Double Exponential Density of States and Modified Charge Carrier Transport in Organic Semiconductors

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Double Exponential Density of States and Modified Charge Carrier Transport in Organic Semiconductors

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Abstract. This paper discusses an approach to use an approximated charge carrier density for organic thin-film transistor (OTFT) using a double exponential density of states. Traditionally the literature has been published using a single exponential density of states and Gaussian density of states but this paper deals with using a double exponential density of states in the Fermi Integral to evaluate the charge carrier density for the OTFT. There are two exponential density of states related to the Tail region and Deep region and various parameters associated with it. The distribution of localized trap states between the highest and lowest orbital is expressed as a density of states. There are two states deep states and tail states. Tail states are better described by the Gaussian function, while Deep states are better described by the Exponential density of states. So, if we require that the two regions be defined by a single function then the function should be a sum of the two, the exponential and the Gaussian to accurately describe the complete region. The double exponential density of states is considered to evaluate and approximate the Fermi Integral using various Mathematical Methods, so that the error is lower for various parameters.

Key Words: Organic thin film transistor (OTFT), Double exponential density of states, Charge Carrier Density, Fermi–Dirac-type integral.

I. INTRODUCTION

The concentration of electrons at various energy levels in a semiconductor material is a very important parameter to determine characteristics of the device manufactured out of that semiconductor material. Now to determine the concentration of electron we need to know the probability of an electron residing at that particular energy level which would tell us what are the chances of finding electron possessing the said amount of energy, in other words, the chances of an electron occupying that particular energy level. Also, the electrons cannot occupy all the energy values in a continuum i.e., there are only predefined states or energy levels which are allowed for an electron to possess. These states are the actual energy levels that are occupied by the electrons. So, in addition to the probability of number of electrons at a particular energy we also need to know the number of states that are allowed in a particular range of energy which are called density of states (number of states per unit volume of semiconductor material).

Now traditionally, the probability of electron in a particular energy level is given by the Fermi-Dirac function: [1]

$$f(E,T) = \frac{1}{1 + e^{\frac{E-E_F}{k_B T}}}$$

Here E is the energy of the electron and T is the temperature at which this energy is attained, k_B is the Boltzmann constant and E_F is the energy associated with the Fermi level of the semiconductor. Fermi level, in semiconductor engineering, is the energy level which has a 50% chance of occupation at finite temperatures. It is known about density of electrons at various energies, coming to density of energy levels or states as we move from lower energy range to higher energy range. This is historically given by a Gaussian Density of States [2-5] or by Exponential Density of States [1], [6-8]. Also, a double Exponential Density of States function will be used as stated in [6] and [9] and given by:

$$g(E) = \frac{N_{Deep}}{\varphi_{Deep}} \cdot e^{\frac{E}{\varphi_{Deep}}} + \frac{N_{Tail}}{\varphi_{Tail}} \cdot e^{\frac{E}{\varphi_{Tail}}}$$

Also to bolster this claim it can be seen in [10-12] that when the current for a TFT is modeled using double exponential density of states it has more resemblance to the actual experimental data than when single exponential density of states is used.
Currently the calculation of charge carrier density, which is basically the integral of f(E,T) and g(E) over all the energies from -∞ to 0, has been done by taking g(E) as Gaussian Density of States and Exponential Density of States as shown in [13] and by single exponential density of states as shown in [1].
Since we are developing Double Exponential Density of States so focus will be kept on Hart [1] in which he has taken the Fermi function: $f(E,T) = \frac{1}{1+e^{\frac{E-E_F}{k_B T}}}$ and the single exponential density of states function as $g(E) = \frac{N_t}{E_0} e^{\frac{E}{E_0}}$. This depiction is correct but this might be made more accurate if we consider it to be summation of two exponentials [14] with different E_0's to characterize both deep and tail states, as deep and tail state both have different energy E_0 associated with it. We will then calculate the charge carrier density by integrating the EDOS and Fermi-Dirac function [2].
Although, above research works are good and fruitful in their own might we needed to have, what we observe a more accurate version of closed form of charge carrier density for the Exponential Density of States can be found. Double Exponential Density of States which we observe a more accurate description of the Density of States.

II. THE VM MODEL [5]

The VM model begins with an assumed exponential density of states of the form where $E_0 = k_B T_0$. The single DOS is given by the following equation and is defined for $-\infty < E \leq 0$.

$$D_e(E, T_0) = \frac{N_t}{E_0} e^{\frac{E}{E_0}}$$

2.1 Approximate Charge Carrier Density

The actual charge density function can be written as the following equation which integrates the product of the density of states and Fermi Dirac function:

$$\boldsymbol{\delta = \frac{1}{N_t} \int_{-\infty}^{0} D_e(E, T_0) f_e(E, T, E_f) dE} \tag{1}$$

Here $\boldsymbol{f_e}$ is the Fermi Dirac function for electron defined as stated:

$$\boldsymbol{f_e = \frac{1}{1 + e^{\frac{E-E_F}{k_B T}}}}$$

Also, N_t is the number of energetic states per unit volume, k_B is the Boltzmann's constant, and $T_0 > 0$ is the representative width of exponential distribution that can be considered a measure of the disorder of the system in question. The energy, E_0, in the denominator of the equation is a *normalizing factor* used to ensure that the total charge carrier density resulting from integration over all energy states is N_t. The EDOS is considered to be zero for all energies $E > 0$. Refer to Figure 1:

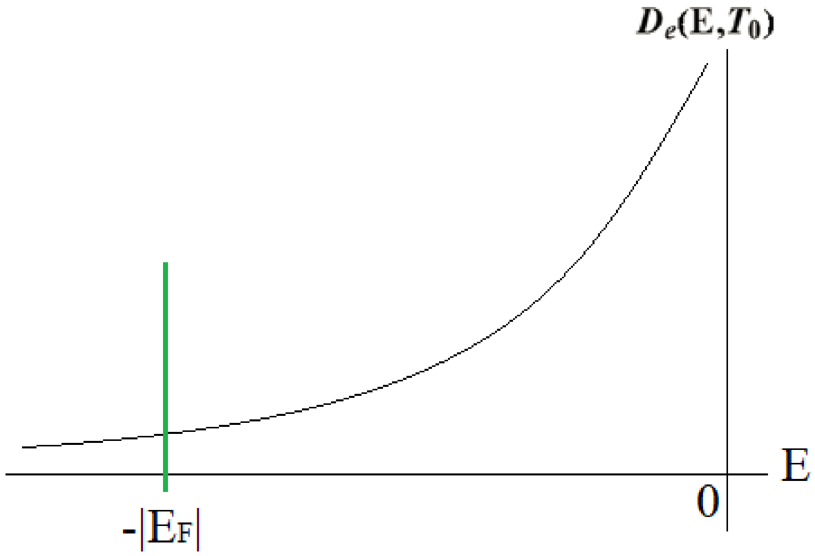


Fig. 1.1 Exponential Density of States in the VM Model

A. Double Exponential Density of States

As introduced in the earlier sections "Double Exponential function" is a better approximation for the Density of States. The equation for this Double-EDOS is considered from [9] and as portrayed in [14], [15-16].

$$g(E) = \frac{N_{Deep}}{\varphi_{Deep}} \cdot e^{\frac{E-E_{LUMO}}{\varphi_{Deep}}} + \frac{N_{Tail}}{\varphi_{Tail}} \cdot e^{\frac{E-E_{LUMO}}{\varphi_{Tail}}}$$

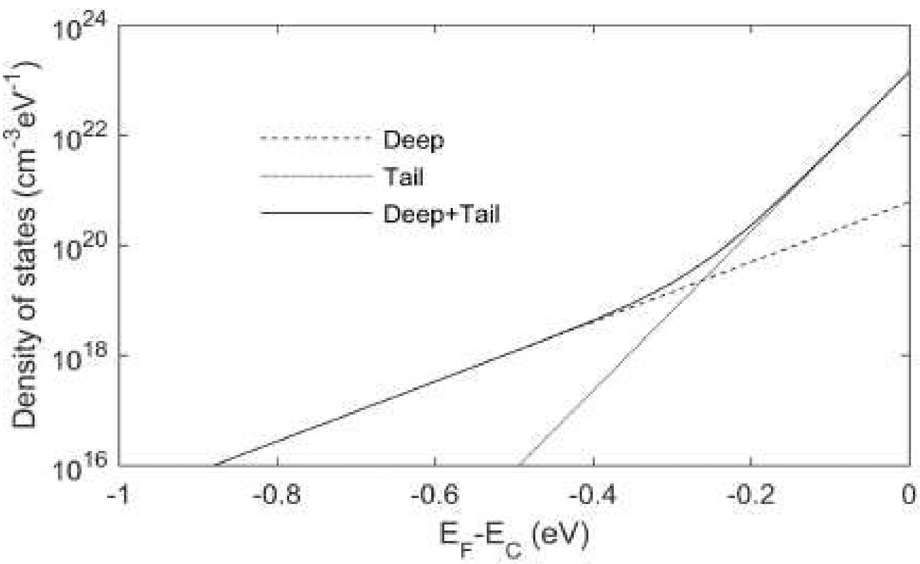


Fig. 2.1 Double exponential distribution density of acceptor trap states in the energy gap.

Here E_{LUMO} is considered to be 0, so it reduces to the form:

$$g(E) = \frac{N_{Deep}}{\varphi_{Deep}} \cdot e^{\frac{E}{\varphi_{Deep}}} + \frac{N_{Tail}}{\varphi_{Tail}} \cdot e^{\frac{E}{\varphi_{Tail}}}$$

So, the exact carrier density for the stated Double-EDOS would be:

$$\delta = \frac{1}{N_t} \int_{-\infty}^{0} g(E) \cdot f_e(E) dE$$

Here N_t is a normalization parameter such that $\int_{-\infty}^{0} g(E) dE$ is 1. Hence $N_t$can be found out as:

$$N_t = N_{Deep} + N_{Tail}$$

$$= \frac{1}{N_t}\int_{-\infty}^{0} \frac{\frac{N_{Deep}}{\varphi_{Deep}} \cdot e^{\frac{E}{\varphi_{Deep}}} + \frac{N_{Tail}}{\varphi_{Tail}} \cdot e^{\frac{E}{\varphi_{Tail}}}}{1 + e^{\frac{E-E_F}{k_B T}}} dE$$

$$= \frac{N_{Deep}}{\varphi_{Deep}} \cdot \frac{1}{N_t}\int_{-\infty}^{0} \frac{e^{\frac{E}{\varphi_{Deep}}}}{1 + e^{\frac{E-E_F}{k_B T}}} dE \; + \frac{N_{Tail}}{\varphi_{Tail}} \cdot \frac{1}{N_t}\int_{-\infty}^{0} \frac{e^{\frac{E}{\varphi_{Tail}}}}{1 + e^{\frac{E-E_F}{k_B T}}} dE$$

$$= \frac{N_{Deep}}{\varphi_{Deep}} \cdot \frac{1}{N_t}\int_{-\infty}^{0} \frac{e^{\frac{E}{\varphi_{Deep}}}}{1 + e^{\frac{E-E_F}{k_B T}}} dE \; + \frac{N_{Tail}}{\varphi_{Tail}} \cdot \frac{1}{N_t}\int_{-\infty}^{0} \frac{e^{\frac{E}{\varphi_{Tail}}}}{1 + e^{\frac{E-E_F}{k_B T}}} dE$$

$$\delta = \frac{N_{Deep}}{\varphi_{Deep}} \cdot \frac{1}{N_t}\int_{0}^{\infty} \frac{e^{\frac{-E}{\varphi_{Deep}}}}{1 + e^{\frac{-(E+E_F)}{k_B T}}} dE \; + \frac{N_{Tail}}{\varphi_{Tail}} \cdot \frac{1}{N_t}\int_{0}^{\infty} \frac{e^{\frac{-E}{\varphi_{Tail}}}}{1 + e^{\frac{-(E+E_F)}{k_B T}}} dE$$

Now terms in both the summation are similar in nature and differ in only coefficients φ_{Deep} and φ_{Tail} and coefficients outside the integral. So, we calculate only one of the terms of the summation and derive the other by simply substituting the parameters.

To solve the above integral let us perform some substitutions:

$$x = \frac{E}{k_B T}, \; \xi = \frac{E_F}{k_B T}, \; \; \varphi_{Deep} = k_B T_{Deep}, \varphi_{Tail} = k_B T_{Tail}$$

$$\delta_1 = \frac{N_{Deep}}{\varphi_{Deep}} \cdot \frac{1}{N_t}\int_{0}^{\infty} \frac{e^{\frac{-E}{\varphi_{Deep}}}}{1 + e^{\frac{-(E+E_F)}{k_B T}}} dE \quad \delta_2 = \frac{N_{Tail}}{\varphi_{Tail}} \cdot \frac{1}{N_t}\int_{0}^{\infty} \frac{e^{\frac{-E}{\varphi_{Tail}}}}{1 + e^{\frac{-(E+E_F)}{k_B T}}} dE$$

$$\delta = \delta_1 + \delta_2$$

B. SOLUTION OF THE INTEGRAL USING EXACT TECHNIQUES

The equation is:

$$\delta_1 = \frac{N_{Deep}}{\varphi_{Deep}} \cdot \frac{1}{N_t}\int_{0}^{\infty} \frac{e^{\frac{-E}{\varphi_{Deep}}}}{1 + e^{\frac{-(E+E_F)}{k_B T}}} dE$$

Performing the substitutions mentioned above we get:

$$\delta_1 = \frac{N_{Deep}}{\varphi_{Deep}} \cdot \frac{1}{N_t}\int_{0}^{\infty} \frac{e^{\frac{-x k_B T}{k_B T_{Deep}}}}{1 + e^{\frac{-(k_B T + \xi k_B T)}{k_B T}}} dE$$

$$= \frac{N_{Deep}}{T_{Deep}} \cdot \frac{1}{N_{Deep} + N_{Tail}} \cdot T \int_{0}^{\infty} \frac{e^{-x \cdot \frac{T}{T_{Deep}}}}{1 + e^{-(x+\xi)}} dx$$

$$= \frac{T}{T_{Deep}} \cdot \frac{N_{Deep}}{N_{Deep} + N_{Tail}} \int_0^\infty \frac{e^{-x \cdot \frac{T}{T_{Deep}}}}{1 + e^{-(x+\xi)}} dx$$

Since $\xi < 0$ for all practical considerations we substitute $\xi \to -|\xi|$ and get the equations as:

$$= \frac{T}{T_{Deep}} \cdot \frac{N_{Deep}}{N_{Deep} + N_{Tail}} \int_0^\infty \frac{e^{-x \cdot \frac{T}{T_{Deep}}}}{1 + e^{-(x-|\xi|)}} dx$$

$$= \frac{T}{T_{Deep}} \cdot \frac{N_{Deep}}{N_{Deep} + N_{Tail}} \cdot e^{-|\xi|} \int_0^\infty \frac{e^{x \cdot \left(1 - \frac{T}{T_{Deep}}\right)}}{1 + e^{(x-|\xi|)}} dx$$

Now consider $\frac{T}{T_{Deep}} \cdot \frac{N_{Deep}}{N_{Deep}+N_{Tail}} = A_{Deep}$ so the equation reduces to:

$$\delta_1 = A_{Deep} \cdot e^{-|\xi|} \int_0^\infty \frac{e^{x \cdot \left(1 - \frac{T}{T_{Deep}}\right)}}{1 + e^{(x-|\xi|)}} dx$$

Now, using the techniques in Selvaggi [13] to evaluate an approximation for this integral for calculation purposes. Let us consider integral $\int_0^\infty \frac{e^{x \cdot \left(1 - \frac{T}{T_{Deep}}\right)}}{1+e^{(x-|\xi|)}} dx$ as I_1 such that $\delta_1 = A_{Deep} \cdot e^{-|\xi|} I_1$, so,

$$I_1 = \int_0^\infty \frac{e^{x \cdot \left(1 - \frac{T}{T_{Deep}}\right)}}{1 + e^{(x-|\xi|)}} dx$$

$$= \int_0^{|\xi|} \frac{e^{x \cdot \left(1 - \frac{T}{T_{Deep}}\right)}}{1 + e^{(x-|\xi|)}} dx + \int_{|\xi|}^\infty \frac{e^{x \cdot \left(1 - \frac{T}{T_{Deep}}\right)}}{1 + e^{(x-|\xi|)}} dx$$

As discussed in [17-18], we have:

$$\frac{1}{1 + e^{z-\eta}} = \lim_{N \to \infty} \sum_{m=0}^{N} f_m(-1) \times \begin{cases} e^{-(1+m)(z-\eta)}, & for\ z \geq \eta \\ e^{(z-\eta)m}, & for\ z \leq \eta \end{cases}$$

It is also known that $f_m(n) = \frac{1}{m!} \prod_{i=0}^{m-1} n - i$, so, $f_m(-1) = (-1)^m$

So, writing I_1 as follows according to the expansion stated above:

$$= \int_0^{|\xi|} \frac{e^{x \cdot \left(1 - \frac{T}{T_{Deep}}\right)}}{1 + e^{(x-|\xi|)}} dx + \int_{|\xi|}^\infty \frac{e^{x \cdot \left(1 - \frac{T}{T_{Deep}}\right)}}{1 + e^{(x-|\xi|)}} dx$$

$$= \int_0^{|\xi|} e^{x \cdot \left(1 - \frac{T}{T_{Deep}}\right)} \cdot \sum_{p=0}^{\infty} (-1)^p \cdot e^{(x-|\xi|) \cdot p}\ dx + \int_{|\xi|}^\infty e^{x \cdot \left(1 - \frac{T}{T_{Deep}}\right)} \cdot \sum_{p=0}^{\infty} (-1)^p \cdot e^{-(x-|\xi|) \cdot (1+p)}\ dx$$

$$= \int_0^{|\xi|} e^{x\cdot\left(1-\frac{T}{T_{Deep}}\right)} + \int_0^{|\xi|} e^{x\cdot\left(1-\frac{T}{T_{Deep}}\right)} \cdot \sum_{p=1}^{\infty} (-1)^p \cdot e^{(x-|\xi|)\cdot p}\ dx$$

$$- \int_{|\xi|}^{\infty} e^{x\cdot\left(1-\frac{T}{T_{Deep}}\right)} \cdot \sum_{p=1}^{\infty} (-1)^p \cdot e^{-(x-|\xi|)\cdot(p)}\, dx$$

$$= \int_0^{|\xi|} e^{x\cdot\left(1-\frac{T}{T_{Deep}}\right)} + \sum_{p=1}^{\infty} (-1)^p$$

$$\times \left[\int_0^{|\xi|} e^{x(1-\frac{T}{T_{Deep}})} \cdot e^{(x-|\xi|)\cdot p}\, dx - \int_{|\xi|}^{\infty} e^{x(1-\frac{T}{T_{Deep}})} \cdot e^{-(x-|\xi|)\cdot p}\, dx\right]$$

$$= \int_0^{|\xi|} e^{x\cdot\left(1-\frac{T}{T_{Deep}}\right)} + \sum_{p=1}^{\infty} (-1)^p \times \left[\int_0^{|\xi|} e^{x(p+1-\frac{T}{T_{Deep}})} \cdot e^{-p|\xi|}\, dx - \int_{|\xi|}^{\infty} e^{-x(p-1+\frac{T}{T_{Deep}})} \cdot e^{p|\xi|}\, dx\right]$$

$$= \int_0^{|\xi|} e^{x\left(1-\frac{T}{T_{Deep}}\right)} + \sum_{p=1}^{\infty} (-1)^p \times \left[e^{-p|\xi|} \int_0^{|\xi|} e^{x(p+1-\frac{T}{T_{Deep}})}\, dx - e^{p|\xi|} \int_{|\xi|}^{\infty} e^{-x(p-1+\frac{T}{T_{Deep}})}\, dx\right]$$

$$= \int_0^{|\xi|} e^{x\left(1-\frac{T}{T_{Deep}}\right)} + \sum_{p=1}^{\infty} (-1)^p \times \left[e^{-p|\xi|} \frac{e^{|\xi|(p+1-\frac{T}{T_{Deep}})} - 1}{p+1-\frac{T}{T_{Deep}}} - e^{p|\xi|} \frac{0 - e^{-|\xi|(p-1+\frac{T}{T_{Deep}})}}{-\left(p-1+\frac{T}{T_{Deep}}\right)}\right]$$

$$= \frac{e^{|\xi|\left(1-\frac{T}{T_{Deep}}\right)} - 1}{\left(1-\frac{T}{T_{Deep}}\right)} + \sum_{p=1}^{\infty} (-1)^p \times \left[\frac{e^{|\xi|(1-\frac{T}{T_{Deep}})} - e^{-p|\xi|}}{p+1-\frac{T}{T_{Deep}}} - \frac{e^{|\xi|(1-\frac{T}{T_{Deep}})}}{p-1+\frac{T}{T_{Deep}}}\right]$$

$$= \frac{e^{|\xi|\left(1-\frac{T}{T_{Deep}}\right)} - 1}{\left(1-\frac{T}{T_{Deep}}\right)} + \sum_{p=1}^{\infty} (-1)^p \times \left[\frac{e^{|\xi|(1-\frac{T}{T_{Deep}})}}{p+1-\frac{T}{T_{Deep}}} - \frac{e^{|\xi|(1-\frac{T}{T_{Deep}})}}{p-1+\frac{T}{T_{Deep}}}\right]$$

$$- \sum_{p=1}^{\infty} (-1)^p \frac{e^{-p|\xi|}}{p+\left(1-\frac{T}{T_{Deep}}\right)}$$

$$= \frac{e^{|\xi|\left(1-\frac{T}{T_{Deep}}\right)} - 1}{\left(1-\frac{T}{T_{Deep}}\right)} + e^{|\xi|(1-\frac{T}{T_{Deep}})} \cdot \sum_{p=1}^{\infty} \left[\frac{(-1)^p}{p+1-\frac{T}{T_{Deep}}} - \frac{(-1)^p}{p-1+\frac{T}{T_{Deep}}}\right]$$

$$- \sum_{p=1}^{\infty} (-1)^p \frac{e^{-p|\xi|}}{p+\left(1-\frac{T}{T_{Deep}}\right)}$$

$$= \frac{e^{|\xi|\left(1-\frac{T}{T_{Deep}}\right)} - 1}{\left(1 - \frac{T}{T_{Deep}}\right)} + e^{|\xi|(1-\frac{T}{T_{Deep}})} \cdot [\phi\left(-1,1,\frac{T}{T_{Deep}}\right) - \phi(-1,1,2 - \frac{T}{T_{Deep}})]$$

$$- \sum_{p=1}^{\infty} (-1)^p \frac{e^{-p|\xi|}}{p + \left(1 - \frac{T}{T_{Deep}}\right)}$$

Here $\phi(z, s, \alpha)$ gives Hurwitz Lerch transcendent [19]

$\phi(z, s, \alpha) = \sum_{p=0}^{\infty} \frac{z^p}{(p+\alpha)^s}$

The expression [20] $[\phi\left(-1,1,\frac{T}{T_{Deep}}\right) - \phi(-1,1,2 - \frac{T}{T_{Deep}})]$ reduces to: $-\frac{1}{1-\frac{T}{T_{Deep}}} + \frac{\pi}{\sin(\frac{\pi T}{T_{Deep}})}$

So,

$$I_1 = \frac{e^{|\xi|\left(1-\frac{T}{T_{Deep}}\right)} - 1}{\left(1 - \frac{T}{T_{Deep}}\right)} + e^{|\xi|(1-\frac{T}{T_{Deep}})} \cdot [-\frac{1}{1 - \frac{T}{T_{Deep}}} + \frac{\pi}{\sin(\frac{\pi T}{T_{Deep}})}] - \sum_{p=1}^{\infty} (-1)^p \frac{e^{-p|\xi|}}{p + \left(1 - \frac{T}{T_{Deep}}\right)}$$

$$I_1 = \frac{e^{|\xi|\left(1-\frac{T}{T_{Deep}}\right)} - 1}{\left(1 - \frac{T}{T_{Deep}}\right)} - \frac{e^{|\xi|\left(1-\frac{T}{T_{Deep}}\right)}}{\left(1 - \frac{T}{T_{Deep}}\right)} + e^{|\xi|\left(1-\frac{T}{T_{Deep}}\right)} \cdot \left[\frac{\pi}{\sin\left(\frac{\pi T}{T_{Deep}}\right)}\right] - \sum_{p=0}^{\infty} (-1)^p \frac{e^{-p|\xi|}}{p + \left(1 - \frac{T}{T_{Deep}}\right)}$$
$$+ \frac{1}{1 - \frac{T}{T_{Deep}}}$$

$$I_1 = e^{|\xi|\left(1-\frac{T}{T_{Deep}}\right)} \cdot \left[\frac{\pi}{\sin\left(\frac{\pi T}{T_{Deep}}\right)}\right] - \sum_{p=0}^{\infty} (-1)^p \frac{e^{-p|\xi|}}{p + \left(1 - \frac{T}{T_{Deep}}\right)}$$

Now since $\delta_1 = A_{Deep} \cdot e^{-|\xi|} I_1$ so computing δ_1 using the simplified value of I_1 we get:

$$\delta_1 = A_{Deep} \cdot e^{-|\xi|} \cdot \left[e^{|\xi|\left(1-\frac{T}{T_{Deep}}\right)} \cdot \left[\frac{\pi}{\sin\left(\frac{\pi T}{T_{Deep}}\right)}\right] - \sum_{p=0}^{\infty} (-1)^p \frac{e^{-p|\xi|}}{p + \left(1 - \frac{T}{T_{Deep}}\right)}\right]$$

$$= \frac{T}{T_{Deep}} \frac{N_{Deep}}{N_{Deep} + N_{Tail}} e^{-|\xi|} \left[e^{|\xi|\left(1-\frac{T}{T_{Deep}}\right)} \cdot \left[\frac{\pi}{\sin\left(\frac{\pi T}{T_{Deep}}\right)}\right] - \sum_{p=0}^{\infty} (-1)^p \frac{e^{-p|\xi|}}{p + \left(1 - \frac{T}{T_{Deep}}\right)}\right]$$

$$\delta_1 = \frac{N_{Deep}}{N_{Deep} + N_{Tail}} \left[e^{-|\xi|\frac{T}{T_{Deep}}} \cdot \left[\frac{\frac{\pi T}{T_{Deep}}}{\sin\left(\frac{\pi T}{T_{Deep}}\right)}\right] - \frac{T}{T_{Deep}} e^{-|\xi|} \sum_{p=0}^{\infty} (-1)^p \frac{e^{-p|\xi|}}{p + \left(1 - \frac{T}{T_{Deep}}\right)}\right]$$

Similarly calculating δ_2 by replacing A_{Deep} by A_{Tail} and T_{Deep} by T_{Tail} in δ_1 , we get:

$$\delta_2 = \frac{N_{Tail}}{N_{Deep}+N_{Tail}}\left[e^{-|\xi|\frac{T}{T_{Tail}}}\cdot\left[\frac{\frac{\pi T}{T_{Tail}}}{\sin\left(\frac{\pi T}{T_{Tail}}\right)}\right]-\frac{T}{T_{Tail}}e^{-|\xi|}\sum_{p=0}^{\infty}(-1)^p\frac{e^{-p|\xi|}}{p+\left(1-\frac{T}{T_{Tail}}\right)}\right]$$

So, $= \delta_1+\delta_2$:

$$\delta = \frac{N_{Deep}}{N_{Deep}+N_{Tail}}\left[e^{-|\xi|\frac{T}{T_{Deep}}}\cdot\left[\frac{\frac{\pi T}{T_{Deep}}}{\sin\left(\frac{\pi T}{T_{Deep}}\right)}\right]-\frac{T}{T_{Deep}}e^{-|\xi|}\sum_{p=0}^{\infty}(-1)^p\frac{e^{-p|\xi|}}{p+\left(1-\frac{T}{T_{Deep}}\right)}\right]$$
$$+\frac{N_{Tail}}{N_{Deep}+N_{Tail}}\left[e^{-|\xi|\frac{T}{T_{Tail}}}\cdot\left[\frac{\frac{\pi T}{T_{Tail}}}{\sin\left(\frac{\pi T}{T_{Tail}}\right)}\right]-\frac{T}{T_{Tail}}e^{-|\xi|}\sum_{p=0}^{\infty}(-1)^p\frac{e^{-p|\xi|}}{p+\left(1-\frac{T}{T_{Tail}}\right)}\right]$$

C. MODIFIED CHARGE CARRIER DENSITY

In order to develop a modified model, we approximate the above exact equation of δ by calculating it only for p=0 and neglecting higher order terms for p = 1,2,3 …

$$\delta \cong \frac{N_{Deep}}{N_{Deep}+N_{Tail}}\left[e^{-|\xi|\frac{T}{T_{Deep}}}\cdot\left[\frac{\frac{\pi T}{T_{Deep}}}{\sin\left(\frac{\pi T}{T_{Deep}}\right)}\right]-e^{-|\xi|}\frac{\frac{T}{T_{Deep}}}{1-\frac{T}{T_{Deep}}}\right]$$
$$+\frac{N_{Tail}}{N_{Deep}+N_{Tail}}\left[e^{-|\xi|\frac{T}{T_{Tail}}}\cdot\left[\frac{\frac{\pi T}{T_{Tail}}}{\sin\left(\frac{\pi T}{T_{Tail}}\right)}\right]-e^{-|\xi|}\frac{\frac{T}{T_{Tail}}}{1-\frac{T}{T_{Tail}}}\right]$$

III. ANALYSIS AND RESULTS

Following value have been used for the delta equation to plot the charge carrier density function for various value of E_F.

Table 1. Values of the physical parameters.

Parameters	Values
N_{Deep}	$4.8 \cdot 10^{19}$
ϕ_{Deep}	$1.28 \cdot 10^{-20}$
N_{Tail}	$4.2 \cdot 10^{21}$
ϕ_{Tail}	$0.48 \cdot 10^{-20}$
E_{LUMO}	0
E_F	$-1.6 \cdot 10^{-19}$
k_B	$1.38 \cdot 10^{-22}$
T	300

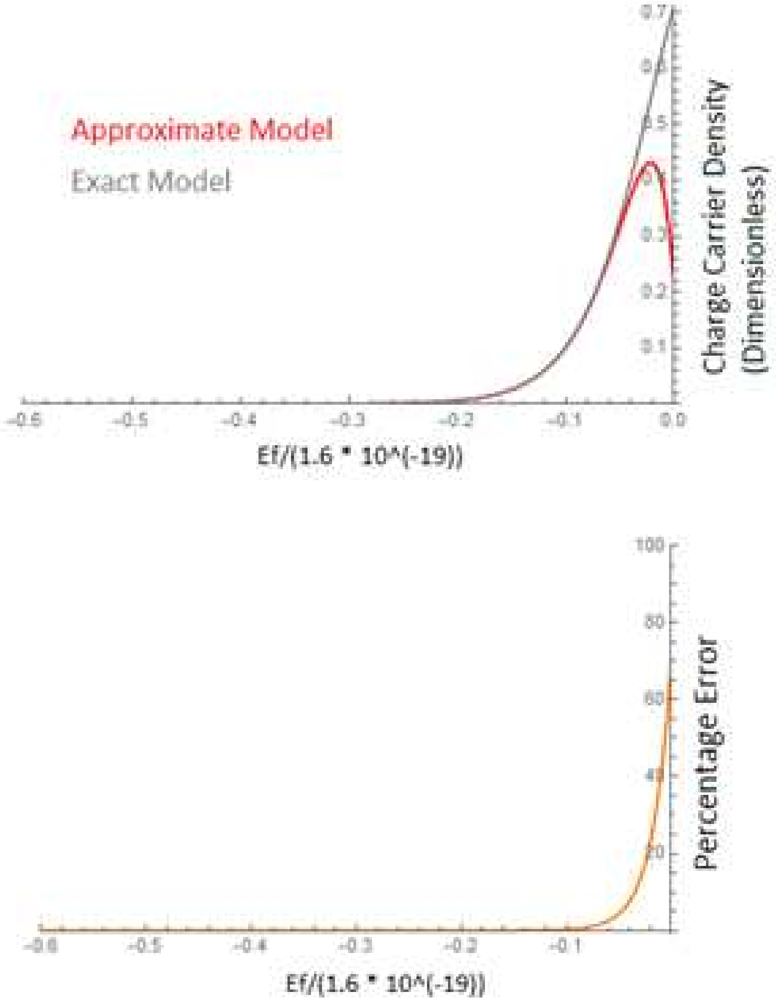


Fig. 3.1 a, b: Exact and Approximate Model and relative error for charge carrier density using Double-EDOS EF is varied

Next we compare the values of charge carrier density for varying values of E_f for both exact and approximated expressions for varying degree of approximation (based on different values of p, 0 being highly approximated and as we increase p, it converges to the actual expression)

Table 2 Deviation from actual values as (E_F) is varied

E_f	Actual value	Percentage deviation in value of approximated expression as p increases						
eV		p=0	p=1	p=2	p=3	p=4	p=5	p=6
0	$3.033\cdot 10^{21}$	71	-34	22	-16	12	-10	9
-0.1	$4.346\cdot 10^{20}$	0.319	-0.003	10^{-5}	10^{-7}	10^{-8}	10^{-10}	10^{-12}
-0.5	$1.122\cdot 10^{17}$	10^{-11}	10^{-11}	10^{-11}	10^{-11}	10^{-11}	10^{-11}	10^{-11}
-1	$2.138\cdot 10^{14}$	10^{-7}	10^{-7}	10^{-7}	10^{-7}	10^{-7}	10^{-7}	10^{-7}
-1.5	$4.127\cdot 10^{11}$	10^{-13}	10^{-13}	10^{-13}	10^{-13}	10^{-13}	10^{-13}	10^{-13}

As it can be seen in Table 2, deviation is quite negligible even for p=0, among values of E_f greater that 10% of 1eV, and the deviation remains fairly constant in order when we increase the value of p, hence we can conclude that as far as E_f is considered the approximated expression for charge carrier density with p=0 would be suited for a fairly accurate representation of the actual integral.

Table 3 Deviation from actual values as ($\phi_{Deep,Tail}$) varied

ϕ_{Deep} (eV)	ϕ_{Tail} (eV)	Actual value	Percentage deviation in value of approximated expression as p increases			
			p=0	p=1	p=2	p=6
0.08	0.03	$2.138 \cdot 10^{14}$	10^{-7}	10^{-7}	10^{-7}	10^{-7}
0.10	0.05	$2.453 \cdot 10^{15}$	10^{-9}	10^{-9}	10^{-9}	10^{-9}
0.12	0.07	$1.579 \cdot 10^{16}$	10^{-10}	10^{-10}	10^{-10}	10^{-10}
0.14	0.09	$1.123 \cdot 10^{17}$	10^{-11}	10^{-11}	10^{-11}	10^{-11}
0.16	0.11	$6.160 \cdot 10^{17}$	10^{-12}	10^{-12}	10^{-12}	10^{-12}

Now we perform a similar analysis for varying temperature, ϕ_{Deep} , ϕ_{Tail} , N_{Deep} and N_{Tail}.

As it can be observed from Table 3, there is minimal effect of approximation as ϕ_{Deep} , ϕ_{Tail} are varied the percentage error is less than 10^{-7} for the most part, and also order of the error remains same for subsequent values of p, hence in this instance too, the result obtained taking p=0 is a good approximation to the actual integration.

Table 4 Deviation from actual values as $N_{Deep,Tail}$ are varied

N_{Deep} x10^{19} (cm^{-3})	N_{Tail} x10^{21} (cm^{-3})	Actual value	Percentage deviation in value of approximated expression as p increases			
			p=0	p=1	p=2	p=6
0.0048	0.0042	$2.138 \cdot 10^{11}$	10^{-7}	10^{-7}	10^{-7}	10^{-7}
0.48	0.42	$2.138 \cdot 10^{13}$	10^{-7}	10^{-7}	10^{-7}	10^{-7}
4.8	4.2	$2.138 \cdot 10^{14}$	10^{-7}	10^{-7}	10^{-7}	10^{-7}
0.48	42	$2.138 \cdot 10^{13}$	10^{-5}	10^{-5}	10^{-5}	10^{-5}
0.0048	4200	$3.045 \cdot 10^{11}$	0.142	0.142	0.142	0.142

From the Table 4 and following two conclusions can be made:

First, that as N_{Tail} increases and N_{Deep} decreases simultaneously, the error in the approximated values from the actual values, regardless of increasing p-values, increases significantly, e.g. when the order of N_{Tail}/N_{Deep} is 100 the error across the approximated values is of order 10^{-7} and when the order of N_{Tail}/N_{Deep} increases to 1000 the order of error increases to 10^{-5}**.** Also we observe that for different values of N_{Deep} and N_{Tail} if the order is constant the order of error is also constant. Next as we increase the order of N_{Tail}/N_{Deep} to 10^{8}, we see a steep rise in the percentage error value which now 0.142, an order of 10^{-1}.

Second, we see that increasing the p-values up to a reasonable level, 6 does not have any effect on deviation, i.e. as we change N_{Deep} and N_{Tail} the approximated expression converges very slowly to the real expression and hence, for we can assume p=0 in this case too and get a reasonably approximate solution.

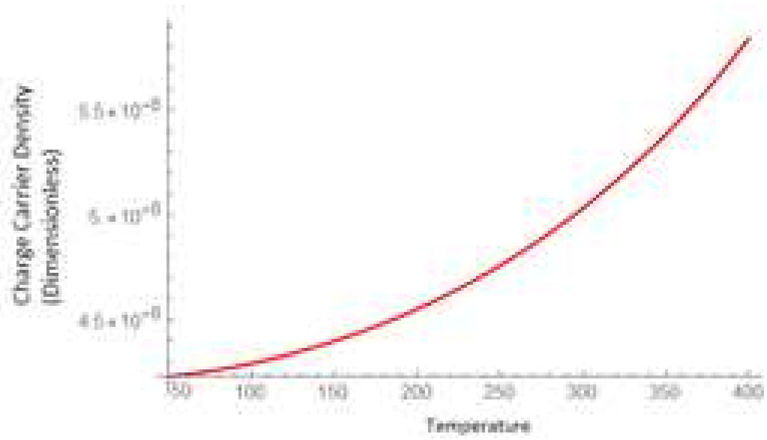
Table 5 represents the variation in temperature from 50K – 500K with deviation in approximate and exact model, keeping all other parameters fixed at the specified values.

Table 5 Deviation from actual values as Temperature varies

Temp. (K)	Actual Value	Percentage deviation in values of approximated expression as p increases			
		p=0	p=1	p=2	p=6
50	$1.797 \cdot 10^{14}$	10^{-12}	10^{-12}	10^{-12}	10^{-12}
100	$1.823 \cdot 10^{14}$	10^{-13}	10^{-13}	10^{-13}	10^{-13}
200	$1.933 \cdot 10^{14}$	10^{-13}	10^{-13}	10^{-13}	10^{-13}
250	$2.021 \cdot 10^{14}$	10^{-11}	10^{-11}	10^{-11}	10^{-11}
300	$2.138 \cdot 10^{14}$	10^{-7}	10^{-7}	10^{-7}	10^{-7}
350	$2.288 \cdot 10^{14}$	10^{-9}	10^{-9}	10^{-9}	10^{-9}
500	$3.063 \cdot 10^{14}$	10^{-10}	10^{-10}	10^{-10}	10^{-10}

As documented in the Table 5, we can see that temperature doesn't affect the charge carrier density as much as the other factors do. Also the error in the approximated expression is less that 10^{-7} for the temperatures between 50K and 500K. We also conclude that increasing the value of p at least till p=6 doesn't contribute much in increasing the accuracy as the order of the error remains the same. Hence p=0 is a good choice for approximation as far as temperature is concerned.

Now, the variation of charge carrier density with temperature and percentage error which corroborates our findings are shown in Fig. 3.2a and 3.2b.



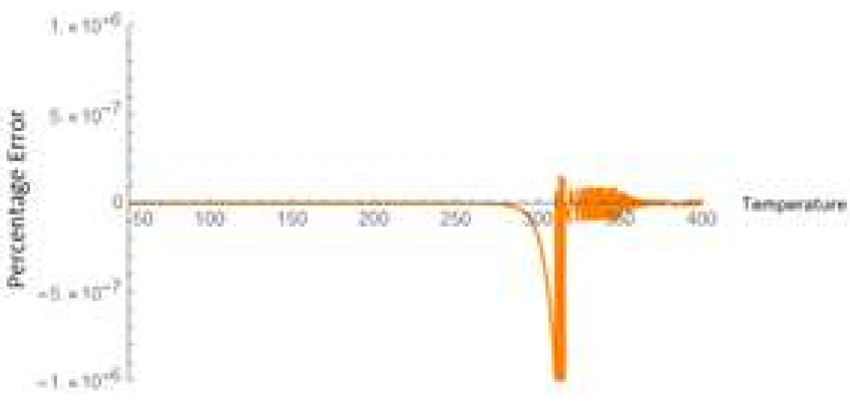


Fig. 3.2 a, b: Exact and Approximate Model for charge carrier density using Double-EDOS temperature

is varied

IV. CONCLUSION

After using various approximation techniques and employing various mathematical methods to do so we have evaluated a fairly simple closed form of charge carrier density function with quite less error range for a wide range of parameter values. Earlier, the literature for Single Exponential Density of States are available and techniques applied for this double exponential density of states is quite similar to those used for single exponential density of states. One of techniques used was expanding $\frac{1}{1+e^{(x-|\xi|)}}$ using binomial expansions. The second technique applied was writing a summation of form $\sum_{n=0}^{\infty}\frac{(-1)^n}{(n+\alpha)^s}$ as a HurwitzLerchPhi transcendental notion. Finally, we put the higher order terms of a diminishing series to zero and took in account only the first term to get a closed form of the integral.

After a detailed error analysis on the approximated charge carrier density expression and the degree of approximation versus the exact expression, it is concluded that approximations are a very computationally-efficient replacement to the exact expressions for a wide range of parameters involved in the charge carrier density evaluation and show a very less relative error.

Also the expression with highest degree of approximation i.e. for p=0 can be selected as the primary expression to evaluate charge carrier density as further increment in the value of p lead to increased computational complexity whereas the increase in accuracy is marginal. Hence, the final approximated expression is obtained by keeping p=0 and neglecting the diminishing higher order terms.

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