General Drift-Diffusion Theory of the Current Density in Schottky Diodes

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Abstract—A new general expression for the current in Schottky diodes due to drift-diffusion but neglecting tunneling is presented. A precise expression for the ideality factor is derived. The temperature dependence of important quantities in both the degenerate (heavy doping) and nondegenerate (Boltzmann) limit is examined. In the degenerate regime, the temperature independence of the saturation current is shown to complicate the extraction of the barrier height from the current-voltage characteristics.

I. INTRODUCTION

ALTHOUGH the theory of Schottky diodes (or more generally metal-semiconductor interfaces) has a long and rich history [1], [2], a complete understanding is still not achieved. Most of the literature concentrates on the determination of the barrier height between the metal and semiconductor interface, but relatively little effort has been devoted to heavily doped diodes. Very often, weak temperature dependence of the ideality factor was ascribed to tunneling [2]. In addition, our analysis emphasizes that the temperature independence of the current for high doping concentrations complicates the extraction of the barrier height from current-voltage characteristics significantly. As a conclusion, we point out that the knowledge of the barrier height alone is insufficient except both the doping concentration and the temperature interval from which the data is extracted are specified.

These new insights may help to improve the current understanding for heavily doped Schottky diodes.

II. INTEGRAL FORM OF THE DRIFT-DIFFUSION EQUATION

When applying a voltage $V$ across a n-type semiconductor, the electric current density due to electrons in one-dimension, $J_n(V)$, satisfies the drift-diffusion equation [5]

$$J_n(V) = q\mu_n(x)n(x;V)\mathcal{E}(x;V) + qD_n(x)\frac{dn(x;V)}{dx}$$

(1)

where $\mu_n(x)$ is the electron mobility, $D_n(x)$ is the electron diffusion coefficient, $n(x;V)$ denotes the density of electrons as a function of distance $x$ and of applied voltage $V$ and $\mathcal{E}(x;V)$ is the electric field at position $x$ corresponding to the applied voltage $V$. For the sake of brevity, we limit the discussion to n-type semiconductors. The adoption of the one-dimensional drift-diffusion equation (1) is the sole approximation made. The voltage independent mobility excludes cases where velocity saturation occurs. But, more important, the drift-diffusion equation (1) does not account for tunneling that undoubtedly plays a role in heavily doped Schottky diodes at low temperatures.

At a constant temperature $T$ in equilibrium ($V = 0$), there is no current or $J_n(0) = 0$. This condition relates the electron mobility and diffusion coefficient as

$$\frac{\mu_n(x)}{D_n(x)} = \frac{\partial \ln[n(x;0)]}{\partial \phi(x;0)} \equiv f(x)$$

(2)

where the electrostatic potential $\phi(x;V)$ and the electric field are linked by $\mathcal{E}(x;V) = -\frac{\partial \phi(x;V)}{\partial x}$. When assuming Boltzmann statistics, (2) reduces to the well known Einstein relation [14] $f(x) = \frac{1}{k_B T}$. With Fermi–Dirac statistics concentrations where Boltzmann statistics are valid to $\beta = 1$ for heavily doped diodes. Previously an inverse $T$-law for the ideality factor was ascribed to tunneling [2].
and a parabolic density of states\(^1\) \(f(x)\) can be rewritten as

\[
f(x) = \frac{q}{k_B T} F^{-1/2}_{-1/2} \left[ \frac{q\psi(x;0) - \phi_n(x;0)}{k_B T} \right] F_{1/2} \left[ \frac{q\psi(x;0) - \phi_n(x;0)}{k_B T} \right]
\]

where \(\phi_n(x; V)\) is the quasi-fermi level for electrons at position \(x\) when the voltage \(V\) is applied over the diode and \(\phi_n(x; 0) = -E_F/q\) for a Fermi level \(E_F\). Since \(F_{-1/2}(y) \leq 1\) for real \(q > p > -1\) we find the upper bound \(f(x) \leq \frac{q}{k_B T} \).

In addition \(f(x)\) is positive. Thus

\[
0 < f(x) \leq \frac{q}{k_B T}.
\]

This implies that the Boltzmann limit gives the maximal value for \(f(x)\).

As demonstrated in the appendix, the electron current density \(J_n(V)\) in (1) can be rewritten as

\[
J_n(V) = J_s(V) \left( \frac{n(b; V)}{N(a; V)} \exp \left[ \int_a^b E(x; V) f(x) dx \right] - 1 \right)
\]

with

\[
J_s(V) = \frac{q n(a; V)}{\int_a^b \frac{d\xi}{D_n(x)} \exp \left[ \int_a^\xi E(u; V) f(u) du \right]}
\]

where \(a\) and \(b\) are arbitrary points in the semiconductor. Relation (5) being mathematically equivalent to (1), can include besides the Fermi–Dirac statistics all heavy doping effects as many body interactions [8] and bandtails [9]. One may wonder if (5) can be expanded around the low density limit (Boltzmann statistics) so that the degenerate case may be treated as a perturbation. Since we can show (see appendix) that the number of electrons can be rewritten in terms of Fermi–Dirac integrals for an arbitrary density of states and since the Fermi–Dirac integrals \(F_p(y)\) do not have a Dirichlet series for \(y > 0\) as shown by Dingle [10], we conclude that the degenerate regime is both mathematically and physically disconnected from the nondegenerate regime.

For Boltzmann statistics where \(n(x; V) = N \exp \left[ \frac{\psi(x; V) - \phi_n(x; V)}{k_B T} \right]\) and \(f(x) = \frac{\phi_n(x)}{D_n(x)} = \frac{q}{k_B T}\) equation

\[
(5) \text{ reduces to}
\]

\[
J_{nB}(V) = J_{sB}(V) \left( \exp \left[ \frac{q \psi_n(a; V) - \phi_n(b; V)}{k_B T} \right] - 1 \right)
\]

with

\[
J_{sB}(V) = \frac{q N \exp \left[ - \frac{q \psi_n(a; V)}{k_B T} \right]}{\int_a^b \frac{d\xi}{D_n(x)} \exp \left[ - \frac{q \psi(x; V)}{k_B T} \right]}
\]

III. CURRENT IN AN N-TYPE SCHOTTKY DIODE

We first consider Boltzmann statistics in order to compare our results with the expression of Crowell and Sze [11] or Taylor and Simmons [12]. Then, we will generalize the Boltzmann results using (6).

A realistic sketch of the conduction band profile is drawn in Fig. 1 (see also Fig. 6 on pp. 253 in [14] and potential profiles computed in [20]). Let us choose \(a < x_0\) and \(b\) in the quasi-neutral region. The point \(x_0\) is the position in the semiconductor close to the metal interface where the potential \(\psi(x) = -E_c(x)/q\) reaches its minimum (see Fig. 1). Initially, we rewrite and physically interpret (8) relying on the shape of the sketch in Fig. 1. Afterwards, we will discuss the influence of the precise location of \(a\) and \(b\) and of the interface boundary conditions.

Equation (8) can be rewritten as (see (9) at bottom of page). The first integral in the denominator \(I_1 = \exp \left[ \frac{q \psi(x_0; V)}{k_B T} \right] \int_a^{x_0} \frac{d\xi}{D_n(x)} \exp \left[ - \frac{q \psi(x; V)}{k_B T} \right]\) can be approximated as follows. Around its minimum \(x_0\) the potential increases rapidly. This observation suggests to use the method of the steepest descent (4.6 in [15]). We expand the potential

\[
J_{sB}(V) = \frac{q N \exp \left[ \frac{q \psi(n; V) - \phi_n(n; V)}{k_B T} \right]}{\exp \left[ \frac{q \psi_n(a; V) - \phi_n(x_0; V)}{k_B T} \right] \int_a^{x_0} \frac{d\xi}{D_n(x)} \exp \left[ - \frac{q \psi(x; V)}{k_B T} \right] + \int_{x_0}^b \frac{d\xi}{D_n(x)} \exp \left[ - \frac{q \psi(x; V)}{k_B T} \right]}
\]
around the minimum $x_0$ where $\psi''(x) > 0$ and obtain

\[
I_1 \approx \int_x^{x_0} \frac{dx}{D_n(x)} \exp \left( -\frac{q\psi''(x;0;V)}{2k_BT}(x-x_0)^2 \right)
\]

\[
\approx \frac{1}{2} \int_x^{x_0} \frac{dx}{D_n(x)} \exp \left( -\frac{q\psi''(x;0;V)}{2k_BT}(x-x_0)^2 \right)
\]

\[
\approx \frac{1}{2D_n(x_0)} \int_{-\infty}^{x_0} dx \exp \left( -\frac{q\psi''(x;0;V)}{2k_BT}(x-x_0)^2 \right)
\]

\[
= \frac{1}{2D_n(x_0)} \sqrt{\frac{2\pi k_BT}{q^2 n_{net}}}.
\]

We use the Poisson equation $\psi''(x) = -\frac{z}{q} q\text{net}(x)$ where $q\text{net}$ denotes the total net charge. Since $\psi''(x_0) > 0$ we have that $n_{net} < 0$ regardless of the doping concentration of the semiconductor. The charge distribution where the curvature of the potential is positive consists mainly of electrons. The underlying physical phenomena, image charge and correlation effects, have been analyzed in detail by Vinter [13]. In this seemingly metallic region we can define a "Debye length $L_{Dm}$" as

\[
L_{Dm} = \sqrt{\frac{e^2 k_BT}{q^2 n_{net}}}
\]

and obtain for $I_1$

\[
I_1 \approx \sqrt{\frac{\pi}{2D_n(x_0)}} v_e^{-1}
\]

The diffusion coefficient can be written as $D_n(x_0) = l_n v_{th}$ where $l_n$ and $v_{th} = \sqrt{\frac{2k_BT}{m^*}}$ denotes the electron mean free path and the thermal velocity in a material with effective mass $m^*$, respectively. Thus, we have

\[
I_1 \approx \sqrt{\frac{\pi}{2} v_{th}^{-1} L_{Dn}} \equiv v_e^{-1}
\]

where $v_e$ describes the velocity of electrons at $x_0$.

The second integral, $I_2 = \exp \left( \frac{-q\psi(x;V)}{k_BT} \right) \int_{x_0}^{x} dx \exp \left( -\frac{q\psi''(x;0;V)}{k_BT} (x-x_0)^2 \right)$, has been thoroughly investigated in the literature [1] and approximated as

\[
v_e \approx 2v_{th} \sqrt{\frac{l_n}{L_D}} \left[ \frac{q[V_{bi}-V]}{k_BT} \right]^{-1}
\]

where $L_D$ denotes the usual Debye length [14] and $V_{bi}$ is the built-in potential. The quantity $v_e$ describes the velocity of electrons in the depletion layer due to a drift-diffusion mechanism. Since both defined velocities are weakly voltage dependent, it is in general difficult to determine which is dominant. The two extreme regimes are broadly discussed in [1]. The approximations for $I_1$ and $I_2$ simplify the expression of the saturation current considerably,

\[
J_{SB}(V) = \frac{qN_c}{v_th} \exp \left( \frac{\Phi_{MS} - \phi_n(a;V)}{k_BT} \right)
\]

\[
\times \exp \left( -\frac{q[\psi(a;V) - \psi(x;0;V)]}{k_BT} \right).
\]

At this point we introduce the concept of a barrier height $\Phi_{MS}$ between the metal and semiconductor. From Fig. 1, we read that $\Phi_{MS} = q[\psi(a;V) - \psi(x;0;V)]$. So far the precise location of the point $a$ was not required. Since the region $[0,x_0]$ is shown to be effectively metallic, the potential $\psi(a;V)$ can be chosen to coincide with the quasi-fermi level in the metal that acts as potential reference ($\phi_n(a;V) = 0$). Hence, we choose the point $a$ sufficiently close to the metallurgical junction. Our final result which was originally due to Crowell and Sze [11] except with $v_m$ replaced by $v_{th}$, is

\[
J_n = \frac{qN_c}{v_th} \frac{\Phi_{MS}}{k_BT} \left[ \exp \left( \frac{qV}{k_BT} \right) - 1 \right]^{-1}
\]

It is instructive to briefly deduce the Simmons and Taylor formula. They essentially make two assumptions. First they neglect the Schottky effect [14] which means that $x_0$ lies precisely at the metallurgical junction and that the potential only exhibits a negative curvature (see dotted curve in Fig. 1). The omission of the Schottky effect causes only a small error as shown by Crowell and Sze [11]. Secondly, the metal interface current is approximated as

\[
J = qv_m[n(a;V) - n(a;0)].
\]

Substituting the expression for the interface density of electrons $n(a;V)$ from (5) into (17) and solving for $J_n = J$ yields

\[
J_n = \frac{qn(a;0)}{v_{th}^{-1} + v_e^{-1}} \left[ \frac{n(b;V)}{n(a;0)} \right] \left[ \exp \left( \int_{a}^{b} \frac{\mathcal{E}(x;V)f(x)dx}{k_BT} \right) - 1 \right].
\]

The Boltzmann approximation of (18) gives the Crowell-Sze or Simmons-Taylor formula

\[
J_n = \frac{qN_c}{v_{th}^{-1} + v_e^{-1}} \exp \left( \frac{-\Phi_{MS}}{k_BT} \right) \left[ \exp \left( \frac{qV}{k_BT} \right) - 1 \right].
\]
This equation implies that the reference for the quasi-fermi level is the Fermi level in the metal ($\phi_m(a;0) = 0$) and that the energy barrier between a metal and semiconductor equals $\Phi_{MS} = q\phi(0;0) - \phi_n(a;0)$. This result (19) only differs from (16) in the denominator. The generalized Simmons–Taylor result (18) is not an exact integral of the drift-diffusion equation (1) in contrast to (5) with the boundary values explained above. The reason for the discrepancy is that they allow (17) to modify the result.

When examining the general relation (5), the saturation current can be rewritten analogously as (see (20) at bottom of previous page) where we have associated the integrals in the denominator with reciprocal velocities found in the Boltzmann nondegenerate case above. We observe that the barrier height $\Phi_{MS}$ does not appear explicitly anymore but that the information is concealed in

$$I_s = \int_{a}^{b} \epsilon(u,V)f(u)du. \quad (21)$$

This dimensionless integral describes the work done when crossing the interface potential barrier, however, modulated by the environment through $f(x)$. The consequence for degenerate Schottky diodes is discussed below.

**IV. THE IDEALITY FACTOR $m(V,T)$**

A commonly used quantity as figure of merit for the Schottky diode is the ideality factor $m(V,T)$ defined as

$$m(V,T) = \left( \frac{k_B T}{qV} \right) \ln \left( \frac{J_n(V)}{J_s(V)} + 1 \right)^{1} \quad (22)$$

or with (5)

$$\frac{1}{m(V,T)} = \frac{k_B T}{qV} \ln \left( \frac{n(b;V)}{n(a;V)} \right) + \int_{a}^{b} \epsilon(x;V)f(x)dx. \quad (23)$$

The definition (22) is often approximated [14] when Boltzmann statistics apply as

$$m(V,T) = \left[ \frac{k_B T}{q} \frac{\partial \ln [J_n(V)]}{\partial V} \right]^{-1} \quad \text{for} \quad V > \frac{k_B T}{q}. \quad (24)$$

Another expression follows from (1). After dividing (1) by $qD_n(x)n(x;V)$ and integrating over $[a, b]$ we obtain using (23)

$$J_n(V) \int_{a}^{b} \frac{dx}{qD_n(x)n(x;V)} = \ln \left( \frac{n(b;V)}{n(a;V)} \right) + \int_{a}^{b} \epsilon(x;V)f(x)dx \quad \equiv \frac{qV}{m(V,T)k_B T}. \quad (25)$$

Defining a voltage dependent 'area' resistance $\rho_A(V) = V/J_n(V)$ in $\Omega \cdot cm^2$, we find from (25) that

$$\rho_A(V) = \frac{m(V,T)k_B T}{q} \int_{a}^{b} \frac{dx}{Q_n(x)n(x;V)}. \quad (26)$$

The current density $J_n(V)$ can also be expressed in terms of the quasi-Fermi levels as $J_n(V) = -q\mu_n(x)n(x;V)\frac{d\phi_n(x)}{dx}$. Performing an analogous operation as explained above yields

$$J_n(V) \int_{a}^{b} \frac{dx}{q\mu_n(x)n(x;V)} = \phi_n(a) - \phi_n(b) \equiv V \quad (27)$$
or

\[ \rho_A(V) = \int_a^b q n(x)V(x) \, dx \]  

From (26) and (28) we find an alternative expression for the ideality factor

\[ m(V, T) = \frac{q}{k_B T} \int_a^b \frac{n(x)}{F_p(y)} \, dx = \frac{q}{k_B T} \int_a^b \frac{n(x)}{F_p(y)} \, dx \]  

Introducing the lower and upper bound (4) for \( f(x) \) we obtain

\[ \frac{d}{dT} \ln \frac{J_n(V)}{T^2} = \frac{k_B}{q} \frac{m(V, T)}{T} \]  

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\[ \frac{d}{dT} \ln \frac{J_n(V)}{T^2} = \frac{k_B}{q} \frac{m(V, T)}{T} \]  

and define an effective barrier height related to a certain temperature range as

\[ \Phi_{\text{eff}}(V, T) = -k_B \frac{d}{dT} \ln \frac{J_n(V)}{T^2} \]  

such that the barrier height \( \Phi_{\text{MS}} \) follows from the extrapolation towards zero voltage.

The temperature independence of degenerate Schottky diodes complicates the extraction of the barrier height \( \Phi_{\text{MS}} \) seriously because the both currents \( J_n(V) \) and \( J_s(V) \) as well as \( I_2 (21) \) become temperature independent. The standard nondegenerate approach that plots \( -k_B \ln \frac{J_n(V)}{T^2} \) versus inverse temperature and then identifies the slope as \( \Phi_{\text{MS}} \) clearly does not apply anymore.

However, the temperature \( T \) can still be used as a tool to extract a high temperature barrier height, because for sufficiently high temperatures a semiconductor becomes again nondegenerate. When plotting \( -k_B \ln \frac{J_n(V)}{T^2} \) versus inverse temperature and then identifies the slope as \( \Phi_{\text{MS}} \) clearly does not apply anymore.

V. THE BARRIER HEIGHT \( \Phi_{\text{MS}} \) IN HEAVILY DOPED SCHOTTKY DIODES

From the previous discussion and the definition of the ideality factor (22) we find that \( J_n(V) / T^2 \) is temperature independent in the degenerate limit. Further, invoking the definition of the voltage dependent resistivity and the temperature dependence of the free carriers, it follows that \( J_n(V) \) is almost temperature independent and, hence, also \( J_s(V) \). A temperature independent current is generally attributed to tunneling only. Our analysis shows that this statement should be revised.

Let us examine

\[ -k_B \ln \frac{J_n(V)}{T^2} = -k_B \ln \frac{J_s(V)}{T^2} - \frac{qV}{T m(V, T)} \]  

and define an effective barrier height related to a certain temperature range as

\[ \Phi_{\text{eff}}(V, T) = -k_B \frac{d}{dT} \ln \frac{J_n(V)}{T^2} \]  

When Boltzmann statistics apply and \( J_n(V) = AT^2 \exp(-\Phi_{\text{MS}} / k_B T) \) [14], we have for voltages larger than \( k_B T / q \)

\[ \Phi_{\text{eff}}(V, T) = \Phi_{\text{MS}} - qV/m \]  

such that the barrier height \( \Phi_{\text{MS}} \) follows from the extrapolation towards zero voltage.

The temperature independence of degenerate Schottky diodes complicates the extraction of the barrier height \( \Phi_{\text{MS}} \), however, because the both currents \( J_n(V) \) and \( J_s(V) \) as well as \( I_2 (21) \) become temperature independent. The standard nondegenerate approach that plots \( -k_B \ln \frac{J_n(V)}{T^2} \) versus inverse temperature and then identifies the slope as \( \Phi_{\text{MS}} \) clearly does not apply anymore.

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Fig. 3. The effective barrier height $\Phi_{\text{eff}}(V, T)$ versus applied voltage for a Au/n$^+$-GaAs Schottky diode extracted from the high-temperature regime by fitting a straight line $A/T + B$. Extrapolation towards zero voltage gives a barrier height of 0.3 eV and the slope indicates that the high temperature ideality factor is about $m = 1.1$.

But as generally believed in literature [21], the Au/GaAs barrier height is around 0.7 eV (Fermi-level pinning due to the high amount of surface states). Clearly the extracted barrier height is both related to the doping concentration and temperature range where the information is obtained from. Moreover, the ideality factor is found to vary as $m(V, T) \sim T^{-0.8}$ when determined from the current-voltage characteristics performed over a broad temperature range [80 K, 340 K]. Pure tunneling gives rise to an ideality factor inversely proportional with temperature [2]. An ideality factor temperature law as $m(V, T) \sim T^{-\beta}$ with $0 \leq \beta \leq 1$ is a natural consequence of the Fermi-Dirac statistics as demonstrated above.

As a conclusion, we have shown that the ideality factor and barrier height essentially dependent on doping concentration and temperature. Moreover, the analysis demonstrates that the influence of the Fermi-Dirac statistics can cause effects previously attributed to tunneling only. Hence, both effects should be considered as suitable explanations for a non-Boltzmannian behavior of the ideality factor.

APPENDIX

MATHEMATICAL DERIVATIONS

A. Derivation of (5)
Combining (1) and (2) yields

$$
\frac{J_n(V)}{q\mu_n(x)} = \left( n(x; V) - \frac{1}{f(x)} \frac{\partial n(x; V)}{\partial \psi(x; V)} \right) \frac{d\psi(x; V)}{dx}.
$$

We use the identity

$$
-\frac{1}{f(x)} \exp \left( -\int_{x_0}^{x} \mathcal{E}(x; V) f(x) dx \right) \frac{\partial}{\partial \psi(x; V)}
\times \left[ n(x; V) \exp \left( \int_{x_0}^{x} \mathcal{E}(x; V) f(x) dx \right) \right]
= \left( n(x; V) - \frac{1}{f(x)} \frac{\partial n(x; V)}{\partial \psi(x; V)} \right)
$$

(34)

to obtain

$$
\frac{J_n(V)}{qD_n(x)} \exp \left( \int_{x_0}^{x} \mathcal{E}(x; V) f(x) dx \right)
= \frac{d}{dx} \left[ n(x; V) \exp \left( \int_{x_0}^{x} \mathcal{E}(x; V) f(x) dx \right) \right].
$$

(35)

We integrate from, say, $a$ to $b$ in the semiconductor side of the Schottky diode,

$$
\int_{a}^{b} \frac{J_n(V) dx}{qD_n(x)} \exp \left( \int_{x_0}^{x} \mathcal{E}(x; V) f(x) dx \right)
= \frac{n(b; V)}{\exp \left( \int_{x_0}^{x} \mathcal{E}(x; V) f(x) dx \right)}
\exp \left( \int_{x_0}^{x} \mathcal{E}(x; V) f(x) dx \right)
- \frac{n(a; V)}{\exp \left( \int_{x_0}^{x} \mathcal{E}(x; V) f(x) dx \right)}.
$$

(36)
Dividing both sides by \( n(a; V) \exp \left( \int_{a}^{b} \mathcal{E}(x; V) f(x) \, dx \right) \) eliminates the arbitrary constant \( x_0 \).

\[
\frac{1}{n(a; V)} \int_{a}^{b} \frac{J_n(x)}{qD_n(x)} \exp \left( \int_{a}^{b} \mathcal{E}(x; V) f(x) \, dx \right) = \frac{n(b; V)}{n(a; V)} \exp \left( \int_{a}^{b} \mathcal{E}(x; V) f(x) \, dx \right) - 1.
\] (37)

The continuity equation for the electric current density, \( \frac{\partial}{\partial x} \mathcal{J}(x; V) = 0 \), indicates that \( \mathcal{I}(a; V) = \mathcal{I}(b; V) \) is independent of position \( x \). Rearrangement of (37) leads to (5). On the other hand, starting from the integral form (5), we easily recover (1).

Indeed, application of theorem of de l'Hôpital and of (2) leads to (1). This demonstrates that (1) and (5) are mathematically equivalent.

**B. Estimates for the Ideality Factor \( m(V, T) \)**

We will present alternative expressions for the ideality factor

\[
\frac{1}{m(V, T)} = \frac{k_B T}{qV} \ln \left( \frac{J_n(V)}{J_n(0)} + 1 \right)
\]

Using the definition (2) of \( f(x) \), (38) rewrites as

\[
\frac{1}{m(V, T)} = \frac{k_B T}{qV} \left( \int_{a}^{b} \left[ \frac{\partial \ln n(x; V)}{\partial \xi(x; V)} - \frac{\partial \ln n(x; 0)}{\partial \xi(0; V)} \right] \right) \mathcal{E}(x; V) \, dx
\]

The point \( b \) must be chosen in the neutral region where \( \mathcal{E}(b; V) = 0 \) for all voltages \( V \). The last integral can be estimated in the assumption of the constant doping profiles and in the depletion approximation. We have that \( \frac{\partial \ln n(x; V)}{\partial \xi(x; V)} = \frac{W_n(0)-W_n(V)}{W_n(0)-W_n(V)} \) and \( \frac{\partial \ln n(x; 0)}{\partial \xi(0; V)} = \frac{W_n(0)}{(W_n(0)-x)^2} < 0 \) in forward bias where \( W_n(V) \) denotes the depletion thickness at applied voltage \( V \).

The last integral is thus negative. A simple estimate is

\[
\int_{a}^{b} \ln n(x; 0) \frac{\partial}{\partial x} \left( \frac{\mathcal{E}(x; V)}{\mathcal{E}(x; 0)} \right) \, dx > \ln n(b; 0) \int_{a}^{b} \frac{\partial}{\partial x} \left( \frac{\mathcal{E}(x; V)}{\mathcal{E}(x; 0)} \right) \, dx
\]

\[
= - \ln n(b; 0) \frac{\mathcal{E}(a; V)}{\mathcal{E}(a; 0)}
\] (40)

such that, because \( 0 < \frac{1}{m(V, T)} \leq 1 \)

\[
\frac{1}{m(V, T)} = \min \left\{ \frac{k_B T}{qV} \ln \left( \frac{n(b; V)}{n(a; V)} \right), 1 \right\}
\] (41)

\[
> \max \left\{ \frac{k_B T}{qV} \ln \left( \frac{n(b; V)}{n(a; V)} \right), 0 \right\}
\] (42)

**C. Short Note on the Fermi-Dirac Integrals \( F_p(y) \)**

A quite different manner to examine properties of Fermi–Dirac integrals consists in studying their generating function. When looking at the definition written as a \( \varphi \)-transform, where \( \{1, \xi(x)\} \) is Heavyside’s stepfunction,

\[
F_p(y) = \frac{x^p \delta(x)}{\Gamma(p+1)} \psi \left( \frac{\mathcal{E}(x; V)}{\mathcal{E}(x; 0)} \right) = \frac{1}{\Gamma(p+1)} \int_{0}^{\infty} x^p \exp(x-y) \, dx
\] (43)

we may interpret \( \Gamma(p+1)F_p(y) \) as the Mellin transform of the function \( (1 + \exp(x-y))^{-1} \), which alternatively means by inversion,

\[
\int_{0}^{\infty} f(x)g(x)x^{s-1} \, dx = \frac{1}{2\pi i} \int_{k-i\infty}^{k+i\infty} F(w)G(s-w) \, dw.
\] (45)

The interest of relation (45) is that using (45) the single sided \( \varphi \)-transform can be written in terms of the Fermi–Dirac integrals provided that the Mellin transform \( G(s) \) of the density function \( g(x) \) exists.²

The point \( b \) must be chosen in the neutral region where \( \mathcal{E}(b; V) = 0 \) for all voltages \( V \). The last integral can be estimated in the assumption of the constant doping profiles and in the depletion approximation. We have that \( \frac{\partial \ln n(x; V)}{\partial \xi(x; V)} = \frac{W_n(0)-W_n(V)}{W_n(0)-W_n(V)} \) and \( \frac{\partial \ln n(x; 0)}{\partial \xi(0; V)} = \frac{W_n(0)}{(W_n(0)-x)^2} < 0 \) in forward bias where \( W_n(V) \) denotes the depletion thickness at applied voltage \( V \). The last integral is thus negative. A simple estimate is

\[
\int_{a}^{b} \ln n(x; 0) \frac{\partial}{\partial x} \left( \frac{\mathcal{E}(x; V)}{\mathcal{E}(x; 0)} \right) \, dx > \ln n(b; 0) \int_{a}^{b} \frac{\partial}{\partial x} \left( \frac{\mathcal{E}(x; V)}{\mathcal{E}(x; 0)} \right) \, dx
\]

\[
= - \ln n(b; 0) \frac{\mathcal{E}(a; V)}{\mathcal{E}(a; 0)}
\] (40)

such that, because \( 0 < \frac{1}{m(V, T)} \leq 1 \)

\[
\frac{1}{m(V, T)} = \min \left\{ \frac{k_B T}{qV} \ln \left( \frac{n(b; V)}{n(a; V)} \right), 1 \right\}
\] (41)

\[
> \max \left\{ \frac{k_B T}{qV} \ln \left( \frac{n(b; V)}{n(a; V)} \right), 0 \right\}
\] (42)

²It is very likely that there exists a nonzero s-interval around \( s = 1 \) where \( G(s) \) converges since for density functions \( f(x) \) the density function \( g(x) \) exists.
This demonstrates that we may rewrite the number of electron \( n(y) \) for an arbitrary density of states in terms of the Fermi-Dirac integrals.

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REFERENCES


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