, there are three cases may be classified as: non-degenerate ($T \gg T_D$ and $N \ll N_e$), moderately degenerate ($T > T_D$ and $N \gg N_e$) and degenerate ($T < T_D$ and $N \gg N_e$)-cases, $T_D$ and $N_e$ being respectively the degenerate temperature defined in Eq. (15) and critical impurity density.

In the present paper, the degenerate d-Si system is considered, noting that all the optical, electrical, and thermoelectric properties given in the degenerate a-Si system can also be investigated by a same treatment.

So, in the degenerate d-Si system, a good knowledge of: (i) energy-band structure parameters such as: the reduced band gap [7-12], $N_{c(d)}$ [11, 12] and effective donor ionization energy [13], (ii) exponential conduction-band tails [14-25] and Fermi energy [26-28], and finally (iii) optical [29-48], electrical [49-69], and thermoelectric [58, 61, 68, 69] properties, due to the effects of donor size [11, 12, 42, 43, 53], heavy doping [14, 17-30, 34, 35, 48-68], and low T [49, 58], is thus necessary for designing new devices and also understanding their performance.

In Section 2, we studied the effects of donor size [or compression (dilatation)], temperature, and heavy doping on the energy-band-structure parameters. At $T = 0$ K, with
increasing values of donor radius \( r_d \), since the effective dielectric constant \( \varepsilon_n(r_d) \), due to the donor-size effect, the effective donor ionization \( \varepsilon_{d0}(r_d) \), unperturbed intrinsic band gap \( \varepsilon_{go}(r_d) \), and critical donor density \( N_{c(d)} \) increase, as seen in Table 1. Then, for a given \( r_d \), the effective intrinsic band gap \( \varepsilon_{go}(r_d,T) \), due to the T-effect, decreases with increasing \( T \), as given in Eq. (3). Finally, due to the heavy doping effect (HDE), for a given \( N \), the effective electron mass \( m_{n}^{\text{HDE}}(N,r_d) \) increases with increasing \( N \), as given in Eq. (8), and for given \( r_d \) and \( T \), the reduced band gap \( \varepsilon_{gn2}(N,T,r_d) \) decreases with increasing \( N \), as given in Eq. (10).

In Section 3, the effective autocorrelation function for potential fluctuations, \( W_n \), was determined and in Eq. (B.6) the appendix B, being a central result of the present paper, as noted in Eq. (20). It was suggested that \( W_n(\varepsilon \rightarrow \pm \infty) \rightarrow \eta_n \), \( \varepsilon \) and \( \eta_n \) being respectively the total electron energy and the energy parameter characteristic of the conduction-band tail states, and \( W_n(\varepsilon \rightarrow \pm 0) \rightarrow 0 \). Therefore, the density of states, the optical absorption coefficient and the electrical conductivity, being proportional to our result (20), vanished at the conduction-band edge \( \varepsilon = 0 \), as given in Eqs. (23, 26). Those results were also compared with other theoretical results, obtained at \( \varepsilon = 0 \), in the small time approximation [21, 29, 30] and in the full ground-state case and deep-tail approximation [21], which were found to be constant, being not correct, as discussed also in Eq. (26). Then, for \( \varepsilon \leq 0 \), their exponential tails were obtained in Figures 1, 4 and 7, in which they increased with increasing \( r_d \) for a given value of \( \varepsilon \), due to the donor-size effect, and further they went to zero as \( \varepsilon \rightarrow -\infty \) and presented the maxima, being found to be in good accordance with an asymptotic form for exponential conduction-band tail, obtained by Halperin and Lax [19], using the minimum counting methods.

In Section 4, we determined the average of \( \varepsilon^P \) at low temperature \( T \) (\( T << T_0 \)), using the Fermi-Dirac distribution function (FDDF), \( \langle \varepsilon^P \rangle^\text{FDDF} = \varepsilon_{FP}^P(\varepsilon) \), for \( p = 3/2 \), as given in Eq. (34) and Table 3, \( \varepsilon_{FP} \) being the Fermi energy determined in Eq. (A10) of the Appendix C.

In Section V, we determined the critical donor density, as given in Table 1, suggesting that its numerical results are in good agreement with the corresponding data given in Ref. 12, and it increases with increasing \( r_d \), due to the donor-size effect [12]. Then, for \( \varepsilon \leq 0 \), the exponential band-tail behaviors were investigated and reported in Table 4, and also in Figures 1 and 2a (b).

In Section 6, various optical functions were determined in band-to-band transitions (\( \varepsilon \geq 0 \)) as found in Figs. 3a, 3b, 3c, and in a simple generalized Mott model, by [12]

\[
N_{c(r_d)} = N_{c(P)} \times \left( \frac{\varepsilon_{n}(r_d)}{\varepsilon_{n}(r_d_0)} \right)^3.
\]

Therefore, with increasing \( r_d \), the effective dielectric constant \( \varepsilon_n(r_d) \) decreases, implying thus that \( \varepsilon_{go}(r_d) \), being compared with other theoretical and experimental works [33-35, 38, 44-48], and also the exponential optical absorption-coefficient tail behaviors were investigated when \( \varepsilon \leq 0 \), as seen in Table 7, and Figures 4 and 5a (b).

In Section 7, for \( \varepsilon \geq 0 \), using the functions \( G_P \) obtained at low \( T \), given in Table 3, we determined various electric functions as those given in Tables 10-13, in good accordance with the corresponding experimental results [50, 53, 54, 56-61], and for \( \varepsilon \leq 0 \), we also studied the exponential conductivity-tail behaviors, as those given in Tables 14 and Figures 7, 8a (b).

In Section 8, for \( \varepsilon \geq 0 \), using also the function \( G_P \), we studied various thermoelectric functions, and reported their numerical results in Table 15 and Figures 9a, 9b, 9c, 9d, 9e, and 9f, noting that for \( \varepsilon \leq 0 \) we could also study the exponential thermoelectric function-tail behaviors by a same treatment, as those obtained in Sections 5-7.

Finally, some concluding remarks were given and discussed in Section 9.

2. Energy-Band-Structure Parameters

Here, we study the effects of donor size, temperature, and heavy doping on the energy-band-structure parameters.

2.1. Donor-Size Effect

In donor-Si systems at \( T=0 \) K, since the d-radius, \( r_d \), in tetrahedral covalent bonds is usually either larger (or smaller) than the Si atom-radius, \( r_a \), assuming that in the P-Si system \( r_p = r_a = 0.117 \) nm, with \( nm = 10^{-9}m \), a local mechanical strain (or deformation potential-or-strained energy) is induced, according to a compression (dilation) for \( r_d > r_p \) \( (r_d < r_a) \), respectively, or to the donor size \( (r_d) \)-effect. In the Appendix A of our recent paper [12], basing on an effective Bohr model, such a compression (dilation) occurring in various donor (d)-Si systems was investigated, suggesting that the effective dielectric constant, \( \varepsilon_n(r_d) \), decreases with increasing \( r_d \). This donor size \( (r_d) \)-effect affects the changes in all the energy-band-structure parameters or the electronic properties of various donor-Si systems, expressed in terms of \( \varepsilon_n(r_d) \), as those investigated in our recent paper [12], noting that \( \varepsilon_n(r_p) = 11.4 \). In particular, the changes in the unperturbed intrinsic band gap, \( \varepsilon_{go}(r_p) = 1170 \) meV , effective donor ionization energy, \( \varepsilon_{d0}(r_p) = 33.58 \) meV , and critical donor (P)-density, \( N_{c(P)} = 3.5 \times 10^{18} \) cm\(^{-3} \), of the P-Si system at 0 K, are obtained in an effective Bohr model, as [12]
results of $N_{\text{EBT}}(r_{n,d},\delta_{e})$ would be more accurate.

Table 1. The following values of $r_{d}$, $\epsilon_{m}$, $a_{sd}$, $E_{po}(r_{d})$, and $N_{(d}\delta_{e})$-data, given in our previous paper [12], are now reported in this TABLE, in which we also include the numerical results of $N_{\text{EBT}}(r_{d},\delta_{e})$ where $\delta_{e} = 1$ or $\delta_{e} = 1.0028637416$, calculated using Eqs. (41, 42), and their absolute relative errors defined by:

$$|RE| = \left|1 - \frac{N_{\text{EBT}}(r_{d},\delta_{e})}{N_{(d}\delta_{e})}\right|.$$ Here, $nm \equiv 10^{-9}$ m.

| Donor | Sb | P | As | Bi | Ti | Te | Se | S |
|-------|----|---|----|----|----|----|----|---|
| $r_{d}$ (nm) | $0.1131$ | $0.1170$ | $0.1277$ | $0.1292$ | $0.1424$ | $0.1546$ | $0.1621$ | $0.1628$ |
| $\epsilon_{m}(r_{d})$ | $12.02$ | $11.40$ | $8.47$ | $7.95$ | $4.71$ | $3.26$ | $2.71$ | $2.67$ |
| $E_{po}(r_{d})$ (meV) | $30.18$ | $33.58$ | $60.82$ | $69$ | $197$ | $411$ | $593$ | $613$ |
| $E_{po}(r_{d})$ (meV) | $1167$ | $1170$ | $1197$ | $1205$ | $1333$ | $1547$ | $1729$ | $1749$ |
| $N_{(d)}$ ($10^{18}$ cm$^{-3}$) | $3$ | $3.52$ | $8.58$ | $10.37$ | $50$ | $150.74$ | $261.24$ | $274.57$ |
| $N_{\text{EBT}}(r_{d},\delta_{e})$ ($10^{18}$ cm$^{-3}$) | $3.00003$ | $3.520005$ | $8.579950$ | $10.368890$ | $10.370000$ | $10.370000$ | $10.370000$ | $10.370000$ |
| $[RE]$ | $1.1 \times 10^{-6}$ | $1.3 \times 10^{-6}$ | $6.1 \times 10^{-6}$ | $1.1 \times 10^{-4}$ | $3.1 \times 10^{-7}$ | $4.1 \times 10^{-6}$ | $2.1 \times 10^{-7}$ | $2.2 \times 10^{-10}$ |
| $N_{\text{EBT}}(r_{d},\delta_{e})$ ($10^{18}$ cm$^{-3}$) | $2.991440$ | $3.509950$ | $8.555450$ | $10.339280$ | $10.370000$ | $10.370000$ | $10.370000$ | $10.370000$ |
| $[RE]$ | $2.8 \times 10^{-3}$ | $2.8 \times 10^{-3}$ | $2.9 \times 10^{-3}$ | $3.0 \times 10^{-3}$ | $2.9 \times 10^{-3}$ | $2.8 \times 10^{-3}$ | $2.8 \times 10^{-3}$ | $2.8 \times 10^{-3}$ |

Moreover, it should be noted that in donor-Si systems such the $E_{boi}(r_{d},300 \text{ K})$-increase with increasing $r_{d}$ as shown in Table 1. $E_{boi}$ being the effective intrinsic band gap given in next Eq. (3), well agrees with a result obtained recently by Ding et al. [42]. In fact, in their study of the optical properties of isolated silicon nano-crystals (nc-Si) with the size of $2r_{nc-Si} = 4.2$ nm ($\gg 2r_{p} = 2 \times 0.117$ nm) embedded in a SiO$_{2}$ matrix, they showed that $E_{boi}(r_{nc-Si},300 \text{ K}) = 1.79 \text{ eV} \gg E_{boi}(r_{d},300 \text{ K}) = 1.12 \text{ eV}$ given in the bulk crystalline Si at room temperature, being also due to the size effect ($r_{nc-Si} \gg r_{p}$).

Now, the effective Bohr radius can be defined by

$$a_{bo}(r_{d},m^{*}) = \frac{m^{2}}{\epsilon_{n}} \times \epsilon_{n}(r_{d}) \times 5.3 \text{ nm}. \tag{1}$$

In Eq. (1), $m^{*}$ is the effective electron mass given in the Si, being equal to: (i) the effective mass $m_{a} = 0.3216 \times m_{o}$, $m_{o}$ being the free electron mass, defined for the calculation of $m_{a}^{\text{HEE}}(N)$, as determined in next Eq. (8), due to the heavy doping effect (HDE), (ii) the reduced effective mass: $m_{r} = \frac{m_{a}^{\text{HEE}}}{m_{a}} \times m_{o}$, $m_{o}$, for the optical absorption-coefficient calculation, where $m_{p} = 0.3664 \times m_{o}$ is the effective hole mass in the silicon [12], (iii) $m_{a}^{\text{HEE}}(N)$, given in next Eq. (8), for the determination of the density of states, as given in Section 5, and finally (iv) the conductivity effective mass: $m_{\text{cond}} = 0.26 \times m_{o}$ for the electrical conductivity calculation [6], as used in Section 7.

Then, in the degenerate case ($N > N_{(d)}$), denoting the Fermi wave number by: $k_{F}\equiv(3\pi^{2}N/g_{c})^{1/3}$, where $g_{c} = 3$ is the effective average number of equivalent conduction-band edges [11, 12], the effective Wigner-Seitz radius $r_{\text{WS}}$ characteristic of the interactions is defined by

$$r_{\text{WS}}(N,r_{d},m^{*}) = \frac{2\pi^{2}N}{g_{c}} \times \frac{1}{m^{*}}, \tag{2}$$

being proportional to $N^{-1/3}$. Here, $\gamma = (4/9\pi)^{1/3}$, and $k_{F}$ means the averaged distance between ionized donors.

2.2. Temperature Effect

Here, in d-Si systems, being inspired from recent works by Pässler [8, 9], we can propose an accurate expression for the effective intrinsic band gap as a function of $r_{d}$ and $T$, as

$$E_{boi}(T,r_{d}) = E_{boi}(r_{d}) - 0.071 (eV) \times \left\{1 + \left(\frac{2T}{440.6913K}\right)^{2.201} \left(\frac{k_{F}^{2}}{2\pi m^{*}}\right)^{2.201} - 1\right\}. \tag{3}$$

For example, in the (P, S)-Si systems, for $0 \leq T(\text{K}) \leq 3500$, the absolute maximal relative errors of $E_{boi}$ are equal to: 0.22%, 0.15%, respectively, calculated using the accurate complicated results given by Pässler [9].

2.3. Heavy Doping Effect (HDE)

HDE on $m_{a}$

Now, using Eq. (2) for $r_{\text{WS}}(N,r_{d},m^{*} = m_{a})$, the ratio of the inverse effective screening length $k_{\text{sn}}$ to Fermi wave number $k_{F}\equiv k_{F}^{2}/2\pi m^{*}$ at 0 K is defined by [12]

$$R_{\text{sn}}(N,r_{d}) \equiv \frac{k_{\text{sn}}}{k_{F}} = \frac{k_{F}^{-1}}{k_{\text{sn}}} = R_{\text{WS}} + \left[R_{\text{snTF}} - R_{\text{WS}}\right]e^{-r_{\text{sn}}}, \tag{4}$$

It is noted that, in the very high electron-density limit [or in the Thomas-Fermi (TF)-approximation], $R_{\text{sn}}$ is reduced to

$$R_{\text{snTF}}(N,r_{d}) \equiv \frac{k_{F}}{k_{F}} = \frac{k_{F}}{k_{\text{sn}}} = \sqrt{\frac{4\pi n}{\pi}} \ll 1, \tag{5}$$

being proportional to $N^{-1/6}$. It should be noted that the effective screening length $k_{\text{snTF}}$ is very larger than the averaged distance between ionized donors $k_{F}^{-1}$ (i.e., this is the TF-condition given in the very degenerate case, $N \gg$
\( N_{e(d)} \), and in the very low electron-density limit [or in the Wigner-Seitz (WS)-approximation], \( R_{sn} \) is reduced to

\[
R_{sn}\text{WS}(N, r_d) \equiv \frac{\text{bs}_{\text{WS}}}{\varepsilon_{p}} = \frac{3}{2\pi^2} - \gamma \frac{d_r s_{\text{WS}}(N, r_d)}{4 R_{sn}}, \quad \gamma = \left(4/9\pi\right)^{1/3}. \tag{6}
\]

Here, when the relative spin polarization \( \zeta \) is equal to zero (paramagnetic state), \( \varepsilon_{CE} \) means the majority-electron correlation energy (CE), determined by as \( [11, 12] \)

\[
\varepsilon_{CE}(N, r_d) = \left[ 1 + \frac{4\pi e^2 N_r \Delta}{3n_l^2 + n_l^2 + n_l^2} \right] m_n. \tag{8}
\]

HDE on \( \varepsilon_{gl} \)

In the degenerate case, the optical band gap is defined by

\[
\varepsilon_{g_{n1}}(N, T, r_d) \equiv \varepsilon_{g_{n2}}(N, T, r_d) + \varepsilon_{F_N}(N, T), \tag{9}
\]

\[
\text{BGN}(N, r_d) \approx C_n \times \left( \frac{N}{10^{18} \text{ cm}^{-3}} \right)^{1/2} \times \left( \frac{\mu_{h_{\text{DE}}}(N, r_d)}{m_n} \right)^{1/2} \times \left[ 1 + \left( \frac{\text{m}_{h_{\text{DE}}}(N, r_d)}{m_p} \right)^{1/2} \right], \tag{11}
\]

which is a very simplified form compared with our previous complicated expression for BGN \([12]\).

Here, the values of effective dielectric constant \( \varepsilon_{gl}(r_d) \) are given in Table 1 and the electron effective mass \( m_{n_{\text{DE}}}(N, r_d) \), due to the heavy doping effect, is determined in Eq. (8). Further, the empirical parameter \( C_n = 0.5 \times 10^{-3} \) (eV) has been chosen so that the absolute maximal relative error \( |R_m| \) of our result \( (9) \), calculated using the optical band-gap \( \varepsilon_{g_{n1}}-\text{data} \) for P-Si systems at 20 K obtained by Wagner \([7]\) are found to be minimized.

In a degenerate P-Si system, with use of the next Eq. (43), obtained for the definition of effective density of free electrons given in the conduction band, \( N^* \approx N - N_{e(P)} \), where the value of \( N_{e(P)} \) is given in Table I, our present results of \( \varepsilon_{g_{n1}}(N^*, T = 20 \text{ K}, r_d) \), computed using Eqs. (9, 11), and their absolute relative errors \( |R_E| \), calculated using the \( \varepsilon_{g_{n1}}-\text{data} \) at 20 K \([12]\), are obtained and reported in Table 2, in which our previous accurate \( \varepsilon_{g_{n1}}(N^*)-\text{results} \) and their \( |R_E| \) are also included \([12]\), for a comparison.

**Table 2.** Numerical results of optical band gap at \( T=20 \text{ K}, \varepsilon_{g_{n1}}(N^*) \), expressed in eV, being investigated in our recent paper \([12]\), and determined in Eq. (9), and finally their absolute relative errors \( |R_E| \), calculated using the \( \varepsilon_{g_{n1}}-\text{data} \). [7]

| \( N (10^{18} \text{ cm}^{-3}) \) | 4 | 8.5 | 15 | 50 | 80 | 150 |
|---|---|---|---|---|---|---|
| \( \varepsilon_{g_{n1}}-\text{data} \) | 1.138 | 1.133 | 1.129 | 1.131 | 1.132 | 1.133 |
| \( \varepsilon_{g_{n1}}(N^*) \) \([12]\) | 1.149 | 1.138 | 1.134 | 1.126 | 1.123 | 1.119 |
| \( |R_E| \) (%) | 0.9 | 0.5 | 0.5 | 0.4 | 0.8 | 1.2 |
| \( \varepsilon_{g_{n1}}(N^*), \text{Eq. (9)} \) | 1.160 | 1.147 | 1.139 | 1.123 | 1.118 | 1.113 |
| \( |R_E| \) (%) | 1.9 | 1.3 | 0.9 | 0.7 | 1.2 | 1.7 |

The underlined \( |R_E| \)-value is the maximal one.

This table indicates that the maximal value of \( |R_E| \), where \( \varepsilon_{F_N} \) is the Fermi energy determined at any \( N \) and \( T \) in Eq. (C.1) of the Appendix C, with an accuracy equal to: \( 2.11 \times 10^{-4} \), and \( \varepsilon_{g_{n2}} \) is the reduced band gap defined as

\[
\varepsilon_{g_{n2}}(N, T, r_d) = \varepsilon_{g}(T, r_d) - \text{BGN}(N, r_d), \tag{10}
\]

where the intrinsic band gap \( \varepsilon_{g}(T, r_d) \) is determined in Eq. (3) and the band gap narrowing (BGN) is determined below.

In our recent paper \([12]\), an accurate formula for the BGN was investigated, being expressed in the following spin-polarized chemical potential-energy contributions, as:

- the exchange energy of an effective electron gas,
- the majority-electron correlation energy of an effective electron gas,
- the minority-hole correlation energy,
- the majority electron-ionized donor interaction screened Coulomb potential energy, and finally
- the minority hole-ionized donor interaction screened Coulomb potential energy.

It should be noted that the two last contributions (iv) and (v) are found to be the most important ones. Therefore, an approximate form for the BGN can be proposed by

\[
\eta_n(N, r_d) = \sqrt{2\pi N} \times q^2 \kappa_{sn}^{-1/2} \varepsilon_{F_N}^{-1}, \tag{12}
\]

where \( \kappa_{\text{sn}}^{-1/2} \) is determined in Eq. (4). Moreover, in highly degenerate case \( (N \gg N_{e(d)}) \) or in the Thomas-Fermi approximation, \( \kappa_{\text{sn}}^{-1/2} \approx \kappa_{\text{snFP}}^{-1/2} \) determined in Eq. (5), \( \eta_n \) is found to be proportional to \( N^{1/2} \).

Then, from Eq. (12) and next Eq. (15), we can obtain another heavy doping condition as

\[
\eta_n \leq \frac{\varepsilon_{F_N}}{\eta_{n}} < 1, \tag{13}
\]

being proportional to \( N^{-1/4} \) in this highly degenerate case.

In summary, in the highly degenerate case \( (N \gg N_{e(d)}) \) and from Eqs. (2, 4, 13), one has

\[
\frac{k_{\text{sn}}^2}{a_B} < \frac{\varepsilon_{F_N}}{\eta_{n}} < \frac{k_{\text{sn}}^2}{\varepsilon_{F_N}}, \tag{14}
\]

where \( \varepsilon_{F_N} \) is the Fermi energy at 0 K, defined by

\[
\varepsilon_{F_N}(N) = k_{\text{sn}}^2 \varepsilon_{F_N}(N)_0 \times n_m^2. \tag{15}
\]

In Eq. (15), \( m^* \) is the electron effective mass, defined in Eq. (1), and in this highly degenerate case one has a low T-condition as: \( T \ll T_D \equiv \varepsilon_{F_N}(N)/k_B, T_D \) and \( k_B \) being the
randomly distributed potential energy, which may be absorbed by a redefinition of the zero energy. Then, the expression for the effective autocorrelation function for potential fluctuations can thus be defined by [25, 58]

$$v_i(t) = -\frac{q^2 \times \exp(-k_{sn} |r - \bar{r}_i|)}{\epsilon_{sn} |r - \bar{r}_i|}.$$  \hspace{1cm} (17)

Further, using a Fourier transform, the $v_i$-representation in wave vector $\mathbf{k}$-space is given by

$$v_i(\mathbf{k}) = -\frac{q^2}{\epsilon_{n0}} \times \frac{4\pi}{\Omega} \times \frac{1}{k^2 + k_{sn}^2},$$ \hspace{1cm} (18)

where $\Omega$ is the total Si-crystal volume and $k_{sn}$ is the inverse screening length determined in Eq. (4). Moreover, in Eqs. (16, 17), $V_o$ is defined as a constant so that $\langle V(r) \rangle = 0$, reflecting a charge neutrality, where the notation $\langle \ldots \rangle$ denotes the configuration average [25, 58]. In fact, from Eq. (17), one has

$$(\mathcal{N} / \Omega) \int_0^\infty v_i(t) \times 4\pi r^2 dr = -4\pi q^2 k_{sn}^2 \epsilon_{n0}^{-1} \equiv -V_o, \mathcal{N} \equiv \mathcal{N} / \Omega,$$

indicating that from Eq. (16) one obtains: $\langle V(r) \rangle = 0$.

Therefore, the effective autocorrelation function for potential fluctuations can thus be defined by [25, 58]

$$W_n(\mathbf{r}, \mathbf{r}') \equiv \langle V(r)V(r') \rangle \equiv \langle V(r) \rangle \times \langle V(r') \rangle + \langle (V(r)V(r')) \rangle = \langle (V(r)V(r')) \rangle,$$

where $\langle (V(r)V(r')) \rangle$ denotes the effective second-order cumulant, and $\mathbf{r}(t)$ and $\mathbf{r}'(t')$ are the electron positions at the times $t$ and $t'$, noting that the cumulant is just the average potential energy, which may be absorbed by a redefinition of the zero energy. Then, the expression for $W_n$ is determined in Eq. (B.6) of the Appendix B, as

$$W_n(v_n, N, r_a) \equiv \langle V(r)V(r') \rangle = \frac{n_a^2 \times \exp \left(-\frac{\mathcal{H}_n \times R_{sn}}{2\sqrt{\mathcal{W}_n}} \right)}{(2\pi\hbar^2)^{3/2}}.$$ \hspace{1cm} (19)

Here, $R_{sn}(N)$ is given in Eq. (4), $n_a$ is determined in Eq. (12), the constant $\mathcal{H}_n$ will be chosen in Section V A as: $\mathcal{H}_n = 5.4370$, such that the determination of the density of electrons localized in the conduction-band tail would be accurate, and finally $v_n \equiv -\frac{E}{\mathcal{W}_{n0}}$, where $E$ is the total electron energy and $E_{F_{n0}}$ is the Fermi energy at 0 K, determined in Eq. (15).

Now, we calculate the ensemble average of the function:

$$\langle (E - V)^{a-\frac{1}{2}} \rangle_{KIM} \equiv \langle E_k^{a-\frac{1}{2}} \rangle_{KIM} = \int_{-\infty}^{\infty} (E - V)^{a-\frac{1}{2}} \times P(V) dV,$$ for $a \geq 1$.

Then, by variable changes: $s = (E - V) / \sqrt{\mathcal{W}_n}$ and $x = -\frac{E}{\sqrt{\mathcal{W}_n}}$, and using an identity [15]:

$$\int_0^\infty s^{a-\frac{1}{2}} \times \exp(-sx^2) ds = \Gamma(a + \frac{3}{2}) \times \exp(x^2/4) \times D_{a-\frac{1}{2}}(x),$$

where $\mathcal{D}_{a-\frac{1}{2}}(x)$ is the parabolic cylinder function, $\Gamma(a + \frac{3}{2})$ is the Gamma function, one thus finds

$$\langle E_k^{a-\frac{1}{2}} \rangle_{KIM} = \frac{\exp(-x^2/4) \times \mathcal{W}_n^{\frac{a}{2}}}{\sqrt{\pi}} \times \Gamma(a + \frac{3}{2}) \times D_{a-\frac{1}{2}}(x).$$ \hspace{1cm} (20)

This result (20) will used to study the optical, electrical, and thermoelectric properties of various degenerate d-Si systems, depending on $W_n$ defined in Eq. (19) and the variable $x$, expressed also in terms of $W_n$, as
\[
\begin{align*}
    x &= -\frac{E}{\sqrt{W_n}} \equiv A_n \times v_n \times \exp \left( \frac{\eta_n \times W_n}{4 \sqrt{W_n}} \right), \quad A_n \equiv \frac{E_{\text{Froo}}}{\eta_n}, \quad v_n \equiv -\frac{E}{E_{\text{Froo}}}, \\
    \text{where } E_{\text{Froo}} \text{ and } \eta_n \text{ are determined in Eqs. (15, 12), respectively. Therefore, the effective autocorrelation function for potential fluctuations } W_n, \text{ defined in Eq. (19), is thus a central result of the present paper.}
\end{align*}
\]
\[ D_{-a^{-\frac{1}{2}}}(x \to \infty) \approx \beta(a) \times \exp \left[ -\left( \sqrt{a} + \frac{1}{16a^2} \right) x - \frac{x^2}{16a^2} - \frac{x^3}{24a^3} \right] \to 0, \quad \beta(a) = -\frac{\sqrt{a}}{2^5a \Gamma\left(\frac{3}{2} + \frac{1}{a^2}\right)}, \]

noting that

\[ \beta(1) = \frac{\sqrt{a}}{2^5 \Gamma(5/4)} \quad \text{and} \quad \beta(5/2) = \frac{\sqrt{a}}{2^{5/2}}. \]

Then, putting \( f(a) \equiv \frac{n_a}{\sqrt{2\pi}} \times \Gamma(a + \frac{1}{2}) \times \beta(a) \), Eq. (25) yields

\[ H_n(v_n \to 0, r_d, a) = \frac{(a_k^L)^{\frac{1}{2}}}{(f(a))} = \exp \left[ -\left( \frac{\eta_a R_n}{2x_{vn}} \right) - \left( \sqrt{a} + \frac{1}{16a^2} \right) x - \left( \frac{1}{2} - \frac{1}{16a^2} \right) x^2 - \frac{x^3}{24a^3} \right] \to 0, \]

which is in good accordance with that given in Eq. (A3) of the Appendix A. In particular, as \( v_n \to 0 \), the first term of \( \ln H_n(v_n \to 0, r_d, a = 1) \) given in Eq. (26), \(-\frac{\eta_a R_n}{2x_{vn}}\), can be compared with the third one given in Eq. (A3), \(-4Bc^2R_n \times |v_n|^{-1/2}\). Moreover, as noted in Eqs. (B.5, B.6) of the Appendix B, when the small time approximation (STA) is used: \( \Delta t \approx 0 \) [17, 21, 22, 29, 30], \( W_n(v_n, N) \approx \eta_n^2 \). Therefore, Eq. (25) now yields [21, 29, 30]:

\[ H_n(\text{STA})(v_n \to 0, r_d, a) = \frac{(a_k^L)^{\frac{1}{2}}}{(f(a))} = \exp \left[ \left( \sqrt{a} + \frac{1}{16a^2} \right) x - \frac{\eta_n^2}{4} \right], \quad E \leq 0, \]

being equal to 1 for \( E = -0 \), which is not correct, since we must have: \( H_n(E \to -0, r_d, a) \to 0 \), as obtained in Eq. (26), due correctly to the Heisenberg uncertainty relation given in Eq. (B.5): \( \Delta r \gg 0 \) as \( E \to -0 \). Finally, we also remark that, in the full ground-state case and deep-tail approximation, the exponential conduction-band-tail states, obtained by Sa-yakamit et al. [23], was also equal to a constant at \( E = -0 \), being not correct.

Further, from Eq. (21), as \( E \to -\infty \), one has: \( v_n \to +\infty \) and \( x \to \infty \). Thus, one gets [15]:

\[ D_{-a^{-\frac{1}{2}}}(x \to \infty) \approx x^{-a^{-\frac{1}{2}}} \times e^{-\frac{x^2}{4}} \to 0. \]

Therefore, Eq. (25) yields

\[ K_n(v_n \to +\infty, r_d, a) \equiv \frac{(a_k^L)^{\frac{1}{2}}}{(f(a))} = \frac{1}{\beta(a)} \times \exp \left( -\frac{(A_n \times v_n)^2}{2} \right) \times (A_n \times v_n)^{-a^{-\frac{1}{2}}} \to 0, \]

being in perfect agreement with a well-known semi-classical Kane’s result [14].

It should be noted that, as \( E \leq 0 \), the ratios (26) and (27) can be taken in an approximate form as

\[ F_n(v_n, r_d, a) = K_n(v_n, r_d, a) + [H_n(v_n, r_d, a) - K_n(v_n, r_d, a)] \times \exp[-c_4 \times (A_n v_n)]c_2]. \]

Here, \( e(r_d, v_1, v_2, z) \) is the slope of this AF-curve, defined by

\[ e(r_d, v_1, v_2, z) \equiv \frac{\ln F_n(v_2, r_d, a) - \ln F_n(v_1, r_d, a)}{v_2^z - v_1^z}, \]

which is negative for \( \nu_n > \nu_{n(M)} \) and positive for \( \nu_n < \nu_{n(M)} \), noting that for \( \nu_n > \nu_{n(M)} \) or in particular \( \nu_n \to +\infty \), from our above results (27, 28), one has: \( z = 2 \). So, for \( \nu_n > \nu_{n(M)} \) the values of exponent \( z = 1, \frac{3}{2}, 1/3 \) and \( \nu_n < \nu_{n(M)} \) those of exponent \( z = 2, 1, \frac{1}{2}, 1/3 \) and \( \frac{1}{4} \) could be considered in next Sections V-VII. Moreover, as \( \nu_n > \nu_{n(M)} \), according to \( e(r_d, v_1, v_2, z = 1) < 0 \), the energy parameter characteristic of \( [-|e| \times \nu_{n(M)}] \) linear exponential tail states of the function \( F_n(v_n, r_d) \) can be defined by

\[ E_{\text{no}}(N, r_d, v_1, v_2) \equiv \frac{E_{\text{no}}(N)}{|e(r_d, v_1, v_2, z = 1)|}, \]

as observed in next Figs. 2, 5, and 8.

It should be noted that the important results (20) obtained for any \( E \)-values, (24) for \( E \geq 0 \), and (28-31) for \( E \leq 0 \), can be used to determine the density of states and the optical,
electrical and thermoelectric functions in Sections V-VIII, respectively.

4. Low Temperature Effect, Due to the Fermi-Dirac Distribution Function

The Fermi-Dirac distribution function (FDDF) is given by

\[
\langle \mathbb{E}^p \rangle_{\text{FDDF}} \equiv G_p(\mathbb{E}_{\text{Fn}}) \times \mathbb{E}_{\text{Fn}}^p \equiv \int_{-\infty}^{\infty} \mathbb{E}^p \times \left( -\frac{\partial f}{\partial \mathbb{E}} \right) \, d\mathbb{E}, \quad -\frac{\partial f}{\partial \mathbb{E}} = \frac{1}{k_B T} \times e^\mathbb{E}_{\text{Fn}}/(1+e^\mathbb{E}_{\text{Fn}})^2.
\]  

(32)

Further, one remarks that, at 0 K, \( -\frac{\partial f}{\partial \mathbb{E}} = \delta(\mathbb{E} - \mathbb{E}_{\text{Fn}}) \), \( \delta(\mathbb{E} - \mathbb{E}_{\text{Fn}}) \) being the Dirac delta (\( \delta \))-function and \( \mathbb{E}_{\text{Fn}} \) is the Fermi energy at \( T=0 \) K defined in Eq. (15). Therefore, \( G_p(\mathbb{E}_{\text{Fn}}) = 1 \).

Then, at low \( T \), by a variable change \( \gamma \equiv (\mathbb{E} - \mathbb{E}_{\text{Fn}})/(k_B T) \), Eq. (32) yields

\[
G_p(\mathbb{E}_{\text{Fn}}) = 1 + \mathbb{E}_{\text{Fn}}^p \times \int_{-\infty}^{\infty} e^\mathbb{E}_{\text{Fn}} \times (k_B T \gamma + \mathbb{E}_{\text{Fn}})^p \, d\gamma = 1 + \mathbb{E}_{\text{Fn}}^p \times \sum_{\mu=1,2,...} C_\mu \times (k_B T)^\mu \times \mathbb{E}_{\text{Fn}}^{-\mu} \times I_\mu,
\]

where \( C_\mu \equiv p(p-1)\ldots(p-\mu+1)/\mu! \) and the integral \( I_\mu \) is given by

\[
I_\mu = \int_{-\infty}^{\infty} \gamma^\mu e^\mathbb{E}_{\text{Fn}} \, d\gamma = \int_{-\infty}^{\infty} \gamma^\mu (e^{T/2} - e^{-\gamma})^\frac{T}{2} \, d\gamma.
\]

(33)

Now, using an identity [15]: \( (1 + e^T) = \sum_{s=0}^{\infty} (-1)^{s+1} s \times e^T(s-1) \), a variable change: \( s \gamma = -t \), the Gamma function: \( \int_{-\infty}^{\infty} t^n e^{-t} \, dt \equiv \Gamma(2n+1) = (2n)! \), and also the definition of the Riemann’s zeta function [15]: \( \zeta(2n) \equiv 2^{2n-1} n 2^{2n} \mid B_{2n} \mid (2n)! \), \( B_{2n} \) being the Bernoulli numbers, one finally gets: \( I_{2n} = (2^{2n} - 2) \times \pi^{2n} \times |B_{2n}| \). So, from (Eq. 32), we get in the degenerate case the following ratio:

\[
G_p(\mathbb{E}_{\text{Fn}}) \equiv \frac{\langle \mathbb{E}^p \rangle_{\text{FDDF}}}{\mathbb{E}_{\text{Fn}}^p} = 1 + \sum_{\mu=1}^{\infty} \frac{p(p-1)\ldots(p-2n+1)}{(2n)!} \times (2^{2n} - 2) \times |B_{2n}| \times \gamma^{2n} \equiv G_p(\mathbb{y}) \equiv y \equiv \frac{\pi k_B T}{\mathbb{E}_{\text{Fn}}} = \frac{\pi k_B T}{\mathbb{E}_{\text{Fn}}},
\]

(34)

It should be noted that our previous expression for \( G_p(x) [58] \) can now be corrected, replacing \( \beta \) by \( 2n \) and the Bernoulli numbers \( B_{2n} \) by \( |B_{2n}| \). Further, Jaffe [49] proposed the following result:

\[
G_p(\text{Jaffe})(\mathbb{E}_{\text{Fn}}, T) = 1 + \mathbb{E}_{\text{Fn}}^p \times \sum_{n=1}^{\infty} (-1)^{2n+1} \times c_{2n} \times (k_B T)^{2n} \times \left( \frac{\mathbb{E}_{\text{Fn}}^2}{\mathbb{E}_{\text{FHo}}^2} \right)^n \equiv G_p(\mathbb{E}_{\text{FHo}}),
\]

(35)

where \( c_{2n} = \frac{(2-2^{2n}) \times 2^{2n} \times |B_{2n}|}{(2n)!} \). Now, using an identity:

\[
\left( \frac{d^2 \mathbb{E}_{\text{FHo}}^2}{d\mathbb{E}_{\text{FHo}}^2} \right)_{\mathbb{E}_{\text{Fn}}} \equiv p(p-1)\ldots(p-2n+1) \times \mathbb{E}_{\text{Fn}}^{-2n}.
\]

Eq. (35) is found to be identical to our above result (34), which is a more practical result. Then, some usual results of \( G_p(\mathbb{y}) \) are given in Table 3.

**Table 3.** The values of absolute Bernoulli numbers \( |B_{2n}|[15] \), and some expressions for \( G_p(\mathbb{y}) \), obtained from Eq. (34) at low \( T \) and for \( p \geq 3/2 \). Here, \( \mathbb{y} = \frac{\mathbb{E}_{\text{FHo}}}{\mathbb{E}_{\text{Fn}}} \equiv \frac{\pi k_B T}{\mathbb{E}_{\text{Fn}}}, \quad \mathbb{y} = \frac{\mathbb{E}_{\text{FHo}}}{\mathbb{E}_{\text{FHo}}} \)

| \( 2n \) | 2 | 4 | 6 | 8 | 10 | 12 |
|---|---|---|---|---|---|---|
| \( |B_{2n}| \) | 1/6 | -1/30 | 1/42 | -1/30 | 5/66 | -69/12730 |

\( G_0(\mathbb{y}) = 1 + \frac{y^2}{8} + \frac{y^4}{440} \), \( G_2(\mathbb{y}) = 1 + \frac{y^2}{2} + \frac{2y^4}{440} \), \( G_4(\mathbb{y}) = 1 + y^2 + \frac{4y^4}{24} + \frac{4y^6}{384} \), \( G_6(\mathbb{y}) = 1 + 2y^2 + \frac{4y^4}{15} + \frac{4y^6}{128} + ... \)

These functions \( G_p(\mathbb{y}) \) obtained in Table 3 will be applied to determine the electrical and thermoelectric properties of the degenerate d-Si systems, being given in Sections 7 and 8, respectively.
5. Determination of Critical Donor Density

In degenerate d-Si systems at T=0 K, due to the heavy doping effect (HDE), using Eq. (20) for a=1, \( \langle E_k \rangle_{KIM} \), the density of states \( \mathcal{D}(\mathcal{E}) \) is given by:

\[
\langle \mathcal{D}(E_k) \rangle_{KIM} = \frac{6c}{2\pi^2} \left( \frac{2m_{\text{HDE}}(N)}{\hbar^2} \right)^{\frac{3}{2}} \times \left( \langle E_k \rangle_{KIM} \right)^{\frac{3}{2}} \times \frac{\exp \left( \frac{-x^2}{2} \right) x W_n^{\frac{1}{2}}}{\sqrt{2\pi}} \times \Gamma \left( \frac{3}{2} \right) \times D_{\frac{1}{2}}(x) = \mathcal{D}(\mathcal{E}),
\]

where \( m_{\text{HDE}}(N) \) is the electron effective mass, due to the HDE, determined in Eq. (8), and the variable \( x \) is defined in Eq. (21), as

\[
x = \frac{-E}{\hbar \omega_n} - \omega_n \times \exp \left( \frac{H_{\text{HDE}}(N)}{4x \sqrt{\omega_n}} \right). \quad A_n = \frac{E_{\text{F0}}}{\omega_n}, \quad \nu_n(N, \mathcal{E}) \equiv -E_{\text{F0}}.
\]

Here, \( E_{\text{F0}} \) is determined in Eq. (15) for \( m^* = m_{\text{HDE}}(N) \), \( m_{\text{HDE}}(N) \) being the electron effective mass due to the HDE and determined in Eq. (8), and the value of Heisenberg empirical parameter \( \H_{n(p)} \) was defined in the Appendix B and proposed here as: \( \H_{n(p)} = 5.4370 \), so that the following determination of the critical density of electrons localized in the exponential conduction-band tail would be accurate. Further, from Eq. (24), one also has

\[
\mathcal{D}(\mathcal{E} \geq 0) = \frac{6c}{2\pi^2} \left( \frac{2m_{\text{HDE}}(N)}{\hbar^2} \right)^{\frac{3}{2}} \times \sqrt{\mathcal{E}}.
\]

Going back to the functions: \( \H_n, K_n \), and \( F_n \), given respectively in Eqs. (26-28), in which the factor \( \frac{\langle E_k \rangle_{KIM}}{E_{\text{F0}}} \) is now replaced by:

\[
\frac{\langle E_k \rangle_{KIM}}{E_{\text{F0}}} = F_n(\nu_n, r_d, a = 1), \quad D_\mathcal{D} = \frac{8c \times (m_{\text{HDE}}^N)^{3/2} \sqrt{\omega_n}}{2\pi^3 \hbar^3}, \quad \beta(a = 1) = \frac{\sqrt{\pi}}{2 \times \Gamma(5/4)},
\]

where the reduced density of exponential-tail states: \( F_n(\nu_n, r_d, a = 1) \equiv F_{n(1)}(\nu_n, r_d) \), for a simplicity of presentation, is determined in Eq. (28). Then, in d-Si systems at 0 K and for \( N = 5 \times 10^{25} \text{ cm}^{-3} \), our results of the functions \( F_{n(1)}(\nu_n, r_d) \) obtained for each \( r_d \)-value, are plotted as functions of \( \nu_n \) in Figure 1.

Figure 1. Our results of \( F_{n(1)} \) increase with increasing \( r_d \) for a given \( \nu_n \), due to the donor-size effect, and present the maxima at \( \nu_n = \nu_{n(1)} \) and go to zero as \( \nu_n \to 0 \) and \( \infty \).
Figure 1 shows that:
(i) our results of $F_n(T)$ increase with increasing $r_d$ for a given $v_n$, due to the donor-size effect, and
(ii) present the maxima at $v_n = v_{n(M)}$ and go to zero as $v_n \to 0$ and $\infty$, being found to be in good agreement with theoretical results obtained by Lifshitz [18], Friedberg and Luttinger [20], our results given in Eq. (A.3) of the Appendix A, and in particular with an asymptotic form for exponential

\[ F_n |_{v_n = v_{n(M)}} \]

For $v_n$, $v_{n(M)}$, and also those of absolute relative errors defined by: $|\langle F_n \rangle | = 1 - \frac{2}{\langle F_n \rangle^2} \langle \Phi_f \rangle$, using the reduced density of state, $|\langle F_n \rangle | = 1 - \frac{2}{\langle F_n \rangle^2} \langle \Phi_f \rangle$.

For $n = 5 \times 10^{28} \text{ cm}^{-3}$, using the reduced density of state, $F_n(v_n, r_d, a = 1)$, determined in Eq. (38), the numerical results of $\ln[F_n(v_n, r_d, a = 1)]$, and its approximate form obtained for $a = 1$: $F_n(v_n, r_d, a = 1)$, determined in Eq. (29), for small $v_n$-intervals: $v_1 \leq v_n \leq v_2$, and those of absolute relative errors defined by: $|\langle F_n \rangle | = 1 - \frac{2}{\langle F_n \rangle^2} \langle \Phi_f \rangle$.

The Theoretical $|\langle F_n \rangle |$-value is the maximal one for each donor-Si system.

Table 4 suggests that: (i) our results of $AF(v_n, r_d, a = 1)$ for given $v_n$, due to the donor-size effect, and (ii) present the maxima at $v_n = v_{n(M)}$ and go to zero as $v_n \to 0$ and $\infty$, being found to be in good agreement with theoretical results obtained by Lifshitz [18], Friedberg and Luttinger [20], our results given in Eq. (A.3) of the Appendix A, and in particular with an asymptotic form for exponential

\[ F_n |_{v_n = v_{n(M)}} \]

For $v_n$, $v_{n(M)}$, and also those of absolute relative errors defined by: $|\langle F_n \rangle | = 1 - \frac{2}{\langle F_n \rangle^2} \langle \Phi_f \rangle$, using the reduced density of state, $F_n(v_n, r_d, a = 1)$, determined in Eq. (38), the numerical results of $\ln[F_n(v_n, r_d, a = 1)]$, and its approximate form obtained for $a = 1$: $F_n(v_n, r_d, a = 1)$, determined in Eq. (29), for small $v_n$-intervals: $v_1 \leq v_n \leq v_2$, and those of absolute relative errors defined by: $|\langle F_n \rangle | = 1 - \frac{2}{\langle F_n \rangle^2} \langle \Phi_f \rangle$. 

Finally, our numerical results of energy parameter, $E_{n0}(N; r_d, a = 1)$, obtained in the small interval: $1.2 \leq v_n \leq 1.25$, using Eq. (31), are plotted as functions of $N$ in Figures 2a and 2b, indicating that, for a given $N$, $E_{n0}$ increases with increasing $r_d$-values, due to the donor-size effect.

The Theoretical $|\langle F_n \rangle |$-value is the maximal one for each donor-Si system.
Our results of energy parameter, $E_{\text{no}}(N; r_d, \alpha = 1)$, are plotted as functions of $N$, indicating that, for a given $N$, $E_{\text{no}}$ increases with increasing $r_d$-values, due to the donor-size effect.

Now, for $E \leq 0$, using Eqs. (27, 28) for the functions $K_n$ and $F_n$ as $\alpha = 1$, the density of electrons localized in the exponential band tail (EBT) is given by

$$N_d^{\text{EBT}}(N, r_d) = \int_{-\infty}^{0} D(E \leq 0) \, dE,$$

where $D(E \leq 0)$ is determined in Eq. (38).
Then, by a variable change: \( \nu_n \equiv -\frac{E}{k_F n_0} \), Eq. (39) yields
\[
N_{E^{d},6}^E (N, r_d) = \frac{g_c \times (m_{H^{d}}^{E})^{3/2}}{2 \pi^{3/2}} \frac{\nu_n \times N_{E^{d}n}}{2 \pi^{3/2}} \times \delta \times \left\{ \int_0^\infty \beta (a = 1) \times F_n (\nu_n, r_d, a = 1) \, d\nu_n + I_n \right\},
\]
where
\[
I_n \equiv \int_0^\infty \beta (a = 1) \times K_n (\nu_n, r_d, a = 1) \, d\nu_n = \int_0^\infty e^{-A_n \nu_n}^2 \times (A_n \nu_n)^{-3/2} \, d\nu_n.
\]
Here, \( \beta (a = 1) = \frac{\sqrt{\gamma}}{2^7 \times \Gamma (5/4)} \) and \( \delta \) is normally equal to 1, but it can be an empirical parameter, being chosen as: \( \delta = \delta_0 = 1.0028637416 \) such that the obtained values of \( N_{E^{d}}^E \) would be accurate.

Then, by another variable change: \( t = \left[ A_n \nu_n / \sqrt{2} \right] \), the integral \( I_n \) yields [15]
\[
I_n = \frac{1}{2^{7/2} A_n} \times \int_0^\infty t^{b-1} e^{-t^2} \, dt \equiv \frac{\Gamma (b, y_n)}{2^{7/2} x A_n}
\]
where \( b = -1/4 \), \( y_n = \left[ 16 A_n / \sqrt{2} \right] \), with \( A_n \) being defined in Eq. (38), and \( \Gamma (b, y_n) \) is the incomplete Gamma function, defined by [15]
\[
\Gamma (b, y_n) \equiv y_n^{b-1} \times e^{-y_n} \left[ 1 + \sum_{i=1}^{\infty} \frac{(b-1)(b-2)\ldots(b-i)}{y_n^i} \right].
\]
Finally, Eq. (40) now yields
\[
N_{E^{d},6}^E (N, r_d) = \frac{g_c \times (m_{H^{d}}^{E})^{3/2}}{2 \pi^{3/2}} \frac{\nu_n \times E_{Fmn}}{2 \pi^{3/2}} \times \delta \times \left\{ \int_0^\infty \beta (a = 1) \times F_n (\nu_n, r_d, a = 1) \, d\nu_n + \frac{\Gamma (b, y_n)}{2^{7/2} x A_n} \right\},
\]
being the density of electrons localized in the exponential conduction-band tail.

Hence, in the degenerate d-Si system, replacing \( N \), given in the parabolic conduction band of an effective electron gas, by the effective density of free electrons defined here by: \( N^* = N - N_{E^{d},6}^E \geq 0 \). So, in this system, the Fermi energy given in Eq. (15) is now rewritten as
\[
E_{Fmn} (N^*) \equiv \frac{\gamma \times k_F \nu_n (N^*)}{2 \pi^{3/2} n_{H^{d}}^{E}} \times \Delta \times \left\{ \int_0^\infty \beta (a = 1) \times F_n (\nu_n, r_d, a = 1) \, d\nu_n + \frac{\Gamma (b, y_n)}{2^{7/2} x A_n} \right\},
\]
where the Fermi wave number \( k_F = \text{constant} \) and \( m_{H^{d}}^{E} \) are respectively determined in Eqs. (2, 8). One notes here that \( E_{Fmn} (N^*) \) vanishes at \( N^* = 0 \), or at the critical donor density defined by: \( N = N_{c(d),6}^E \equiv N_{E^{d},6}^E (N = N_{c(d),6}, r_d, r_d) \), at which the metal-insulator transition thus occurs. Then, the numerical results of \( N_{c(d),6}^E \), for \( \delta = 1 \) and \( \delta_0 = 1.0028637416 \), and their absolute relative errors \( \text{[RE]} \), calculated using the \( E_{Fmn} (N^*) \)-data given in Table I, are obtained and also reported in this Table 1, indicating that those of \( N_{c(d),6}^E \) and \( N_{c(d),1}^E \) are obtained respectively with accuracies of the orders of \( 1.1 \times 10^{-4} \) and \( 3 \times 10^{-3} \). Hence, these results of \( N_{c(d),6}^E \) thus confirm our above choice of Heisenberg parameter value: \( H_n = 5.4370 \), as that proposed in Eq. (19) and also in the Appendix B. Furthermore, our numerical calculation indicates that, in all the d-Si systems for \( N \geq 1.15 \times N_{c(d)} \), if defining the absolute relative deviations between \( N - N_{E^{d},6}^E \) and \( N_{c(d)} \) by: \( |\text{RD}| \equiv \left| 1 - \frac{N_{E^{d},6}^E}{N_{c(d)}^E} \right| \), the maximal \( |\text{RD}| \)-values, which occur at \( N = 1.15 \times N_{c(d)} \), are approximately equal to 3.2%. So, \( N^* \) given in the parabolic conduction band of the degenerate d-Si systems can be approximated by [22]
\[
N^* = N - N_{c(d),6}^E \approx N - N_{c(d)}^E.
\]

Here, this notion of effective density of free electrons \( N^* \) defined by Eq. (43) should be equivalent to that of \( (N_d - N_a) \) given in the n-type compensated Si, in which \( N_d \) is the total density of donors (or majority electrons) and \( N_a \) is the total density of acceptors (or minority holes), assuming that all the impurities are ionized [22]. Finally, in degenerate d-Si systems, in which \( N > N_{c(d)} \) and \( T \leq 77 K \) or \( T < T_D \), \( T_D \) being the degeneracy temperature defined in Eq. (15), this result (43) will be used in all the following Sections.

6. Optical Properties

The problem of exponential optical absorption-coefficient tails has by now a rather long history. We will limit our study here to the degenerate d-Si systems, although the band structure of random alloys and amorphous materials is a problem with many common features [41].

Optical properties of any medium can be described by the complex refraction index \( n \) and the complex dielectric function \( \varepsilon \), defined by: \( n \equiv n - i \kappa \) and \( \varepsilon \equiv \varepsilon_1 - i \varepsilon_2 \), where \( \kappa^2 = -1 \) and \( \varepsilon \equiv \varepsilon_2 ^2 \), and by the optical absorption coefficient \( \alpha \), which is related to the imaginary part of \( \varepsilon_2 \), the refraction index \( n \), the extinction coefficient \( k \), and the conductivity \( \sigma_0 \), due to the electro-optical effect, as [29-48]
\[
\alpha (E) \equiv \frac{h \nu |\text{ev}(E)|^2}{m(E) \times \varepsilon_0 \times c} \times (E) = \frac{E \times \varepsilon_0 (E)}{h c} = 2 \times \varepsilon_0 (E) = 4 \times \pi \times \varepsilon_0 (E) = 4 \times \pi \times \varepsilon_0 (E). \quad (44)
\]
One remarks that the real part of $\varepsilon$ is defined by
\[ \varepsilon_1(E) \equiv n(E)^2 - \kappa(E)^2, \tag{45} \]
and the normal-incidence reflectance $R(E)$, by
\[ R(E) = \frac{[n(E) - 1]^2 + \kappa(E)^2}{[n(E) + 1]^2 + \kappa(E)^2}, \tag{46} \]
which are the optical dispersion relations since in general the values of those optical functions are expressed as functions of the multi-photon energy [46], $E \equiv \hbar \omega$, $2\hbar \omega$, $3\hbar \omega$, $4\hbar \omega$, .... In the present work, we only focus our attention to the case of photon energy $E \equiv \hbar \omega$. Here, $-q$, $h$, $[v(E)]$, $\omega$, $\varepsilon_a$, $c$, $|v(E)|$, respectively represent the electron charge, Dirac's constant, matrix elements of the velocity operator between valence- and conduction bands in $n$-type semiconductors, photon frequency, permittivity of free space, velocity of light, and joint density of states (JDOS). One remarks here that: (i) if some optical functions are known such as: $(J, n, a=1, 2, 5/2, 7/2$ and $9/2$ correspond to the allowed-direct [29-31], the result (49) is reduced to Eq. (48). Here, the values of $0.171 \times m_0^a$, $m_0^a$, are determined respectively in Eqs. (3, 10, 11), we can now determine the extinction coefficient $\kappa$, defined in Eq. (1), as $\kappa(E, a=1, 2, 5/2, 7/2$ and $9/2$, respectively.

Further, for any $E$ or $\varepsilon_a$, using Eq. (20), Eq. (48) becomes
\[ \alpha(E \geq \varepsilon_{gn}) \equiv \frac{n_a^2 \times |v(E)|^2}{n(E) \times \varepsilon_a \times \hbar^2} \times \alpha \left( \frac{2\varepsilon_a}{\hbar^2} \right) \times \frac{1}{\varepsilon_{fp}} \times (\varepsilon - \varepsilon_{gn})^{s+a-1}, \tag{49} \]
where $x$ is defined in Eq. (21), as $x = \frac{-\varepsilon}{\sqrt{\varepsilon_n}} \equiv A_n \times \varepsilon_n$, then, all other ones are determined, and (ii) in $n$-type semiconductor, $\kappa(E \geq \varepsilon_{gn}, a=1, 2, 5/2, 7/2$ and $9/2$, respectively.

Then, one also remarks that:
(i) when $a=1$, according to allowed direct transitions for $n$-type (GaAs, GaSb, InP, InAs and InSb)-semiconductors [31], $\kappa(E \geq \varepsilon_{gn}, a=1)$, being thus expressed in terms of $(E - \varepsilon_{gn})^{1/2}$, is identical to those obtained by Lukes et Somaratna [29], and Van Cong [30], and
(ii) when $a=5/2$, according to allowed indirect transitions for $n$-type (Si, Ge and GaP)-semiconductors [31], $\kappa(E \geq \varepsilon_{gn}, a=5/2)$ is now expressed in terms of $(E - \varepsilon_{gn})^2$.

In 1984, Forouhi- Bloomer (FB) [40] proposed in his FB-method (FB-M) a familiar four-term expression for extinction coefficient, $\kappa(E, 5/2)$, expressed in terms of $(E - \varepsilon_{gn})^2$ for both direct-and-indirect bandgap semiconductors, being thus correct only in indirect band-gap ones. Further, their result is not correct when $E \rightarrow \infty$. Hence, one must have: $\kappa(E \rightarrow \infty) \rightarrow 0$ [36, 41]. Furthermore, in the d-Si systems, from Eqs. (44, 48) one can determine the extinction coefficient $\kappa$, obtained for $a=5/2$, as
\[ \kappa(E \geq \varepsilon_{gn}) \equiv \frac{q^2 \times m_n^a}{2 \times \pi^2 \times \hbar^2} \times \varepsilon_{fp}^{n_a} \times (\varepsilon - \varepsilon_{gn})^{s+a-1}, \tag{50} \]

We now propose an improved FB-M (IFB-M).

First, if putting $F(E) \equiv \sum_{i=1}^{4} A_i(\varepsilon_{FB}) \times \frac{E^2}{\varepsilon_{FB}^2 - B_{i(\varepsilon_{FB})} \times C_{i(\varepsilon_{FB})}}$, where the values of empirical parameters: $A_i(\varepsilon_{FB})$, $B_{i(\varepsilon_{FB})}$ and $C_{i(\varepsilon_{FB})}$, are given in the FB-M for the Si [40], and simply replacing the band-gap energy $E_g = 1.06 \text{ eV}$ [40] by $E_{\text{gn}}$, which can be equal to: $\varepsilon_{gn1}$ and $\varepsilon_{gn2}$, which are determined respectively in Eqs. (3, 10, 11), we can now propose, as that done by O’Leary et al. for very large values of $E$, [39]
for our IFB-M, we can further propose

\[ \kappa_{\text{IFB-M}}(E \geq E_{\text{gn}}) = f(E) \times \frac{(E-E_{\text{gn}})^2}{E^2} \times \left(\frac{6 \text{ eV}}{E}\right)^2, \]

for \( E \geq 6 \text{ eV} \), so that \( \kappa_{\text{IFB-M}}(E \to \infty) \) goes to 0 as \( E^{-3} \), in good accordance with both experimental [36] and theoretical [41] results.

Secondly, by putting

\[ \Delta n(E, A_i(\text{FB}), B_i(\text{FB}), C_i(\text{FB}), E_{\text{gn}}) = \sum_{i=1}^{4} \frac{B_iE + C_iO}{E^2 - B_i(E) + C_i(O)} = \Delta n, \]

for a simplicity of presentation, where the empirical parameters, \( B_i(O), B_i(FB), C_i(O), C_i(FB), E_{\text{gn}} \), are determined respectively in the FB-M [40], in which we now replace \( E_g = 1.06 \text{ eV} \) by \( E_{\text{gn}} \) for our IFB-M, we can further propose

\[ n_{\text{IFB-M}}(E) = n_{\infty} + n_o \times \Delta n, \text{ for } E \geq 6 \text{ eV}, \]

so that \( n_{\text{IFB-M}}(E \to \infty) \to \sqrt{E_{\infty}} \), where the values of \( n_{\infty} \) are given in Table I, giving a correct asymptotic behavior of \( n_{\text{IFB-M}}(E) \). Here, \( n_o \) is the factor to be determined so that the function \( n_{\text{IFB-M}}(E) \) for \( E \geq 6 \text{ eV} \) is continuous at \( E = 6 \text{ eV} \), depending on \( T, r_d, \) and \( N \).

For example, in intrinsic d-Si systems at 298 K, in which \( E_{\text{gn}} = E_{\text{gl}}(T = 298 \text{ K}, r_d) = 1.125 \text{ eV} \) is determined in Eq. (3), the values of \( n_o(r_d) \) are evaluated and tabulated in Table 5.

**Table 5.** In intrinsic donor-Si systems at 298 K, the numerical results of Factor \( n_o(r_d) \), being due to the donor-size effect and expressed as functions of donor-radius \( r_d \), are determined so that the function \( n_{\text{IFB-M}}(E) \) given in Eq. (52) for \( E \geq 6 \text{ eV} \) is continuous at \( E = 6 \text{ eV} \).

| Donor | Sb | P | As | Bi | Ti | Te | Se | S |
|-------|----|---|----|----|----|----|----|---|
| \( n_o(r_d) \) | 2.571289 | 2.482479 | 2.032121 | 1.944450 | 1.290620 | 0.805033 | 0.384780 |

As noted in Eqs. (44-46), if from Eqs. (51, 52) the values of \( \kappa_{\text{IFB-M}}(E) \) and \( n_{\text{IFB-M}}(E) \) are evaluated, all other optical functions can thus be determined. So, at 298 K and \( 1.5 \leq E(\text{eV}) \leq 6 \), in the intrinsic P-Si systems, in which \( E_{\text{gn}} = E_{\text{gl}}(T = 298 \text{ K}, r_d) = 1.125 \text{ eV} \) is evaluated using Eq. (3), our results of all the optical functions and the corresponding ones obtained from the FB-M, and the absolute errors of those, calculated using the optical-function data obtained by Aspnes and Studna [33], are tabulated in the Table 6.

**Table 6.** In intrinsic P-Si systems at 298 K and for \( 1.5 \leq E(\text{eV}) \leq 6 \), our numerical results of all the optical functions (OF) are calculated, using Eqs. (44-46, 51, 52) obtained in our IFB-M, and using the OF-data obtained by Aspnes and Studna [33], their absolute maximal relative errors ([MREs]) determined at the photon energy \( E(\text{eV}) \) are also evaluated and tabulated in this Table, in which the corresponding [MREs] obtained in FB-M are also included.

| MRE | \( E(\text{eV}) \) | \( \epsilon_2\text{-MRE} \) | \( \epsilon_3\text{-MRE} \) | \( n\text{-MRE} \) | \( \kappa\text{-MRE} \) | \( R\text{-MRE} \) | \( \alpha\text{-MRE} \) |
|-----|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| FB-M | 1.5 | 2.2 | 4.2 | 5.0 | 0.66 | 0.57 | 0.58 | 0.58 |
| \( n_o = 1.95, E_{\text{gn}} = 1.06 \text{ eV} \) | 2.2 | 4.2 | 5.0 | 0.66 | 0.57 | 0.58 | 0.58 |
| Our IFB-M | 1.5 | 4.2 | 5.0 | 0.66 | 0.57 | 0.58 | 0.58 |
| \( n_o = \sqrt{11.4}, E_{\text{gl}} = 1.125 \text{ eV} \) | 2.6 | 4.3 | 5.0 | 0.66 | 0.57 | 0.58 | 0.58 |

The underlined [MRE]-value is the maximal one for each optical function.

Table 6 indicates that our results in our IFB-M are found to be more accurate than those obtained in the FB-M. Further, our numerical calculation indicates that, for a given \( E \), since \( \kappa_{\text{IFB-M}}(E) \) given in Eq. (51) is expressed in terms of \( (E - E_{\text{gn}})^2 \), if \( E_{\text{gn}} \) increases (decreases), then other functions such as: \( (E - E_{\text{gn}})^2 \), \( \kappa_{\text{IFB-M}}(E) \), \( \epsilon_2(\text{IFB-M}) \) and \( \epsilon_3(\text{IFB-M}) \) decrease (increase), respectively. This useful remark will be used in our IFB-M to explain all the following results.

In the intrinsic P-Si system, \( E_{\text{gn}} = E_{\text{gl}}(T, r_p) \), calculated from Eq. (3), decreases with increasing \( T \). So, for a given \( E \), our results of \( (E - E_{\text{gn}}(T, r_p))^2 \) and \( \epsilon_3(\text{IFB-M}) \), obtained in absolute values, increase with increasing \( T \), in good...
accordance with experimental results [32, 38, 44, 48], as observed in the following Figure 3a.

In intrinsic donor-Si systems, \( E_{\text{gn}} \equiv E_{\text{g0}}(r_0, T = 298 \, \text{K}) \), calculated from Eq. (3), increases with increasing \( r_0 \), as seen in Table 1. Thus, for a given \( E \), our results of \( \varepsilon_1(\text{IBF-M})(E) \) in absolute values, increase with increasing \( q_1 \).

In degenerate P-Si systems, \( E_{\text{g0}} \equiv E_{\text{g0}}(r_0, T = 298 \, \text{K})^2 \) and \( E_{\text{g1}}(\text{IBF-M})(E) \), in absolute values, decrease with increasing \( r_0 \), as observed in the following Figure 3b, in which we also observe the correct asymptotic results: \( \varepsilon_1(\text{IBF-M})(E \to \infty) \to \varepsilon_n \), being identical to the values of \( \varepsilon_n \) given in Table 1, and \( \varepsilon_2(\text{IBF-M})(E \to \infty) \to 0 \).

So, for a given \( E \), the absolute values of \( [E - E_{\text{gn1}}(N)]^2 \) and \( \varepsilon_1(\text{IBF-M})(E) \) decrease with increasing \( N \), in good accordance with experiments by Aspnes et al. [34], and Vina and Cardona [35], as seen in the following Figure 3c.

Finally, in degenerate P-Si systems, in which \( E_{\text{gn}} \equiv E_{\text{gn2}}(N) \), being the reduced band gap determined in Eq. (10), decreases with increasing \( N \), due to the heavy-doping effect. Consequently, for a given \( E \), the absolute values of \( [E - E_{\text{gn2}}(N)]^2 \) and \( E_{\text{g1}}(\text{IBF-M})(E) \) increase with increasing \( N \).

Now, identifying our above results (50, 51) and using Eq. (52), we can propose an useful expression for \(|\nu(E)|^2\) as

\[
|\nu(E)|^2 = \sqrt{\frac{2}{\pi} A \times n_{\text{IBF-M}}(E)} \times \frac{F_{\text{IBF-M}}(E)}{q^2 \times m^*} \times \frac{1}{E} , \text{ for } E \geq 6 \, \text{eV} \],
\[
= \sqrt{\frac{2}{\pi} A \times n_{\text{IBF-M}}(E)} \times \frac{F_{\text{IBF-M}}(E)}{q^2 \times m^*} \times \frac{1}{E} , \text{ for } E_{\text{gn}} \leq E \leq 6 \, \text{eV} \],
\[
= \frac{\sqrt{2}}{\pi} A \times n_{\text{IBF-M}}(E) \times \frac{F_{\text{IBF-M}}(E)}{q^2 \times m^*} \times \frac{1}{E} , \text{ for } E \leq E_{\text{gn}} \text{ or for } \ E \leq 0. \quad (53)
\]

6.2. Behaviors of Optical Functions Obtained for \( E \leq E_{\text{gn}} \) or \( E \leq 0 \)

Here, going back to the functions: \( H_n \), \( K_n \), and \( F_n \), given respectively in Eqs. (26-28) for \( a=5/2 \), in which the factor \( (\frac{E}{E_{\text{g0}}})^{(a=5/2)} \) is now replaced by: \( (\frac{E}{E_{\text{g0}}})^{(a=5/2)} = \alpha(E_{\text{g0}}) = F_n(\nu, r_0, a = 5/2) \equiv F_n^{(5/2)}(\nu, r_0, a = 5/2) \) calculated using Eq. (28), for a simplicity of presentation, \( \alpha(E_{\text{g0}}) = \alpha(E_{\text{g0}}) \) being determined from Eqs. (26, 49, 53) as: \( \alpha(E_{\text{g0}}) = \frac{\alpha(E_{\text{g0}})}{\alpha(E_{\text{g0}})} \), then our numerical results of reduced optical absorption coefficient given in degenerate P-Si systems at 0 K and for \( N = 5 \times 10^{20} \, \text{cm}^{-3} \), \( F_n^{(5/2)}(\nu, r_0) \), are plotted in Figure 4, as functions of \( \nu_n \).
Figure 4. Our results of $F_{n_{d}}$ increase with increasing $r_{d}$ for a given $v_{n}$, due to the donor-size effect, and present the maxima at $v_{n} = v_{n(m)}$ and go to zero as $v_{n} \rightarrow 0$ and $\infty$.

Table 7. In the d-Si systems at $T=0$ K and for $N = 5 \times 10^{20}$ cm$^{-3}$, our numerical results of $\ln[F_{n}(v_{n}, r_{d}, a = 5/2)]$ and its approximate form for $a = 5/2$. $AF(v_{n}, r_{d}, v_{1}, v_{2}, z, f) = e(v_{n}, v_{1}, v_{2}, z) \times v_{n}^2 + f$, determined in Eqs. (29, 30) for small $v_{n}$-intervals: $v_{1} \leq v_{n} \leq v_{2}$, and those of absolute relative errors defined by $|RE| = 1 - \frac{AF(v_{n}, r_{d}, v_{1}, v_{2}, z, f)}{AF_{0}(v_{n}, r_{d}, v_{1}, v_{2}, z, f)}$ are calculated and tabulated below.

| Donor | Sb | P | As | Bi | Te | Se | S |
|-------|----|---|----|----|----|----|---|
| $v_{n(m)}$ | 0.20000 | 0.23000 | 0.25100 | 0.25000 | 0.36930 | 0.50457 | 0.63809 | 0.65575 |
| For $1.20 \leq v_{n} \leq 1.25$, $AF = (e \times v_{n} + f)$ is accurate to within $1.5 \times 10^{-4}$, where |
| $e$ | 41.048 | 37.467 | 22.309 | 19.884 | 6.959 | 2.089 | 1.025 | 1.344 |
| $f$ | -8.071 | 7.066 | 0.610 | -0.268 | -3.580 | -3.690 | -3.498 | -3.476 |
| $|RE| | 1.5 \times 10^{-4} | 9.5 \times 10^{-5} | 1.4 \times 10^{-4} | 8.4 \times 10^{-5} | 7.7 \times 10^{-5} | 9.4 \times 10^{-5} | 7.2 \times 10^{-5} | 7.7 \times 10^{-5} |
| For $1.10 \leq v_{n} \leq 1.20$, $AF = (e \times v_{n}^{1/2} + f)$ is accurate to within $7.8 \times 10^{-4}$, where |
| $e$ | 83.727 | 76.598 | 45.797 | 40.849 | 14.399 | 5.729 | 2.905 | 2.672 |
| $f$ | 51.300 | 46.035 | 24.020 | 20.630 | 3.803 | -0.784 | -2.061 | -2.161 |
| $|RE| | 7.8 \times 10^{-4} | 7.0 \times 10^{-4} | 5.8 \times 10^{-4} | 5.6 \times 10^{-4} | 3.9 \times 10^{-4} | 3.1 \times 10^{-4} | 2.7 \times 10^{-4} | 2.4 \times 10^{-4} |
| For $1.07 \leq v_{n} \leq 1.09$, $AF = (e \times v_{n}^{1/3} + f)$ is accurate to within $6.7 \times 10^{-5}$, where |
| $e$ | 117.594 | 107.704 | 64.640 | 57.691 | 20.350 | 8.001 | 3.950 | 3.614 |
| $f$ | 84.856 | 76.863 | 42.706 | 37.332 | 9.706 | 1.466 | -1.031 | -1.233 |
| $|RE| | 4.0 \times 10^{-5} | 4.4 \times 10^{-5} | 3.6 \times 10^{-5} | 2.7 \times 10^{-5} | 5.6 \times 10^{-5} | 6.7 \times 10^{-5} | 1.1 \times 10^{-4} | 1.5 \times 10^{-5} |
| For $v_{n(M)} < 1.00 \leq v_{n} \leq 1.05$, $AF = (e \times v_{n}^{1/4} + f)$ is accurate to within $2.5 \times 10^{-4}$, where |
| $e$ | 146.037 | 133.830 | 80.538 | 71.909 | 25.343 | 9.835 | 4.719 | 4.294 |
| $f$ | 113.151 | 102.853 | 58.526 | 51.481 | 14.674 | 3.288 | -0.269 | -0.561 |
| $|RE| | 2.5 \times 10^{-4} | 2.5 \times 10^{-4} | 2.1 \times 10^{-4} | 2.0 \times 10^{-4} | 1.4 \times 10^{-4} | 1.3 \times 10^{-4} | 1.7 \times 10^{-4} | 7.5 \times 10^{-5} |
| For $0.090 \leq v_{n} \leq 0.095 < v_{n(M)}$, $AF = (e \times v_{n}^{1/5} + f)$ is accurate to within $2.5 \times 10^{-4}$, where |
| $e$ | 61.911 | 64.563 | 73.471 | 73.821 | 58.071 | 40.661 | 33.954 | 33.436 |
| $f$ | -51.196 | -52.643 | -56.888 | -56.805 | -44.514 | -32.149 | -27.297 | -26.916 |
| $|RE| | 2.3 \times 10^{-4} | 2.1 \times 10^{-4} | 2.5 \times 10^{-4} | 2.5 \times 10^{-4} | 2.4 \times 10^{-4} | 1.6 \times 10^{-4} | 1.6 \times 10^{-4} | 1.6 \times 10^{-4} |
| For $0.088 \leq v_{n} \leq 0.090$, $AF = (e \times v_{n}^{1/5} + f)$ is accurate to within $7.8 \times 10^{-5}$, where |
| $e$ | 61.933 | 64.532 | 73.219 | 73.525 | 57.271 | 39.554 | 32.765 | 32.240 |
| $f$ | -45.044 | -46.203 | -49.462 | -49.324 | -38.375 | -27.605 | -23.384 | -23.052 |
| $|RE| | 4.7 \times 10^{-5} | 5.4 \times 10^{-5} | 6.8 \times 10^{-5} | 5.6 \times 10^{-5} | 7.5 \times 10^{-5} | 3.6 \times 10^{-5} | 4.3 \times 10^{-5} | 7.8 \times 10^{-5} |
| For $0.080 \leq v_{n} \leq 0.083$, $AF = (e \times v_{n}^{1/5} + f)$ is accurate to within $1.5 \times 10^{-4}$, where.
Table 7 suggests that: (i) our results of \(AF(v_n, r_d, \nu_e, \nu_g, z, f)\) given for \((z=1)\)-exponent agree with the Urbach law obtained from linear exponential conduction-tail-behaviors by some workers [21, 29, 30, 37], (ii) ours for \((z=1/2)\)-exponent and \(v_n > v_n(M)\) agree with other theoretical results [19, 37], and finally (iii) ours for \((z=1/3, 1/4)\)-exponents when \(v_n > v_n(M)\), and for \((z=1/4, 1/3, 1/2, 1, 2)\)-exponents when \(v_n < v_n(M)\) may thus be new.

Finally, our numerical results of energy parameter, \(E_{no}(N; r_d, a = 5/2)\), obtained in the small interval: \(1.2 \leq v_n \leq 1.25\), using Eq. (31), are plotted as functions of \(N\) in Figures 5a and 5b, indicating that, for a given \(N\), \(E_{no}\) increases with increasing \(r_d\)-values, due to the donor-size effect.

### 7. Electrical Properties

Here, \(m^* = m_{\text{cond}} = 0.26 \times m_0\). Then, the electrical functions, obtained in the two cases: \(\mathbb{E} \geq 0\) and \(\mathbb{E} \leq 0\), will be considered as follows.

#### 7.1. Electrical Functions Obtained as \(\mathbb{E} \geq 0\)

In the effective electron gas at 0 K [66], denoting the relaxation time by \(\tau\), the mobility is defined by

\[\mu \equiv \frac{A|\tau|}{m_{\text{cond}}},\]  

the conductivity \(\sigma\) (or resistivity \(\rho \equiv 1/\sigma\)), given in the Drude model, by
\[ \sigma \equiv q \times N \times \mu = q^2 \times N \times \frac{\tau}{m_{\text{cond}}}, \]  
(55)

the Hall conductivity \( \sigma_H \), by

\[ \sigma_H \equiv -\sigma \times \mu = -\frac{q^2 \times N \times \tau}{(m_{\text{cond}})^2} < 0, \]  
(56)

and finally, from Eqs. (55, 56), the Hall coefficient at 0 K, by

\[ R_H(0) \equiv \frac{\sigma_H}{\langle \sigma \rangle^2} = -\frac{1}{N\times q} \times \frac{\langle \tau^2 \rangle}{\langle \tau \rangle^2} < 0, \]  
(57)

This result (57) is not correct for the degenerate donor (d)-Si systems at low temperatures, where \( N \) may be replaced by the total effective density of free electrons given in the conduction band, \( N' = N - N_c(d) \), as that given in Eq. (43), in which the values of critical donor density \( N_c(d) \) are given in Table I. In those degenerate d-Si systems, the relaxation time can be defined by

\[ \frac{1}{\langle \tau(k) \rangle} = N' \times \frac{\hbar}{m_{\text{cond}}} \times \pi(C \times k)^{-2} \times \prod_{i=1}^{\infty} x_i, \]  
(58)

where \( \hbar/(m_{\text{cond}} \times m) \) is the electron velocity, \( C \) is an empirical parameter, \( (C \times k)^{-2} \) is the scattering cross section, and finally the factors \( x_i \) are included to represent the high donor-density conditions when \( k = k_{\text{Fn}} \), as those given in Eq. (14), such that \( \frac{1}{\langle \tau(k_{\text{Fn}}) \rangle} < 1 \).

We now report and discuss the results of \( \tau \), being obtained by Van Cong and Mesnard method (VCMM) [58] and also by Yussouff and Zittarz [59], as follows.

By a Green function (G)-method, assuming that the Gaussian ensemble average of GG as: \( \langle GG \rangle \equiv \langle G \rangle \times \langle G \rangle + \Delta G \approx (G) \times (G) \), Van Cong and Mesnard obtained [58]

\[ \frac{1}{\langle \tau(k_{\text{Fn}}) \rangle} = N' \times \frac{\hbar k_{\text{Fn}}}{m_{\text{cond}}} \times \pi \left( \frac{4\pi}{\hbar^2} \times k_{\text{Fn}} \right)^{-2} \times \frac{\eta_n}{E_{\text{Fn}}} < 1, \]  
(59)

where \( \mu_{\text{VCMM}} \) and \( \sigma_{\text{VCMM}} \) are respectively determined in Eqs. (60, 61) and the function \( G_1(y) \) is given in Table III, with \( y = \frac{\pi k_{\text{Fn}} T}{E_{\text{Fn}}} \equiv \frac{\pi k_{\text{Fn}} T}{E_{\text{Fn}}} \), noting that \( G_1(y) = 1 \).

Further, the Hall coefficient is defined by

\[ R_H(\text{PVCMM})(N', T, r_d) \equiv \frac{\langle \sigma_{\text{PVCMM}} \rangle \times \langle \mu_{\text{PVCMM}} \rangle}{\langle \sigma_{\text{PVCMM}} \rangle^2} = -\frac{1}{N\times q} \times \frac{\langle \tau^2 \rangle}{\langle \tau \rangle^2} < 0, \]  
(60)

where the Hall factor is found to be given by

\[ \frac{\langle \sigma \rangle}{\langle \mu \rangle} \equiv \frac{\langle \tau^2 \rangle}{\langle \tau \rangle^2} = \frac{G_1(y)+\Delta_{\text{PVCMM}}G_2(y)}{G_1(y)+\Delta_{\text{PVCMM}}G_2(y)} \times \frac{G_1(y)+\Delta_{\text{PVCMM}}G_2(y)}{G_1(y)+\Delta_{\text{PVCMM}}G_2(y)}. \]  
(64)

Furthermore, the Hall mobility is given by

\[ \mu_{\text{HPVCMM}}(N', T, r_d) = \mu_{\text{PVCMM}} \times r_{H(\text{PVCMM})}. \]  
(66)

We now propose our present method (PM) to determine all the electrical functions as follows.

First of all, one remarks that in Section 6 all the optical functions, given in Eq. (44) and obtained in d-Si systems, are found to be proportional to \( E^0 \) or to \( E^0_{\text{Fn}} \), as \( E = E_{\text{Fn}} \). Then, in the PM, we propose both principal parts of \( \mu \) and \( \sigma \), being

\[ \mu_{\text{PM}} = \frac{4}{3\sqrt{3}} \times \frac{q^2 k_{\text{Fn}}}{N'h} \times \frac{E_{\text{Fn}}}{\eta_n}, \]  
(60)

\[ \sigma_{\text{PM}} = \frac{4}{3\sqrt{3}} \times \frac{q^2 k_{\text{Fn}}}{h} \times \frac{E_{\text{Fn}}}{\eta_n}, \]  
(61)

which is proportional to \( E^0_{\text{Fn}} \), where the Fermi energy \( E_{\text{Fn}}(N') \) is determined in Eq. (42).
found to be proportional to $E_{F\text{no}}^2$. Further, using now the total correction given by:

$$\Delta_{PM} = 0.04 \times \frac{k_F^3}{k_{\text{F}n}} + 0.2 \times \frac{k_F^3}{\sqrt{\sigma (r_d, \rho_{\text{cond}})}} - 0.03 \times \frac{\eta_n}{E_{F\text{no}}}$$

which is proportional to $E_{F\text{no}}^{-1/2}$,

$$\mu_{PM}(N', T, r_d) \approx \frac{(0.85)^2}{\pi} \times \frac{q^2 \epsilon_{F\text{no}}}{\hbar N} \sqrt{\eta_n} \times \frac{1}{E_{F\text{no}}} \times \frac{k_F^3}{\sqrt{k_{\text{F}n}}}$$

where $(0.85)^2$ is the empirical parameter chosen to minimize the absolute deviations between the numerical results of $\mu_{PM}$ and the corresponding $\mu$-data, and the functions $G_2(y)$ and $G_2'(y)$ are given in Table III. Then, the expression for electrical conductivity is given by

$$\sigma_{PM}(N', T, r_d) = \sigma_0(\mu_{F\text{no}}) \times \left\{G_2'(y) + \Delta_{PM} \times G_2'(y)\right\}.$$  

(68)

where $\sigma_0(\mu_{F\text{no}}) = \frac{(0.85)^2}{\pi} \times \frac{q^2 \epsilon_{F\text{no}}}{\hbar N} \times \frac{1}{E_{F\text{no}}} \times \frac{k_F^3}{\sqrt{k_{\text{F}n}}}$, being proportional to $E_{F\text{no}}^{-2}$.

Further, the Hall coefficient is defined by

$$R_{H}(N', T, r_d) \equiv \frac{-\langle\sigma_{PM} \times \mu_{PM}\rangle}{\langle\sigma_{PM}\rangle^2} = -\frac{1}{N' \times q} \times r_{H}(PM) < 0.$$  

(69)

where the Hall factor is given by

$$r_{H}(PM)(N', T, r_d) \equiv \frac{(r_j^2)}{(n^2)} \times \frac{G_2'(y) + \Delta_{PM} \times G_2'(y)}{[G_2'(y) + \Delta_{PM} \times G_2'(y)]^2}.$$  

(70)

Furthermore, the Hall mobility yields

$$\mu_{H}(PM)(N', T, r_d) = \mu_{PM} \times r_{H}(PM).$$  

(71)

Our numerical calculation indicates that in degenerate d-Si systems the $r_H$-behaviors obtained in PVCMM and PM, using Eqs. (65, 70), are almost the same. So, in the PM, our numerical results of Hall factors $r_H$ obtained in various d-Si systems at 77 K, using Eq. (70), are plotted as functions of $N$ in Figures 6a and 6b.

and also using our result (34) for $G_p(\epsilon_{F\text{no}}) \equiv \langle\epsilon F_{\text{FDDF}}\rangle_{\parallel}$ given for $p=2$ and $p=3/2$, we propose the expression for electron mobility, obtained for $p=2$ and $p=3/2$ as

$$\mu_{PM}(N', T, r_d) \approx \left\{G_2(y) + \Delta_{PM} \times G_2'(y)\right\}.$$  

(67)

Figures 6. In the PM, our results of Hall factors $r_H$ obtained in various d-Si systems are plotted as functions of $N$, decreasing with increasing $N$, increasing with increasing $r_d$ for a given $N$, and tend towards 1 at very high $N$.

Figures 6a and 6b indicate that those results of $r_H$ are positive, decrease with increasing $N$, increase with increasing $r_d$ for a given $N$, and tend towards 1 at very high values of $N$, in good agreement with the result obtained in an effective electron gas [66].

Then, in particular, in the As-Si system at $T=10$ K and for $N = 2.7 \times 10^{19}$ cm$^{-3}$, the numerical results of Hall coefficient, $|R_H(N')|$, where $N' \equiv N - N_{c(\text{As})}$, $N_{c(\text{As})} = 8.58 \times 10^{18}$ cm$^{-3}$, and Hall mobility, $\mu_{H}(N')$, obtained using Eqs. (64, 66) for the PVCMM, and Eqs. (69, 71) for the PM, and their absolute relative errors, $|\text{REs}|$, calculated using the corresponding data obtained by Morin and Maita [50], are tabulated in Table 8.

Table 8. In the As-Si system at $T=10$ K and for $N = 2.7 \times 10^{19}$ cm$^{-3}$, the numerical results of Hall mobility $\mu_{H}(N')$ and Hall coefficient $|R_H(N')|$, obtained in the PM and PVCMM, and their absolute relative errors, $|\text{REs}|$, calculated using the corresponding data obtained by Morin and Maita [50], $\mu_{H}(\text{data}) = 155 (\text{cm}^2/\text{V}\cdot\text{s})$ and $|R_H(\text{data})| = 0.33 (\text{cm}^2/\text{V}\cdot\text{s})$, are calculated and tabulated.

| $N'$ (10$^{19}$ cm$^{-3}$) | $\mu_{H}$ (RE) | $|R_H|$ (RE) | PVCMM | $\mu_{H}$ (RE) | $|R_H|$ (RE) |
|--------------------------|----------------|----------------|--------|----------------|----------------|
| 129.2                    | 0.340          |                 | 156.5  | 0.340          |                |
| [0.17]                   | [0.03]         |                | [0.01] | [0.03]         |                |

Table 8 indicates $|\text{REs}|$ of $\mu_{H}(N')$ and $|R_H(N')|$ are equal to 17% and 3% obtained for the PM, and 0.6% and 3% for PVCMM, respectively, confirming thus the use of $N'$ for the effective density of free electrons given in the conduction band when $N > N_{c(\text{As})}$, given in Eq. (43).
In the P (As)-Si systems at $T=4.2$ K, $n_{c(P)} = 3.52 \times 10^{18}$ cm$^{-3}$ and $n_{c(As)} = 8.58 \times 10^{18}$ cm$^{-3}$, as given in Table 1, the numerical results of resistivity $\rho(N^*) = 1/\sigma(N^*)$, $\sigma(N^*)$ being determined in Eq. (63) for the PVCMM and in Eq. (68) for the PM, are tabulated in Table 9, in which their absolute relative errors $|REs|$, calculated using the data obtained by Chapman et al. [54], are also included, suggesting that the maximal $|REs|$ of $\rho(N^*)$ are equal to 10% (11%), obtained respectively for the PM (PVCMM).

Table 9. In the P (As)-Si systems at $T=4.2$ K, the numerical results of resistivity $\rho(N^*)$, obtained for the PM and PVCMM and expressed in $10^{-4}$ ohm $\times$ cm, are tabulated in this Table IX, in which their absolute relative errors $|REs|$, calculated using the data obtained by Chapman et al. [54], are also included, suggesting that the maximal $|REs|$ of $\rho(N^*)$ are equal to 10% (11%), obtained respectively for the PM (PVCMM).

| $N$ (10$^{19}$ cm$^{-3}$) | 1.1 | 1.6 | 2.7 | 3.9 | 5 | 7 | 13 |
|-------------------------|-----|-----|-----|-----|---|---|----|
| $\rho_{exp}$ (donor) | 33 (P) | 23 (P) | 13 (P) | 9.4 (P) | 13 (As) | 6 (P) | 3.8 (P) |
| In the PM, the results of $\rho$ are accompanied by their $|REs|$ as: $\rho(N^*) (|RE|)$ | 35.8 (0.08) | 23.9 (0.04) | 14.5 (0.10) | 10.4 (0.10) | 13.9 (0.07) | 6.2 (0.03) | 3.6 (0.05) |
| In the PVCMM, the results of $\rho$ are accompanied by their $|REs|$ as: $\rho(N^*) (|RE|)$ | 29.5 (0.10) | 20.5 (0.11) | 13.2 (0.01) | 9.9 (0.05) | 12.3 (0.06) | 6.5 (0.08) | 4.2 (0.11) |

The underlined $|RE|$-value is the maximal one.

In the P-Si system at $T=77$ K and for $n_{c(P)} = 3.52 \times 10^{18}$ cm$^{-3}$, the numerical results of conductivity $\sigma(N^*)$, obtained respectively from Eqs. (63, 68) for the PVCMM and PM, are tabulated in this Table 10, in which their absolute relative errors $|REs|$, calculated using the $\sigma$-data obtained by Finetti and Mazzone [60], are also included. This indicates that the maximal $|RE|$ of $\sigma(N^*)$ are equal to 12% and 14% for PM and PVCMM, respectively.

Table 10. In the P-Si system at $T=77$ K, the numerical results of conductivity $\sigma(N^*)$, obtained respectively for the PVCMM and PM, are tabulated in this Table X, in which their absolute relative errors $|REs|$, calculated using the $\sigma$-data obtained by Finetti and Mazzone [60], are also included, indicating that its maximal $|REs|$ are equal to 12% and 14% for PM and PVCMM, respectively.

| $N$ (10$^{19}$ cm$^{-3}$) | 1.85 | 5.55 | 8.65 |
|-------------------------|------|------|------|
| $\sigma_{donor}$ (ohm$^{-1}$ cm$^{-1}$) | 559 | 1500 | 2000 |
| In the PM, the results of $\sigma$ are accompanied by their $|REs|$ as: $\sigma(N^*) (|RE|)$ | 520 (0.07) | 1339 (0.12) | 1962 (0.02) |
| In the PVCMM, the results of $\sigma$ are accompanied by their $|REs|$ as: $\sigma(N^*) (|RE|)$ | 575 (0.03) | 1318 (0.14) | 1799 (0.11) |

The underlined $|RE|$-value is the maximal one.

As noted above, in the following, we will only present the numerical results of various electrical and thermoelectric functions obtained in the PM, since those obtained in the PVCMM can also be investigated by a same treatment.

In the degenerate d-Si systems at $77$ K, the numerical results of resistivity $\rho(N^*,T,r_d) = 1/\sigma(N^*,T,r_d)$, $\sigma(N^*,T,r_d)$ being calculated from Eq. (68), and those of mobility $\mu(N^*,T,r_d)$ and Hall mobility $\mu_h(N^*,T,r_d)$ obtained respectively from Eqs. (67, 71), are tabulated in Tables 11 and 12.

Table 11. In the degenerate d-Si systems at $77$ K, the numerical results of resistivity $\rho(N^*,T,r_d)$ are expressed in $10^{-4}$ ohm$\times$ cm.

| Donor | Sb | P | As | Bi | Ti | Te | Se | S |
|-------|----|---|----|----|----|----|----|---|
| $N$ (10$^{19}$ cm$^{-3}$) | $\rho$ | $\rho$ | $\rho$ | $\rho$ | $\rho$ | $\rho$ | $\rho$ | $\rho$ |
| 3 | 11.58 | 12.68 | 22.37 | 25.92 |
| 6 | 6.40 | 6.98 | 11.56 | 12.97 |
| 10 | 4.12 | 4.49 | 7.32 | 8.14 |
| 40 | 1.22 | 1.33 | 2.18 | 2.41 |
| 70 | 0.74 | 0.81 | 1.33 | 1.48 |
| 100 | 0.53 | 0.58 | 0.97 | 1.08 |

Table 12. In the degenerate d-Si systems at $77$ K, the numerical results of mobility $\mu(N^*,T,r_d)$ and Hall mobility $\mu_h(N^*,T,r_d)$, both expressed in cm$^2$/V$\times$sec, and obtained respectively from Eqs. (67, 71), are tabulated here. This indicates that $\mu_h = \mu$ at $N = 10^{21}$ cm$^{-3}$.

| Donor | Sb | P | As | Bi | Ti | Te | Se | S |
|-------|----|---|----|----|----|----|----|---|
| $N$ (10$^{19}$ cm$^{-3}$) | $\mu$ ($\mu_h$) | $\mu$ ($\mu_h$) | $\mu$ ($\mu_h$) | $\mu$ ($\mu_h$) | $\mu$ ($\mu_h$) | $\mu$ ($\mu_h$) | $\mu$ ($\mu_h$) |
| 3 | 200 (228) | 186 (213) | 130 (155) | 123 (148) |
| 6 | 171 (180) | 158 (167) | 105 (111) | 97 (103) |
| 10 | 156 (160) | 144 (148) | 93 (96) | 85 (88) |
| 40 | 129 (129) | 118 (119) | 73 (74) | 66 (67) |
| 70 | 121 (122) | 111 (111) | 68 (68) | 61 (61) |
| 100 | 117 (117) | 107 (107) | 65 (65) | 59 (59) |

Table 11 indicates that (i) at a given $r_d$, the resistivity decreases with increasing $N$, and (ii) at a given $N$, it increases with increasing $r_d$. That means: $\rho(r_{sd}) < \rho(r_p) < \rho(r_{As}) < \cdots < \rho(r_{Se}) < \rho(r_s)$ , in good agreement with the observations by Logan et al. [53].

Table 12 suggests that (i) for a given $r_d$, the mobility and the Hall mobility decrease with increasing $N$, (ii) for given $N$, they decrease with increasing $r_d$, since $\mu$ (or $\mu_h$) is proportional to $\sigma \equiv 1/\rho$, where $\rho$ increases with increasing $r_d$, as observed in above Table XI, (iii) for given $N$ and $r_d$, their absolute relative errors $|REs|$, calculated using the data obtained by Chapman et al. [54], are also included, suggesting that the maximal $|REs|$ of $\rho(N^*)$ are equal to 10% (11%), obtained respectively for the PM (PVCMM).
expressed in terms of $\frac{5}{2}$ and $a = 2$, respectively.

Now, in degenerate (d)-Si systems at 77 K, from the generalized Einstein relation [62-67], it is interesting to present in following Table 13 our numerical results of diffusion coefficients: $D(N^*, T, r_d)$, $D_o(N^*, T, r_d)$, and $D_1(N^*, T, r_d)$, determined respectively in Eqs. (A15, A16, A17) of the Appendix C, being related to the mobility $\mu(N^*, T, r_d)$ given in Eq. (67).

Table 13. In degenerate (d)-Si systems at 77 K, our numerical results of diffusion coefficients ($\frac{\text{cm}^2}{\text{s}}$), $D$, $D_o$, and $D_1$ determined respectively in Eqs. (A15, A16, A17) of the Appendix C, being related to the mobility $\mu$ determined in Eq. (67), are tabulated here.

| Donor | Sb | P | As | Bi | Ti | Te | Se | S |
|-------|----|---|----|----|----|----|----|---|
| N   | $D_1$ | $D_1$ | $D_1$ | $D_1$ | $D_1$ | $D_1$ | $D_1$ | $D_1$ |
| 3    | 5.795 | (5.793) | 5.296 | (5.288) | 3.074 | (3.069) | 2.701 | (2.695) |
| 6    | 8.264 | (8.266) | 7.559 | (7.560) | 4.539 | (4.539) | 4.049 | (4.049) |
| 10   | 10.873 | (10.876) | 9.947 | (9.949) | 6.036 | (6.037) | 5.415 | (5.416) |
| 40   | 23.587 | (23.593) | 21.523 | (21.528) | 13.004 | (13.007) | 11.697 | (11.699) |
| 70   | 32.576 | (32.583) | 29.684 | (29.691) | 17.809 | (17.813) | 16.000 | (16.004) |
| 100  | 40.129 | (40.138) | 36.535 | (36.544) | 21.814 | (21.819) | 19.579 | (19.584) |
| N   | $D_o$ | $D_o$ | $D_o$ | $D_o$ | $D_o$ | $D_o$ | $D_o$ | $D_o$ |
| 3    | 10.000 | (10.004) | 9.440 | (9.443) | 6.650 | (6.651) | 5.630 | (5.631) |
| 6    | 15.000 | (15.004) | 14.060 | (14.063) | 9.000 | (9.003) | 7.900 | (7.903) |
| 10   | 20.000 | (20.004) | 19.230 | (19.233) | 12.00 | (12.03) | 10.90 | (10.93) |
| 40   | 50.000 | (50.004) | 48.010 | (48.013) | 32.00 | (32.03) | 30.90 | (30.93) |
| 70   | 70.000 | (70.004) | 68.000 | (68.003) | 44.00 | (44.03) | 42.90 | (42.93) |
| 100  | 100.000 | (100.004) | 98.000 | (98.003) | 64.00 | (64.03) | 62.90 | (62.93) |

Table 13 indicates that: (i) for a given $r_d$, $D$ and $D_1$ increase with increasing $N$, (ii) for a given $N$, since $D$, $D_1$ and $\mu$ are expressed in terms of $\sigma \equiv 1/\rho$, where $\rho$ increases with increasing $r_d$, as observed in above Table 11, our results of $D$ and $D_1$ thus decrease with increasing $r_d$, due to the donor-size effect, and finally (iii) for $N = 10^{22}$ cm$^{-3}$, all the results of $D$, $D_1$ and $D_o$ are found to be almost the same, suggesting that the asymptotic behaviors of $D$ and $D_1$ are correct.

7.2. Behaviors of Electrical Functions Obtained for $\mathbf{E} \leq 0$

First of all, it should be noted from Eqs. (26, 68) that for any $\mathbf{E}$ the conductivity can be rewritten in a general form as

$$\sigma_{PM}(E, r_d) \equiv \sigma(E, r_d) = \sigma_0(E_{Fno}) \times \left\{ \frac{E_{KIM}}{E_{Fno}} + \Delta \rho \times \frac{E_{Fno}}{\eta_{Fno}} \right\}, \tag{72}$$

where $\sigma_0(E_{Fno}) = \frac{(0.85)^2}{\pi} \times \frac{a^2}{h^2} \times \frac{a^2}{h^2} \times \frac{\eta_{Fno}}{\eta_{Fno}}$, is proportional to $E_{Fno}^2$, and $\left\{ \frac{E_{KIM}}{E_{Fno}} \right\}$ is determined in Eq. (26) for $a = 5/2$ and $a = 2$, respectively.

Here, as $E \leq 0$, using the functions: $H_n$, $K_n$ and $F_n$, given respectively in Eqs. (26-28) for $a = 5/2$ and 2, the conductivity, given in Eq. (72), is now rewritten by

$$\sigma(v_n, r_d) \equiv \frac{\sigma_0(E_{Fno})}{\sqrt{\pi}} \times \left\{ \frac{\Gamma(3/2)\times\beta_t^2}{\alpha_{F}} \times F_n(a = 5/2) + \Delta \rho \times \frac{\Gamma(3/2)\times\beta_t^2}{\alpha_{F}} \times F_n(a = 2) \right\}, A_n \equiv \frac{E_{Fno}}{\eta_{Fno}}. \tag{73}$$

So, our numerical results of exponential tails of the electrical conductivity $\sigma(v_n, r_d)$ at 0 K and for $N = 5 \times 10^{20}$ cm$^{-3}$, calculated using Eq. (73), are plotted in Figure 7, as functions of $v_n$.

Figure 7 shows that:

(i) our results of $\sigma(v_n, r_d)$ increase with increasing $r_d$ for a given $v_n$, due to the donor-size effect, and

(ii) present the maxima at $v_n = v_{n(0)}$ and go to zero as $v_n \to 0$ and $\infty$.

Further, our numerical results of the function $\ln(\sigma(v_n, r_d)) < 0$, which can take its approximate form as

$$\ln(\sigma(v_n, r_d)) \approx \ln\left(\frac{e(v_n)_{min}}{v_n^2} \right),$$

are evaluated in small $v_n$-intervals: $v_n \leq v_n \leq v_2$, using Eqs. (29) and (30), being now defined as:

$$e(v_n, v_1, v_2, z) \equiv \ln\left[\frac{\ln(e(v_n)_{min})}{v_n^2 - v_1^2} \right],$$

are tabulated in Table 14.
Table 14. In the d-Si systems at T=0 K and for N = 5 × 10²⁰ cm⁻³, using the expression for electrical conductivity determined in Eq. (73), σ[ν(νₖ), the numerical results of ln(σ[ν,νₖ]) and its approximate form: AF[νₖ,νₖ,ν₋₂,ν₋₃] = e(νₖ,ν₋₂,ν₋₃ × ν₋₂ + ν₋₃) determined in Eq. (29) for small ν₋₃-intervals: ν₋₁ ≤ ν₋₂ ≤ ν₋₃ and those of absolute relative errors: |RE| = 1 - AF[νₖ,ν₋₂,ν₋₃]/n[ln(σ[ν,νₖ])], are evaluated and tabulated below:

| Donor | Sb | P | As | Bi | Ti | Te | Se | S |
|-------|----|---|----|----|----|----|----|----|
| νₖ(M) | 0.24145 | 0.25005 | 0.31043 | 0.32482 | 0.48207 | 0.67829 | 0.86355 | 0.88790 |

For 1.37 ≤ ν₋₁ ≤ 1.42, AF = (e × ν₋₁ + f) is accurate to within 1.9 × 10⁻⁴, where

- e = 17.734, 16.287, 9.955, 8.926
- f = 9.234, 8.507, 5.708, 5.338
- |RE| = 1.2 × 10⁻⁴, 1.2 × 10⁻⁴, 1.0 × 10⁻⁴, 1.2 × 10⁻⁴
- 1.9 × 10⁻³, 2.4 × 10⁻⁴, 1.2 × 10⁻⁴, 1.2 × 10⁻⁴

For 1.28 ≤ ν₋₁ ≤ 1.30, AF = (e × ν₋₁/¹/² + f) is accurate to within 1.5 × 10⁻⁴, where

- e = 38.134, 35.052, 21.508, 19.293
- f = 29.621, 27.264, 17.269, 15.714
- |RE| = 4.7 × 10⁻⁵, 4.8 × 10⁻⁵, 1.2 × 10⁻⁴, 4.7 × 10⁻⁵
- 1.5 × 10⁻³, 6.2 × 10⁻⁵, 3.1 × 10⁻⁵, 1.3 × 10⁻⁴

For 1.180 ≤ ν₋₁ ≤ 1.185, AF = (e × ν₋₁/¹/³ + f) is accurate to within 9.4 × 10⁻⁵, where

- e = 53.080, 48.832, 30.060, 26.972
- f = 44.192, 40.703, 25.620, 23.212
- |RE| = 3.2 × 10⁻⁵, 2.7 × 10⁻⁵, 7.1 × 10⁻⁵, 9.0 × 10⁻⁵
- 9.4 × 10⁻⁴, 1.5 × 10⁻⁴, 5.5 × 10⁻⁵, 1.7 × 10⁻⁵

For ν₋₁ < 1.155 ≤ ν₋₁ ≤ 1.165, AF = (e × ν₋₁/¹/4 + f) is accurate to within 1.4 × 10⁻³, where

- e = 69.838, 64.260, 39.580, 35.514
- f = 60.894, 56.079, 35.109, 31.727
- |RE| = 4.1 × 10⁻¹, 1.8 × 10⁻⁵, 6.9 × 10⁻⁵, 6.7 × 10⁻⁵
- 1.4 × 10⁻³, 6.8 × 10⁻⁵, 1.8 × 10⁻⁵, 7.9 × 10⁻⁵

For 0.110 ≤ ν₋₁ ≤ 0.115 < ν₋₁(M), AF = (e × ν₋₁/¹/³ + f) is accurate to within 2.1 × 10⁻³, where

- e = 26.262, 27.342, 31.423, 31.800
- f = -18.507, -19.124, -21.180, -21.273
- |RE| = 2.8 × 10⁻¹, 1.5 × 10⁻⁴, 5.3 × 10⁻⁴, 4.9 × 10⁻⁴
- 8.2 × 10⁻⁴, 2.1 × 10⁻³, 8.3 × 10⁻⁴, 4.3 × 10⁻⁴

For 0.088 ≤ ν₋₁ ≤ 0.090, AF = (e × ν₋₁/¹/³ + f) is accurate to within 4.3 × 10⁻³, where

- e = 37.452, 38.777, 43.541, 43.855
- f = -21.105, -21.729, -23.698, -23.724
- |RE| = 9.5 × 10⁻⁵, 1.4 × 10⁻⁴, 9.7 × 10⁻⁵, 1.6 × 10⁻⁴
- 3.0 × 10⁻⁴, 4.1 × 10⁻³, 4.3 × 10⁻³, 9.5 × 10⁻⁴

For 0.070 ≤ ν₋₁ ≤ 0.073, AF = (e × ν₋₁/¹/² + f) is accurate to within 1.6 × 10⁻³, where

- e = 59.884, 62.021, 69.660, 70.074
- f = -21.865, -22.520, -24.590, -24.595
- |RE| = 3.6 × 10⁻⁴, 3.9 × 10⁻⁴, 4.5 × 10⁻⁴, 7.5 × 10⁻⁴
- 8.9 × 10⁻⁴, 6.1 × 10⁻⁴, 1.6 × 10⁻³, 9.2 × 10⁻⁴

For 0.061 ≤ ν₋₁ ≤ 0.064, AF = (e × ν₋₁ + f) is accurate to within 1.5 × 10⁻², where

- e = 162.658, 168.842, 191.433, 192.696
- f = -17.234, -17.750, -19.349, -19.334
- |RE| = 5.9 × 10⁻⁴, 6.7 × 10⁻⁴, 7.3 × 10⁻⁴, 6.9 × 10⁻⁴
- 8.3 × 10⁻⁴, 9.3 × 10⁻⁴, 1.1 × 10⁻³, 1.5 × 10⁻³

For 0.054 ≤ ν₋₁ ≤ 0.056, AF = (e × ν₋₁² + f) is accurate to within 9.9 × 10⁻⁴, where

- e = 2147.55, 2236.99, 2576.10, 2597.50
- f = -15.033, -15.491, -16.923, -16.906
- |RE| = 5.4 × 10⁻⁴, 5.2 × 10⁻⁴, 6.5 × 10⁻⁴, 6.2 × 10⁻⁴
- 6.6 × 10⁻⁴, 8.6 × 10⁻⁴, 8.8 × 10⁻⁴, 9.9 × 10⁻⁴

The underlined |RE|-value is the maximal one for each donor-Si system.

Table 14 suggests that: (i) our results of AF[ν₋₁,ν₋₂,ν₋₃] given for (z=1)-exponent agree with the Urbach law obtained from linear exponential conduction-band tail-behaviors by some workers [21, 29, 30, 37], (ii) ours for (z=1/2)-exponent and ν₋₁ > ν₋₁(M) agree with other theoretical results [19, 37], and finally (iii) ours for (z=1/3, 1/4)-exponents when ν₋₁ > ν₋₁(M), and for (z=1/4, 1/3, 1/2, 1, 2)-exponents when ν₋₁ < ν₋₁(M) may thus be new.

Finally, our numerical results of energy parameter, Eₜoₜ(N; ν₋₁), obtained in the small interval: 1.37 ≤ ν₋₁ ≤ 1.42, using Eq. (31), are plotted as functions of N in Figures 8a and 8b, indicating that, for a given N, Eₜoₜ increases with
increasing \( r_d \)-values, due to the donor-size effect.

\[
\vec{j}(\vec{r}) = L^{(3)} \times \vec{E} + L^{(4)} \times T \times \vec{V}(T^{-1}),
\]

where \( \vec{j} \) is the electric current density, \( \vec{E} \) is the electric field, and \( L^{(i)} \) is the transport coefficient determined in an isotropic system. Now, using the average of \( (\mathbb{E}^p)_{\text{FDDF}} \equiv g_p(y) \times \mathbb{E}^p_{\text{Fano}} \), where the expressions for \( g_p(y) \), \( y = \frac{\pi k_B T}{\mathbb{E}^p_{\text{Fano}}} \), are determined in Eq. (34) and given in Table III, calculated using the Fermi-Dirac distribution function (FDDF), and using also the expression for electrical conductivity as a function of \( \mathbb{E} \), derived from Eq. (72) for \( E \geq 0 \), as

\[
\sigma(\mathbb{E}, r_d) = \sigma_0 (\mathbb{E}_{\text{Fano}}) \left\{ \frac{\mathbb{E}^2}{\mathbb{E}^2_{\text{Fano}}} + \Delta_{PM} \times \left( \frac{\mathbb{E}^2}{\mathbb{E}^2_{\text{Fano}}} \right)^{\frac{3}{2}} \right\},
\]

the Onsager relations are found to be given as follows.

First, one has [58, 61]

\[
L^{(1)} \equiv \langle (\mathbb{E}_x,y_0,r_d) \rangle_{\text{FDDF}} = \sigma_0 (\mathbb{E}_{\text{Fano}}) \left\{ \frac{\mathbb{E}^2}{\mathbb{E}^2_{\text{Fano}}} + \Delta_{PM} \times \left( \frac{\mathbb{E}^2}{\mathbb{E}^2_{\text{Fano}}} \right)^{\frac{3}{2}} \right\},
\]

which is just the result obtained in Eq. (68).

Then, one gets [58]

\[
L^{(2)} = L^{(3)} = - \frac{1}{q} \times \langle (\mathbb{E} \times \sigma(\mathbb{E}, r_d))_{\text{FDDF}} = - \frac{\sigma_0 (\mathbb{E}_{\text{Fano}})}{q} \times \left\{ G_4(y) + \Delta_{PM} \times G_2(y) \right\},
\]

Finally, one obtains [58]

\[
L^{(4)} = \frac{1}{q} \times \langle (\mathbb{E}^2 \times \sigma(\mathbb{E}, r_d))_{\text{FDDF}} = \frac{\sigma_0 (\mathbb{E}_{\text{Fano}})}{q} \times \left\{ G_4(y) + \Delta_{PM} \times G_2(y) \right\}.
\]

Now, from Eqs. (77-79), one can define the thermal conductivity by [58, 61]

\[
K_T(N',T,r_d) \equiv \frac{1}{T} \times \left\{ L^{(4)} - \frac{L^{(2)} L^{(3)}}{L^{(1)}} \right\}.
\]

Some remarks obtained from Eq. (80) are given as follows.

(i) First, our numerical calculation indicates that, in the degenerate (P)-Si system, for \( N = 10^{21} \text{ cm}^{-3} \) and at \( T=3 \text{ K} \) and \( 300 \text{ K} \), noting that at 300 K the degenerate temperature \( T_D \) is equal to \( 7895 \gt 300 \text{ K} \), our results of \( K_T \) are equal to \( 8 \times 10^{-4} \) and 0.125 W/(cm.K), in good agreement with the experimental results obtained by Slack [68]: \( 5 \times 10^{-4} \) and between 0.1 and 0.2 W/(cm.K), respectively.

(ii) Second, at \( N = 10^{21} \text{ cm}^{-3} \) and \( T=3 \text{ K} \), the values of relative deviations between our results of \( K_T(N',T,r_d)/[T \times \sigma(N',T,r_d)] \), calculated using Eqs. (68) and (80), and the constant: \( \frac{\pi^2 k_B T}{3 q} \times 2.443 \times 10^{-8} \text{ W. \Omega. K}^{-2} \), being obtained from the Wiedemann-Franck law for metals [58, 61], are tabulated in Table 15, indicating that our result (80) well verifies this law, with a precision of the order of 6.52 \times 10^{-7}.

Figures 8. Our results of energy parameter, \( E_{\text{ano}}(N,r_d) \), are plotted as functions of \( N \), indicating that, for a given \( N \), \( E_{\text{ano}} \) increases with increasing \( r_d \)-values, due to the donor-size effect.

8. Thermoelectric Properties

When the electron-electron and electron-phonon interactions are neglected, the Kubo formulae for the thermal transport coefficients [51], derived by very general arguments of Luttinger [55], are found to be reduced to the Greenwood ones [52]. Then, the phenomenological equations are written as [58]

\[
\vec{j}(\vec{r}) = L^{(3)} \times \vec{E} + L^{(4)} \times T \times \vec{V}(T^{-1}),
\]
Table 15. For \( N = 10^{21} \text{ cm}^{-3} \) and \( T=3 \text{ K} \), the values of the relative deviations (RD) between our results of \( \frac{K_T}{C_T} \) obtained in various degenerate donor-Si systems, and the constant \( \frac{n_0^2}{\eta q} = 2.443 \times 10^{-8} \text{W} \text{cm}^{-2} \text{K}^{-2} \), obtained from the Wiedemann-Frank law for metals, indicating a perfect agreement between those results.

| Donor | Sb   | P   | As  | Bi  | Ti  | Te  | Se  | S   |
|-------|------|-----|-----|-----|-----|-----|-----|-----|
| RE    | 4.72 \times 10^{-7} | -9.40 \times 10^{-8} | -3.51 \times 10^{-8} | 3.79 \times 10^{-7} | 1.67 \times 10^{-7} | -6.52 \times 10^{-7} | -1.53 \times 10^{-7} | -5.95 \times 10^{-8} |

The underlined \(|\text{RE}|\) value is the maximal one for each donor-Si system.

(ii) Finally, our numerical calculation shows that, in degenerate (d)-Si systems, for \( N = 10^{21} \text{ cm}^{-3} \) and in the temperature range from \( T=3 \) to 300 K, the maximal value of absolute deviations between \( K_T(N', T, r_d) \) given in Eq. (80) and its approximate form \( K_T(N', T, r_d) \approx C_K \times T \) is found to be equal to \( 9.9 \times 10^{-4} \), in good agreement with our previous result [58, 61]. Then, those are plotted in Figure 9a as functions of \( T \), suggesting that at a given \( T \) the thermal conductivity \( K_T \) decreases with increasing \( r_d \), due to the donor-size effect.

\[ K_T(N', T, r_d) \approx C_K \times T \]

![Figure 9a](image-url)

Figure 9a. Our results of \( K_T(N', T, r_d) \approx C_K \times T \) are plotted as functions of \( T \), suggesting that at a given \( T \) the thermal conductivity \( K_T \) decreases with increasing \( r_d \), due to the donor-size effect.

Then, from Eqs. (77, 78) for \( L^{(1)} \) and \( L^{(2)} \), and Eq. (D1) of the Appendix D for \( E_{\text{Fmax}} \), the absolute thermoelectric power \( Q \) can be defined by [58, 61]

\[ Q(N', T, r_d) \equiv \frac{1}{4} \times \left( \frac{L^{(2)}}{L^{(1)}} + \frac{E_{\text{Fmax}}}{q} \right). \]  

This result (81) is a function commonly used to describe the following thermoelectric coefficients [58, 61], such as: the Thomson coefficient,

\[ T_S(N', T, r_d) \equiv \frac{dQ(N', T, r_d)}{dT}, \]  

the Seebeck thermoelectric potential,

\[ S_p(N', T, r_d) \equiv \int_0^T Q(N', T, r_d) dT, \]  

and finally the dimensionless figure of merit,

\[ ZT(N', T, r_d) \equiv \frac{T \times S_p^2(N', T, r_d) \times \sigma(N', T, r_d)}{K_T(N', T, r_d)}. \]  

We now evaluate the above results (81-85) in the following.

In degenerate (d)-Si systems, for \( N = 10^{21} \text{ cm}^{-3} \) and in the temperature range from \( T=3 \) to 300 K, our numerical calculation indicates that: (i) the maximal value of absolute relative deviations between \( Q \) determined in Eq. (81) and its approximate form: \(-C_Q \times T \) is found to be equal to \( 6.16 \times 10^{-3} \), and (ii) the maximal value of absolute relative deviations between \( T_S \) determined in Eq. (82) and its approximate form: \(-C_S \times T \) is equal to 0.019. So, our numerical results of \( Q = -C_Q \times T \) and \( T_S = -C_S \times T \) are plotted in Figures 9b and 9c, as functions of \( T \), respectively, suggesting that at a given \( T \), \( Q \) and \( T_S \) both decrease with increasing \( r_d \), due to the donor-size effect.

\[ \text{Figure 9b} \]

![Figure 9b](image-url)

Figure 9b. Our results of \( Q = -C_Q \times T \) are plotted as functions of \( T \), suggesting that, at a given \( T \), \( Q \) decreases with increasing \( r_d \), due to the donor-size effect.
Finally, in the following Figures 9d, 9e and 9f, our numerical results of Peltier coefficient $P_T$, Seebeck thermoelectric potential $S_B$, and dimensionless figure of merit $ZT$, calculated using Eqs. (83-85), are plotted as functions of $T$, respectively.

9. Concluding Remarks

Using the effective autocorrelation function for potential fluctuations $W_n$, developed in Eq. (B.6) of the Appendix B, expressed in terms of the Heisenberg uncertainty relation given in Eq. (B.5), and an expression for the Gaussian average of $\langle \xi k^2 \rangle$, $\langle \xi k^2 \rangle_{\text{KIM}}$, obtained in Eq. (20) by the Kane integration method (KIM), we developed the expressions for density of states, optical absorption coefficient, and electrical conductivity, obtained in various degenerate d-Si systems,
being due to the effects of donor-size and heavy doping, as given respectively in Eqs. (36, 49, 72). It should be noted that this average expression was found to be equivalent to that obtained by the Feynman path-integral method. Then, those above results were expressed in terms of \( \Xi^{\pm (1/2)} \), as given in Eq. (24) for \( \Xi \geq 0 \) and \( a \geq 1 \), vanished at the band edge: \( \Xi = 0 \), and exhibited their exponential tail behaviors for \( \Xi \leq 0 \), as obtained in Eqs. (28-31), in Tables 4, 7, 14, and in Figures 1, 2a (b), 3a (b, c), 4, 5a (b), 7 and 8a (b). Furthermore, in Figures 1, 4, and 7, some important conclusions were obtained as follows.

1. First, for a given value of \( -\Xi \), those exponential tails increased with increasing \( r_g \), being due to the donor-size effect.

2. Secondly, they vanished at the conduction-band edge \( \Xi = -0 \), as given in Eq. (26), in good accordance with our other results obtained in Eq. (A3) of the Appendix A. Furthermore, those exponential tail-results were also compared with other theoretical ones, being found to be constant, at \( \Xi = -0 \), obtained in the small time approximation \([21, 29, 30]\) and in the full ground-state case and deep-tail approximation \([21]\). Thus, their results should not be correct, as discussed in Eq. (26).

3. Finally, for \( \Xi \leq 0 \), they went to zero as \( \Xi \rightarrow -0 \) and \( -\infty \) and presented the maxima, being found to be in good accordance with an asymptotic form for the exponential conduction-band tail, obtained by Halperin and Lax \([19]\), using the minimum counting methods. Hence, the problem posed in the past for those exponential tails \([14, 17, 19, 21, 23, 25, 29, 30, 37] \) should now be solved.

Then, an expression for the average of \( \Xi^p \), at low temperatures and for \( p \geq 3/2 \), calculated by the Fermi-Dirac distribution function, was determined in Eq. (34), being used to evaluate, in degenerate d-Si systems, the mobility, conductivity, resistivity, Hall coefficient, Hall factor, Hall mobility, thermal conductivity, diffusion coefficient, absolute thermoelectric power, Thomson coefficient, Peltier coefficient, Seebeck thermoelectric potential, and finally also the density of states \((DOS)\) or the joint DOS \((JDO)\), reformulating the problem conjectured by Lifshitz (L) \([18]\) as that given in the Brownian motion. Here, they showed that \( J_n(\Xi \rightarrow 0, \Xi) \rightarrow 0 \), and \( J_n(\Xi \rightarrow 0, \Xi) \) vanishes for \( \Xi \leq 0 \), neglecting the exponential conduction-band tail, due to the heavy doping effect, \( \Xi \) being the total electron energy. Then, these LFL results were reviewed by Mieghm \([24]\). In Sections III-VI, since \((DOS)\) and \((JDO)\) given in Eq. (36) for \( a=1 \), is proportional to \((\pi/E)^{1/2}\)\((\Xi)/\Xi, \Xi \), being defined in Eq. (20), we obtained: \((DOS)\) \( n \rightarrow 0 \) when \( \Xi \rightarrow +0 \) and \( -0 \), as discussed in Eqs. (23, 26), respectively. In other words, \((DOS)\) \( n \rightarrow 0 \), when \( |\Xi| \rightarrow 0 \) or \((DOS)\) vanishes at the conduction-band edge \( (\Xi = 0) \), suggesting thus a generalized (LFL)-method (GLFLM) to be study as follows.

In the very large volume \( V_o \equiv (4\pi)^l R_o^l \) of radius \( R_o \), being empty of donors, and for lowest \( |\Xi| \equiv \frac{h^2 \pi^2}{2 m_H^H \pi^2 R_o^2} \equiv \frac{h^2 \pi^2}{2 m_H^H \pi^2 R_o^2} \), \( R_o \) is thus defined by \([18, 20]\)

\[
\Xi = \frac{B}{k} \frac{1}{|\Xi_n|} \quad \Xi = \frac{B}{k} \frac{1}{|\Xi_n|}
\]

where from the LFL-method \([18, 20]\): \( B = B_{LFL} = \pi \) and \( R_o = R_{o(LFL)} = \frac{B_{LFL}}{k} \), \( k \) being the wave number. Here, \( n_{H^D}(N, r_d) \) is determined in Eq. (8), and \( |\Xi_n| \equiv \frac{|\Xi|}{|\Xi_n|} \) is determined in Eq. (21). In fact, Eq. (A1) is thus the Heisenberg uncertainty relation, which can be compared with that given in next Eq. (A8) of the Appendix B, as: \( \Delta r \equiv \Xi \).
Now, in our GLFLM, in which the very large volume is
\[ V = \frac{4\pi}{3} \times \mathbb{R}^3, \]
\[ \mathbb{R} \equiv (\mathbb{R}_{GLFLM} - d\Omega) \] being its radius, where \( d\Omega \ll \mathbb{R} \), the low-lying levels for states localized in it will
\[ V \equiv \frac{4\pi}{3} \times \mathbb{R}^3 = \frac{4\pi}{3} \times [(R_{GLFLM})^3 - 3(R_\text{eff})^2 \times d\Omega + 3(R_\text{eff})GLFLM \times (d\Omega)^2 - (d\Omega)^3]. \]

The probability of such a large region is proportional to:
\[ \exp(-\frac{N}{\delta c} \times V), \]
where \( \frac{N}{\delta c} = \frac{V_4}{\mathbb{R}^3} \), such that the reduced \( J_n \) can be defined by:
\[ \ln_{\text{GLFLM}}[|\nu_{n,p}^\text{GLFLM}|; B] = \exp(-\frac{N}{\delta c} \times V) \]
[20]. Here, \( d\Omega \ll \mathbb{R} \) is determined from the FL-results as [20]:
\[ d\Omega \equiv 2\alpha_0 \approx \lambda_0, \]
where \( c = 0.628 \) and \( \lambda_0 \equiv 1/\sqrt{4\pi L \times (\frac{N}{\delta c})} \) is the skin depth, \( L \) being the scattering length. Moreover, in degenerate d-Si systems, the scattering length \( L \) could be replaced by the effective screening length, \( k_{sn} \), where \( k_{sn} \) is determined in Eq. (4). So, in this GLFLM, for lowest \( |E| \) (or \( |\nu_{n,p}| \to 0 \)), defining the kinetic energy of localization by:
\[ E_{k_{sn}} \equiv \frac{\hbar^2 k_{sn}^2}{2m_\text{n}}, \]
one thus obtains

\[ \ln_{\text{GLFLM}}[|\nu_{n,p}|; B] \to 0, \]
where \( R_{sn} \equiv \frac{k_{sn}}{k_{0}} \) is determined in Eq. (4), in good accordance with our results (23, 26). Furthermore, for \( a=1 \) and \( B = B_{\text{FL}} = \pi \), the first-and-second terms of the last member of Eq. (A3) are found to be identical to the L-and-FL results, respectively.

**Appendix B: Effective Autocorrelation Function**

In degenerate d-Si systems, if denoting the electron positions and the corresponding wave vectors, according to the first-and-second scatterings at the times \( t \) and \( t' \) by \( (\vec{r}, \vec{k}) \) and \( (\vec{r}', \vec{k}') \), and working with the Fourier transform given in Eq. (18), the effective autocorrelation function for potential fluctuations is then defined by [25]

\[ W_n \equiv \langle V(\vec{r})V(\vec{r}')\rangle = \sum (\delta_{\vec{k}\vec{k}'}) v_j(\vec{k})v_j(\vec{k}') \times e^{i(\vec{k}\cdot\vec{r} + \vec{k}'\cdot\vec{r}')} \times \sum (\delta_{j\prime j}) (e^{-i(\vec{k}R_j + \vec{k}'R_{j'})}), \]

where the total potential energy \( V(\vec{r}) \) is defined in Eq. (16), and \( \vec{k}' = -\vec{k}' \). Then, since \( \langle V(\vec{r}) \rangle = \langle V(\vec{r}') \rangle = 0 \) as remarked in Eqs. (16, 17), \( W_n \) is non-zero only when \( \vec{k}' = \vec{k}' \), \( R_j = R_{j'} \), and \( \vec{k} = -\vec{k}' \), meaning that the electron scattered on each donor twice, and giving:

\[ \Delta k = |\vec{k}' - \vec{k}| = 2k. \]

Hence, for \( W_n(|\vec{r}' - \vec{r}|) \neq 0 \), Eq. (A4) thus becomes

\[ W_n(|\vec{r}' - \vec{r}|) = \mathcal{N} \sum_{\vec{k}} (v_j(\vec{k}))^2 \times \exp[i \vec{k} \cdot (\vec{r} - \vec{r}')] \] \[(A6)\]
noting that \( v_j(\vec{k})v_j(\vec{k}') = v_j(\vec{k})v_j(\vec{k}') = |v_j(\vec{k})|^2 \) for real potential energies. Here, \( v_j(\vec{k}) \) is determined in Eq. (18) and \( \mathcal{N} \) is the total number of donors. Further, from the Fourier transform [25], one has

\[ \exp(-k_{sn}^2|\vec{r}' - \vec{r}|^2) \equiv \sum k \frac{n}{\pi} \times \frac{1}{k^2 + k_{sn}^2} \times \exp[i \vec{k} \cdot (\vec{r} - \vec{r}')], \]
where \( \Omega \) is the total crystal volume, and taking its partial derivative (i.e., \( \partial/ \partial k_{sn} \)), one finally finds

\[ W_n(|\vec{r}' - \vec{r}|) \equiv n^2 \exp(-k_{sn}^2|\vec{r}' - \vec{r}|^2). \]

Here, \( n^2 \equiv N \int_{\mathbb{R}} v_j(\vec{r})^2 \times 4\pi m^2 d\vec{r} = 2\pi Nq^4k_{sn}^{-2} \), where \( q \) is the electron charge, \( v_j(\vec{r}) \) is determined in Eq. (17) and the accurate screening length \( k_{sn}^{-1} \) is determined in Eq. (4). Then, some concluding remarks can be obtained below:

(i) In the small time approximation, \( |\vec{r}' - \vec{r}| = 0 \), Eq. (A7) is thus reduced to \( n^2 \) \[17, 21, 22, 29, 30]\.

(ii) Using Eq. (A5), the Heisenberg uncertainty relation between \( \Delta r \equiv |\vec{r}' - \vec{r}| \) and \( \Delta k = 2k \) is given by

\[ \Delta r \times \Delta k = \mathcal{H}_n \geq \frac{1}{2} \Rightarrow \Delta r = B_n/k, \]

where \( B_n = \mathcal{H}_n/2 \).

(A8) which can be compared with that given in Eq. (A1), as discussed above. Here, the values of empirical Heisenberg parameter \( \mathcal{H}_n \) was proposed in Section V as: \( \mathcal{H}_n = 5.4370 \). Further, if replacing the constant \( B \) given in above Eqs. (A1-A3) by \( B = B_n = \mathcal{H}_n/2 = 2.7185 \), which gives: \( B_{\text{FL}} = \pi = 3.1416 > B_n \), then, from Eq. (A3), we also obtain:

\[ \ln_{\text{GLFLM}}[|\nu_{n,p}|; B_n] \to -\infty \text{ or } \ln_{\text{GLFLM}}[|\nu_{n,p}|; B] \to -\infty. \]
0, in good accordance with our results (23, 26).

(iii) Finally, using Eq. (A8) and defining the kinetic energy of localization by: \( E_{\text{kin}} \equiv \frac{k_B^2 z^4}{2m^2 \epsilon_{\text{D}E}(N,r_d)} \), the effective autocorrelation function for potential fluctuations (A7) can be rewritten as

\[
W_n(v_n, N, r_d) = \eta_n^2 \times \exp\left(\frac{-N_{\text{eff}}}{2 \eta_n^2 v_n}\right), \tag{A9}
\]

where the ratio \( R_{\text{eff}} \equiv \frac{k_B^2 z^4}{2m^2 \epsilon_{\text{D}E}} \) is determined in Eq. (4). Here, one remarks that \( W_n(v_n, N, r_d) \to 0 \) and \( \eta_n^2 \), as \( v_n \to 0 \) and \( \infty \), respectively, while in many other works for any \( v_n \)-values, \( W_n(v_n, N) \approx \eta_n^2 \), obtained in the small time approximation [17, 21, 22, 29, 30]: \( \Delta r \sim 0 \), being only valid as \( v_n \to \infty \), but is not correct as \( v_n \to 0 \), since from Eq. (A8), \( \Delta r \gg 0 \). Therefore, Eq. (A9) is an important result of the present paper.

\[
\theta_n(u) = \frac{E_{\text{F}}(u)}{k_B T} = \frac{G(u) + \mu + U^B(u)}{1 + \mu U^B}, \quad A = 0.0005372, \quad B = 4.82842262, \tag{A10}
\]

where, in the degenerate case or as \( \theta_n(u \gg 1) \to \infty \), Eq. (A10) is reduced to

\[
F(u) = u^{2/3} (1 + Bu^{-4/3} + Cu^{-8/3})^{-2/3}, \quad a = 3\sqrt{\pi}/4, \quad b = \frac{1}{8} (2)^2, \quad c = \frac{6.3739855}{1920}, \tag{A11}
\]

and in the non-degenerate case or for \( \theta_n(u_n \ll 1) \ll 0 \), to

\[
G(u) \approx \ln(u) + 2.3^2 u + e^{-du}, \quad d = 2^{3/2} \left[\frac{1}{\sqrt{2}} - \frac{2}{15}\right] > 0. \tag{A12}
\]

Further, one notes that Eq. (A11) can thus be rewritten as

\[
E_{\text{F}n} (u) = E_{\text{F}no} \times (1 + Bu^{-4/3} + Cu^{-8/3})^{-2/3}, \tag{A13}
\]

being the Fermi energy given in the degenerate d-Si systems.

For example, in the Fermi region in the degenerate P-Si system at \( T=77 \) K and \( N(10^{19} \text{ cm}^{-3}) = 3 \) and 100, the relative deviations between \( E_{\text{F}n}(N^*, T, r_d) \) determined in Eq. (A13) and \( E_{\text{F}n}(N^*, T, r_d) = \theta_n \times k_B T \) in Eq. (A10), defined by: \( 1 - \frac{E_{\text{F}n}(u)}{E_{\text{F}n}(u_n)} \), are equal to 0.052 and 4.6 \times 10^{-4}, respectively.

Generalized Einstein Relation

The generalized Einstein relation is defined by \([51, 62-67]\)

\[
\frac{D(u)}{\mu} = \frac{N}{q} \times \frac{\delta E}{\delta u} \equiv \frac{k_B z^2}{q} \times \left( u \frac{\delta \theta_u}{\delta u} \right), \tag{A14}
\]

where \( \mu \) is the mobility and in particular in the degenerate case it is determined in Eq. (67), \( \theta_n(u) \equiv \frac{V(u)}{W(u)} = G(u) + Au^B F(u) \), and \( W(u) = 1 + Au^B \) \( [27, 63] \) as those given in Eqs. (A10, A11, A12). Then, differentiating this function \( \theta_n(u) \) with respect to \( u \), one thus obtains \( \frac{\theta_u}{\delta u} \). Therefore, Eq. (A14) becomes \([63]\)

\[
\frac{D(u)}{\mu} = \frac{k_B z^2}{q} \times u \left[ \frac{V'(u) W(u) - V(u) W'(u)}{W^2(u)} \right], \tag{A15}
\]

where \( W'(u) = A u^B - 1 \) and \( V'(u) = u^{-1} + 2.3^2 u^{-du} (1 - \)}
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