Generalized semiclassical model for the density of states in heavily doped semiconductors

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An accurate description of the density of states, properly combining both statistical and many-particle effects, seems not available for heavily doped semiconductors. We propose a semiclassical approach which exhibits a number of attractive features. First of all, the resulting density of states is easily computed in contrast to quantum-mechanical models. The proposed model describes the exact high-density limit and simply includes the many-body effects, yielding still an analytical expression. Two-dimensional systems appear to be best described. The model approximates the number of the majority carriers very well. The main drawback lies in an overestimation of the number of deep energy states. A formula to estimate the Fermi-level shift purely due to band tailing is derived which allows the easy incorporation of the effect of band tails in a device simulator.

I. INTRODUCTION

In a heavily doped semiconductor, the density of states (DOS) differs from that of the pure crystal due to a number of different physical mechanisms. The electron-electron interactions[1] mainly shift the conduction and valence bands towards each other, but also slightly deform the DOS through a modification of the quasiparticle energies. A stronger distorting of the DOS occurs when electrons interact with impurities. This electron-impurity scattering has been calculated in detail by Serre and Ghazali in three dimensions (3D) and by Ghazali, Gold, and Serre[3] in 2D. Beside these many-body effects, the random distribution of impurities, a statistical effect, introduces band tails in the DOS.

A detailed description that rigorously combines both many-body and statistical fluctuation effects must be exceedingly complicated, if it exists. A theory[4] that partially includes many-body effects with statistical effects has been given, but this requires huge numerical calculations and a number of approximations. A totally different approach would be an introduction of many-body effects into a Feynman path integral because in the absence of many-body effects, an exact path-integral formula exists,[5] which was the basis of the work of Sayakanit.[6–10] However, it is known that the path-integral method is not the best one to describe many-fermion systems.

The discouraging difficulties arising in first-principles models suggest approximate techniques. We would like to demonstrate that a combination of both the electron medium and the statistical fluctuations can be comprised in a semiclassical model. Because band-tail effects as well as many-body effects only significantly alter the DOS at high doping concentrations, a semiclassical approach[11] (SA) looks highly suitable, since it covers the high-density limit (HDL) exactly.[9] The major advantages of the generalized semiclassical DOS are its simple physical interpretation and the explicit use of an arbitrary isotropical energy versus wave vector, $E(k)$, relation, necessary to include many-body effects and to deal with nonparabolic unperturbed DOS's (such as the DOS of $InSb_xAs_{1-x}$). Moreover, the expression for the DOS can be written as a closed analytical formula. In addition, the semiclassical model is the only existing simple formula that covers the whole energy range. The analyticity of our approach introduces the possibility to present DOS expressions in different dimensions. However, it does not describe impurity bands, nor the deep energy tail region.

In material research, one is mainly interested in estimations of the expected band-gap narrowing (BGN). In order to make quick estimations of the band-tailing effect, an analytical closed formula is presented. All numerical results are calculated for n-type GaAs.

II. THE GENERALIZED SEMICLASSICAL DOS

A. The SA

Kane[12] and Shlovskii and Efros[13] have applied the semiclassical method to the calculation of the DOS in heavily doped semiconductors. Our approach generalizes their result to different dimensions, interacting Fermi liquids, and arbitrary initially unperturbed DOS's.

The SA assumes basically one approximation: the classical description of the electron wave packet. The potential fluctuations caused by the charged impurities are assumed to be smooth in the sense that they change little over the electron wavelength. The electron only "feels" the potential of the point where it is located. This approximation considers electrons with energies sufficiently higher than the average potential V_{av} in Fig. 1 such that the actual potential $V(\mathbf{r})$ can be replaced by the smoothed, slowly varying potential $V_s(\mathbf{r})$. Let $\rho_0(E)$ denote the DOS in the crystal not perturbed by impurities. The energy E is measured from the bottom of the band in the noninteracting electron system, which will be represented by the subscript n while the interacting electron system will be denoted by the subscript i. From Fig. 1 and Refs. 11 and 12, we obtain a semiclassical expression for the DOS:

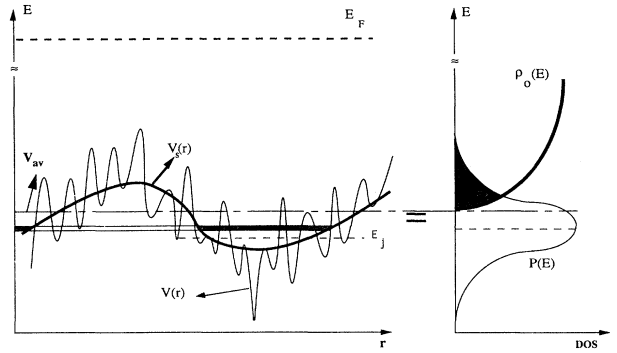

FIG. 1. Sketch of the semiclassical method: all states with energy above the smoothed potential $V_s(r)$ are counted. The summation of states within the shaded infinitesimal energy strip in coordinate space is equivalent to the shaded area (convolution) of the right-hand-side plot.

$$\rho(E)=\int_{-\infty}^{E-\rho_0^{-1}(0)}\rho_0(E-V)P(V)dV$$
$$=\int_{\rho_0^{-1}(0)}^{\infty}\rho_0(\nu)P(E-\nu)d\nu\ , \tag{2.1}$$

where $P(V)$ is the distribution function for the potential energy $V(\mathbf{r})$ which is to be determined, and where $x=\rho_0^{-1}(y)$ is the inverse DOS function or solution of $y=\rho_0(x)$. This notation is required for interacting electron systems, where the DOS shifts down to lower energies due to many-body interactions. Hence, $\rho_{0i}^{-1}(0)<0$, in contrast to $\rho_{0n}^{-1}(0)=0$, by definition as reference energy.

Figure 1 illustrates that in the SA, all energies above $V_s(r)$ contribute to the DOS. The actual energy levels as E_j are discrete and spaced farther from each other as the potential well gets narrower, which happens for lower energies. As the SA ignores this quantum-mechanical effect, the semiclassical DOS overestimates the number of electrons in the deep tails, but gains accuracy for increasing energies and finally becomes exact in the HDL. For degenerate semiconductors, most of the physics will be included if the electron can be regarded as classical. Energy states deep under the unperturbed energy band surely need a quantum-mechanical description, such as that given by Halperin and Lax.[14] Because these deep-lying energy states are not properly taken into account in a SA, the presented model will only describe majority carriers (with Fermi level above the unperturbed band edge) sufficiently well.

Let us now assume that the energy versus wave vector relation is isotropic in k space, then $E(\mathbf{k})=E(|\mathbf{k}|)=E(k)$. From the Bloch theorem, we can derive an explicit relation between the DOS expressed as a function of k and the band structure.[15,16] For a different dimension d, $\rho_{0;kd}(k)$ yields

$$\rho_{0;k3}(k)=\frac{k^2}{\pi^2E'(k)}\ , \tag{2.2a}$$

$$\rho_{0;k2}(k)=\frac{k}{2\pi E'(k)}\ , \tag{2.2b}$$

$$\rho_{0;k1}(k)=\frac{1}{\pi E'(k)}\ , \tag{2.2c}$$

where $E'(k)$ denotes the derivative of $E(k)$ with respect to k. Observe that

$$\rho_{0;k}(k)=\rho_0(E(k))\ . \tag{2.3}$$

A substitution of the independent variable V by $E-E(k)$ in (2.1), yields

$$\rho(E)=\int_0^{\infty}\rho_0(E(k))P(E-E(k))E'(k)dk\ , \tag{2.4}$$

since the lowest-energy $\rho_0^{-1}(0)$ corresponds to $k=0$. Applying (2.2) and (2.3) finally gives $\rho_d(E)$ in different dimensions,

$$\rho_3(E)=\frac{1}{\pi^2}\int_0^{\infty}k^2P(E-E(k))dk\ , \tag{2.5a}$$

$$\rho_2(E)=\frac{1}{2\pi}\int_0^{\infty}k\,P(E-E(k))dk\ , \tag{2.5b}$$

$$\rho_1(E)=\frac{1}{\pi}\int_0^{\infty}P(E-E(k))dk\ . \tag{2.5c}$$

From these relations we conclude that, if the distribution function $P(V)$ and the $E(k)$ relation of electrons in an unperturbed crystal are known, the DOS for majority carriers can be calculated.

B. The distribution function $P(V)$ of the potential energy V in an interacting Fermi system

There only exists an analytical, exact expression for $P(V)$ on the condition that the potential at a certain point $\mathbf{r}$ can be written as a superposition of the influences of all impurities in a system with volume V_0. For, if the probability $p(\mathbf{r}_i)$ having an impurity at an arbitrary point $\mathbf{r}_i$ is constant and, hence, equals V_0^{-1} and if the potential energy $V(\mathbf{r},\{\mathbf{r}_i\})$ at $\mathbf{r}$, caused by a configuration of N impurities at positions $\{\mathbf{r}_i\}$, can be written as a superposition,

$$V(\mathbf{r},\{\mathbf{r}_i\})=\sum_{i=1}^{N}v(\mathbf{r}-\mathbf{r}_i)\ , \tag{2.6}$$

where $v(\mathbf{r})$ is an arbitrary well-behaved function, then an exact expression for the probability distribution function $P(V)$ can be derived[17–20], yielding

$$P(V)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\left[iVt+n\int d\mathbf{R}(e^{-iv(\mathbf{R})t}-1)\right]dt\ , \tag{2.7}$$

whose properties are further explored in Appendix A. The superposition (2.6) implies a superposition of the charge densities, indicating that the Poisson equation must be linear, which generally is not the case in an electron medium.[21] As long as the potential fluctuations are small, linear-response theory[22,23] applies, providing a general expression for the potential induced by an impurity charge $Ze\delta(\mathbf{r})$ in an electron medium,

$$v(\mathbf{r})=Z\int\frac{d\mathbf{q}}{(2\pi)^d}e^{i\mathbf{q}\cdot\mathbf{r}}\frac{v_q}{\epsilon(q)}\ , \tag{2.8}$$

with v_q the Fourier transform of the bare Coulomb po-

tential and $\varepsilon(q)$ the static dielectric function of the surrounding electrons. With an explicit expression for $E(k)$,

$$E(\mathbf{k})=\frac{\hbar^2k^2}{2m}+\hbar\Sigma(\mathbf{k},E) \tag{2.9}$$

where $\hbar\Sigma(\mathbf{k},E)$ denotes the system's self-energy due to many-body interactions, all quantities to calculate (2.5) are defined. In this general form, as both $\hbar\Sigma(\mathbf{k},E)$ and $\varepsilon(q)$ depend on the number of electrons and thus on $\rho(E)$, Eqs. (2.5) and (2.7)–(2.9) represent a coupled system of equations.

The assumption of linearity is, of course, an approximation, but a very good one for heavily doped but noncompensated[24] semiconductors and becomes exact in the HDL. Thus, the proposed model based on the SA and the requirement of linearity describes exactly band tailing and many-body interactions in the HDL. In the following, we will illustrate the proposed model for a simple case of a 3D interacting system and a 2D noninteracting system.

III. THE INTERACTING FERMI LIQUID IN 3D

Since a detailed discussion of the self-energy is beyond the scope of this paper, the calculation will be demonstrated for the simplest expression of the self-energy. We confine ourselves to exchange effects because they dominate in the HDL. We neglect the correlation influence and describe the exchange effect by the simple Hartree model[25] (at $T=0$ K)

$$\Sigma(\mathbf{k},E)=-\frac{e^2}{2\pi^2\epsilon_3}k_F F\left(\frac{|\mathbf{k}|}{k_F}\right), \tag{3.1}$$

where

$$F(x)=\frac{1}{2}+\frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right| . \tag{3.2}$$

Further, we choose the Thomas-Fermi dielectric function,[20,21]

$$\epsilon(q)=1+\frac{\kappa_3^2}{q^2} , \tag{3.3}$$

yielding for the potential (2.8),

$$v(\mathbf{r})=\frac{e^2}{4\pi\epsilon_3 r}\exp(-\kappa_3 r) , \tag{3.4}$$

with κ_3 the inverse screening length in 3D, which obeys

$$\kappa_3=\left[\frac{e^2}{\epsilon_3}\frac{dn_{\rm el}(E_F)}{dE_F}\right]^{1/2} \tag{3.5a}$$

or, worked out,

$$\kappa_3^2=\frac{e^2}{\epsilon_3}\int_{-\infty}^{\infty}\rho(E)\frac{df_{\rm FD}(E-E_F)}{dE_F}dE , \tag{3.5b}$$

where $f_{\rm FD}(x)=[1+\exp(x/k_BT)]^{-1}$ is the Fermi-Dirac distribution function. At this point, we have the problem that (2.7) diverges for the screened Coulomb potential (3.4) because all semi-invariants (A5) of order higher than 2 diverge. The same problem occurs in Kane's model.[11] Restricting ourselves to the HDL, however, $P(V)$ reduces to a Gaussian (A12) that only needs the knowledge of κ_3. Although (3.5) reveals that κ_3 has to be solved self-consistently, we argue that this self-consistent procedure is needlessly sophisticated compared to the approximations already made. Indeed, in Fig. 2 we show the 3D noninteracting screening length, calculated both self-consistently (κ_{3ns}) with (3.5) and not self-consistently (κ_{3n}), where

$$\kappa_{3n}^2=\frac{e^2}{\epsilon_3}\int_{\rho_0^{-1}(0)}^{\infty}\rho_0(E)\frac{df_{\rm FD}(E-E_F)}{dE_F}dE , \tag{3.6}$$

while in Fig. 3, the relative difference $\Delta\kappa_{3n}/\kappa_{3ns}$ is drawn, where $\Delta\kappa_{3n}=\kappa_{3n}-\kappa_{3ns}$. For heavily doped materials, where $na_B^3>1$ with $a_B=4\pi\epsilon_3\hbar^2/me^2$ is the effective Bohr radius (or $n_{\rm GaAs}>10^{18}$ cm^{-3}) this difference is obviously negligible.[26] Moreover, in the HDL, we prove in Appendix B that (3.5) tends to (3.6). Consequently, further calculations invoke (3.6) rather than the unattractive (3.5).

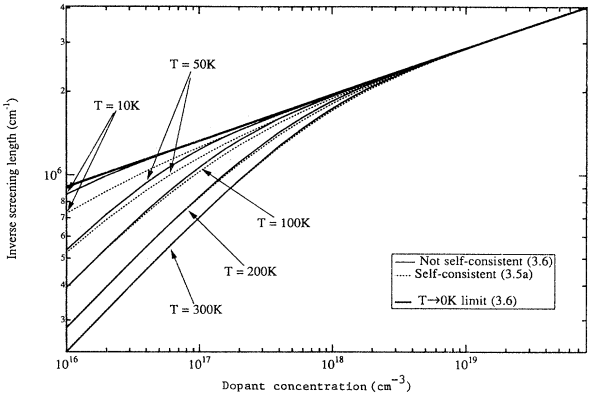

FIG. 2. The 3D noninteracting screening length, calculated both self-consistently (κ_{3ns}) and not self-consistently (κ_{3n}) vs versus doping concentration for different temperatures. Notice that in the HDL, the screening length becomes temperature independent.

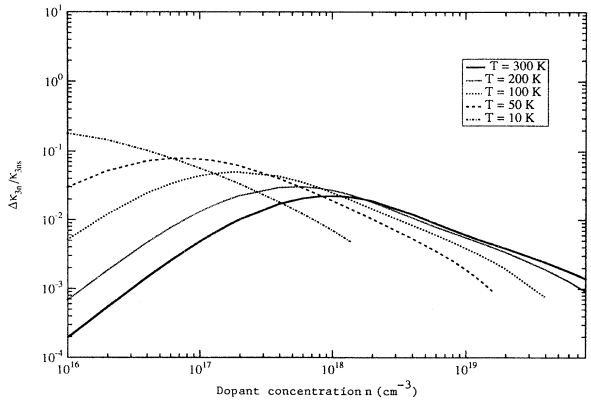

FIG. 3. The relative difference $\Delta\kappa_{3n}/\kappa_{3ns}$ vs doping concentration for different temperatures.

We still have to determine the interacting inverse screening length (at $T=0$ K). If the $E(k)$ relation is isotropic, the number of carriers at zero K equals

$$n_{\rm el}=\frac{1}{3\pi^2}k_F^3 . \tag{3.7}$$

Plugging the Hartree 3D expression for the exchange (3.1) into (2.9), we find

$$E_F=\frac{\hbar^2}{2m}k_F^2-\frac{e^2}{4\pi^2\epsilon}k_F . \tag{3.8}$$

Solving this equation for k_F results in

$$k_F=\frac{1}{\pi a_B}+\left[\left[\frac{1}{\pi a_B}\right]^2+\frac{2\hbar^2}{m}E_F\right]^{1/2} . \tag{3.9}$$

Substituting (3.9) into (3.7) and using (3.5a) not self-consistently, we find the zero-temperature inverse screening length for the interacting system

$$\kappa_{3i}=\frac{2k_F}{\sqrt{\pi a_B k_F-1}} . \tag{3.10}$$

A comparison with the noninteracting DOS and free-electron DOS, shown in Fig. 4, shows the supplementary downwards shift due the electron exchange,[22] $\Delta E_{\rm ex}=(3e^2/16\pi^2\epsilon_3)k_F$. Besides the low-energy band tail, a stronger nonparabolical behavior around the Fermi level is observed. At high energies, all DOS functions tend to the free-electron DOS.

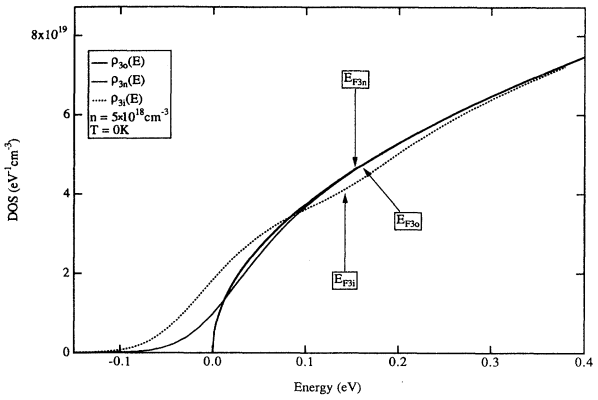

FIG. 4. A comparison between the DOS and the corresonding Fermi levels for the unperturbed [$\rho_{3o}(E)$: free electron], the noninteracting [$\rho_{3n}(E)$: Kane (DOS)], and the interacting [$\rho_{3i}(E)$] electron system for $n=5\times10^{18}$ cm^{-3} in GaAs. The Hartree exchange shift equals $\Delta E_{\rm ex}=13.8$ meV and agrees with $E_{F3n}-E_{F3i}$.

IV. THE NONINTERACTING 2D FERMI GAS

Assuming a noninteracting system [$\hbar\Sigma(\mathbf{k},E)=0$], the potential energy $v(\mathbf{r})$ is readily obtained from the Poisson equation or equivalently from (2.8) with (3.3) in 2D, yielding[27]

$$v(\mathbf{r})=\frac{e^2}{2\pi\epsilon_2}K_0(\kappa_2 r) , \tag{4.1}$$

where $K_0(x)$ denotes the modified Bessel function of zero order and κ_2, not self-consistently,

$$\kappa_{2n}=\left[\frac{me^2}{\pi\hbar^2\epsilon_2}\frac{1}{1+\exp(E_{F_{\rm on}}/k_BT)}\right]^{1/2} . \tag{4.2}$$

The charge density, neglecting self-consistency, equals,

$$\gamma(\mathbf{r})=e^2\left[\delta(\mathbf{r})+\frac{mk_BT}{\pi\hbar^2}\left\{\ln\left[1+\exp\left[\frac{E_{F_{0n}}}{k_BT}\right]\right]-\ln\left[1+\exp\left[\frac{E_{F_{on}}+v(\mathbf{r})}{k_BT}\right]\right]\right\}\right] , \tag{4.3}$$

which is perfectly linear in $v(\mathbf{r})$ at $T=0$ K and almost linear if $E_{F_{on}}/k_BT>1$ (equivalent to a doping concentration $>2.5\times10^{11}$ cm^{-2} in GaAs at 300 K), a condition very well fulfilled in the study of band tails. Hence, the Poisson equation is linear at $T=0$ K, perfectly satisfying the required linearity for $P(V)$. For a 2D noninteracting system, the SA clearly is best suited. Within the SA, all impurity densities are exactly treated, in contrast to 3D, where only the HDL is properly described through linearization of Poisson's equation. Equation (2.1) then reads

$$\rho_{2n}(E)=\frac{m}{\pi\hbar^2}\int_{-\infty}^{E}P(V)dV , \tag{4.4}$$

which demonstrates that $\rho_{2n}(-\infty)=0$, $\rho_{2n}(\infty)=m/\pi\hbar^2$ and that $\rho_{2n}(E)$ continuously increases from 0 to $m/\pi\hbar^2$, since $P(V)>0$. The analytical expression for the 2D DOS is obtained after performing one integration invoking the relation $\int_0^\infty e^{-iut}du=(1/it)+\pi\delta(t)$ and reads as a function of a dimensionless energy,

$$E^*=\frac{2\pi\epsilon_2 E}{e^2} , \tag{4.5}$$

and a dimensionless density,

$$\nu=\frac{2\pi n_2}{\kappa_{2n}^2} , \tag{4.6}$$

$$\rho_{2n}(E^*)=\frac{m}{2\pi\hbar^2}\left[1+\frac{1}{\pi i}\int_{-\infty}^{\infty}dt\frac{1}{t}\exp\left[iE^*t+\nu\int_0^\infty drr\{\exp[-itK_0(t)]-1\}\right]\right] , \tag{4.7}$$

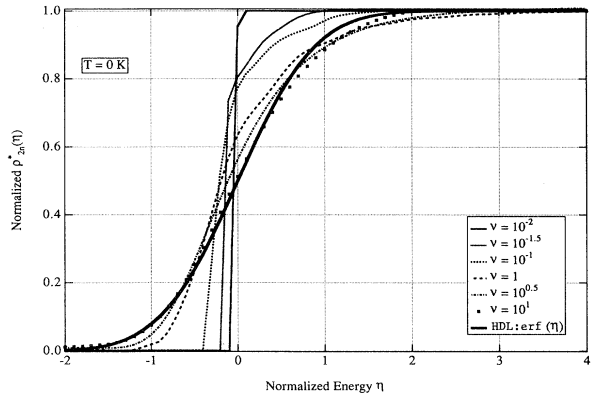

FIG. 5. The normalized $\rho^*_{2n}(\eta)=(\pi\hbar^2/m)\rho_{2n}(E^*)$, where $\eta=(E^*-\nu)/\sqrt{\nu}$ for different dimensionless densities ν. Apart from the HDL, an asymmetry of the step round $E^*=0$ is observed.

and is shown in Fig. 5. The unperturbed Fermi level in dimensionless quantities is found to be $E^*_{Fo}=\nu$ combining (4.5), (4.6), $E_{Fo}=(\hbar^2/2m)k^2_{Fo}$, $k_{Fo}=\sqrt{2\pi n_2}$, and $\kappa_{2n}(0)=(me^2/\pi\hbar^2\epsilon_2)^{1/2}$. In the HDL (see Appendix A), invoking (4.5) and (4.7) reduces to

$$\rho_{2n}(E)=\frac{m}{2\pi\hbar^2}\left[1+\mathrm{erf}\left[\frac{E}{\sigma_{2n}\sqrt{2}}\right]\right], \tag{4.8}$$

where

$$\sigma_{2n}=\frac{e^2}{2\epsilon_2\kappa_{2n}}\left[\frac{n_2}{\pi}\right]^{1/2}. \tag{4.9}$$

Physically, the DOS (4.7) may be used to explain the asymmetry observed in absorption data[28] of doped quantum wells. For a pure 2D system, however, it is not possible to calculate the purely 2D Hartree-Fock exchange energy as it diverges.

V. AN ESTIMATION OF BGN PURELY DUE TO BAND TAILING

The tailing of the DOS induces a Fermi-level shift $\Delta E_F=E_{Fon}-E_{Ftn}$. The indices indicate that we confine ourselves to noninteracting systems. Assuming complete ionization,[29] both introduced Fermi levels are easily calculated from the impurity concentration n, preserving electrical neutrality, as

$$\begin{aligned} n=n_{\mathrm{el}}&=\int_{-\infty}^{\infty}\rho(E)f_{\mathrm{FD}}(E-E_{Ftn})dE \\ &=\int_{-\infty}^{0}\rho(E)f_{\mathrm{FD}}(E-E_{Ftn})dE \\ &\quad+\int_{0}^{\infty}\rho(E)f_{\mathrm{FD}}(E-E_{Ftn})dE\ , \end{aligned} \tag{5.1}$$

where E_{Ftn} denotes the Fermi level using the tailed distribution, whereas E_{Fon} is defined by

$$n=\int_0^\infty\rho_0(E)f_{\mathrm{FD}}(E-E_{Fon})dE\ . \tag{5.2}$$

Combining (2.1) and (5.1), we obtain

$$\begin{aligned} n=&\int_0^\infty dx\, f_{\mathrm{FD}}(-(x+E_{Ftn}))\int_0^\infty dt\,\rho_0(t)P(-(x+t)) \\ &+\int_0^\infty dE\, f_{\mathrm{FD}}(E-E_{Ftn})\int_0^\infty dt\,\rho_0(t)P(E-t)\ . \end{aligned} \tag{5.3}$$

For energies above the unperturbed band edge ($E>0$), $\rho_0(E)$ varies much more slowly than $P(E)$, which is peaked as a Gaussian (A9), justifying the following approximation:

$$\int_0^\infty\rho_0(t)P(E-t)dt\approx\rho_0(E)\int_0^\infty P(E-t)dt\ .$$

For sufficiently high energies, we have to an excellent approximation

$$\int_0^\infty P(E-t)dt\approx\int_{-\infty}^\infty P(E-t)dt=1\ .$$

Hence, for sufficiently high energies, the distribution function $P(V)$ may be approximated by a Dirac function $\delta(V)$, yielding

$$\int_0^\infty dt\,\rho_0(t)P(E-t)\approx\rho_0(E)\ . \tag{5.4}$$

Substitution of (5.4) and (5.2) in (5.3) gives

$$\begin{aligned} &\int_0^\infty\rho_0(E)[f_{\mathrm{FD}}(E-E_{Fon})-f_{\mathrm{FD}}(E-E_{Ftn})]dE \\ &\quad=\int_0^\infty dx\int_0^\infty dt\,\rho_0(t)P(-(x+t))f_{\mathrm{FD}}(-(x+E_{Ftn}))\ . \end{aligned} \tag{5.5}$$

In the HDL, the Fermi level lies in the conduction band ($E_F>0$), providing a simplification for the right side of (5.5) as

$$f_{\mathrm{FD}}(-(x+E_{Ftn}))\approx 1 \tag{5.6}$$

for all $x>0$.

In general, the effect of tailing is relatively small, so that $\Delta E_F=E_{Fon}-E_{Ftn}$ is small. A first-order development of $f_{\mathrm{FD}}(E-E_{Fon})-f_{\mathrm{FD}}(E-E_{Ftn})$ is therefore adequate, reducing (5.5) to

$$\begin{aligned} &\Delta E_F\int_0^\infty\rho_0(E)[-f'_{\mathrm{FD}}(E-E_{Fon})]dE \\ &\qquad\approx\int_0^\infty dx\int_0^\infty dt\,\rho_0(t)P(-(x+t))\ . \end{aligned} \tag{5.7}$$

Integrating the right side of (5.7) by part, defining

$$M_0(E)=\int_0^E\rho_0(t)dt\ ,$$

and applying (3.6) not self-consistently, we find

$$\Delta E_F\approx\frac{e^2}{\epsilon\kappa^2}\int_0^\infty dt\,M_0(t)P(-t)\ . \tag{5.8}$$

Invoking (A12) finally gives the desired estimate for ΔE_F,

$$\Delta E_F\approx\frac{e^2}{\epsilon\kappa^2}\frac{1}{\sqrt{\pi}}\int_0^\infty dt\,M_0(\sqrt{2}\sigma t)\exp(-t^2)\ . \tag{5.9}$$

In two dimensions, only two approximations, (5.4) and (5.6), lead to

$$\begin{aligned} \Delta E_{F2}=E_{F2on}-k_BT\Bigg[\ln\Bigg\{\Bigg[1+\exp\left[\frac{E_{F2on}}{k_BT}\right]\Bigg] \\ \times\exp\left[-\frac{\sigma_{2n}}{\sqrt{2\pi k_BT}}\right]-1\Bigg\}\Bigg]\ , \end{aligned} \tag{5.10}$$

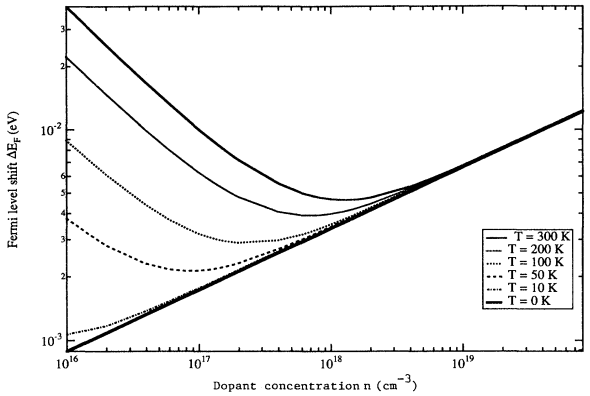

FIG. 6. The ΔE_{F3} in GaAs vs doping concentration for different temperatures. It should be stressed that ΔE_{F3} is only valid at the high-density region ($n_3 > a_B^{-3}$), as clearly demonstrated by extrapolations to low doping regions.

while the zero-temperature $\Delta E_{F2}(0)=\sigma_{2n}(0)/\sqrt{2\pi}$ varies as a square root of doping concentration.

Formula (5.9) is calculated for GaAs in 3D and is shown in Fig. 6. Values of BGN in the literature[30] indicate that the maximum band tailing contributes to BGN at $T=0$ K for approximately one seventh of the many-body interactions.

In the validity region (HDL), BGN due to band tailing barely depends on temperature, a feature that seems to characterize the complete BGN. Estimations of the band-tailing effect in $InSb_xAs_{1-x}$, which exhibits a strong nonparabolicity, are discussed elsewhere.[31] We have built this formula (5.9) into a device simulator in order to extract influences of band tailing on the performances of recent bipolar transistors.[32] Usually, the band-tail effect is neglected because it has a smaller impact than does the BGN. We showed, however, that for heavily doped devices, majority band tailing is too significant to neglect.

VI. CONCLUSION

We have demonstrated that both the band-tail effect in many-body interactions in different dimensions can be included in an analytical model. Despite the semiclassical approximation, the model is simple and very appropriate for majority carriers.

Notwithstanding its unrealistic properties, a 2D system turns out to be best described by our model, since $P(V)$ converges fastest to a Gaussian, and the superposition principle for the potential is best satisfied. In order to estimate the Fermi-level shift due to the random distribution of impurities, an analytical expression is given, that may easily introduce the band-tail effect into device simulators.

APPENDIX A: PROPERTIES OF $P(V)$

The distribution function $P(V)$ can be written as the Fourier transform of a characteristic function

$$\phi(t)=\exp\left[n\int d\mathbf{R}(e^{-iv(\mathbf{R})t}-1)\right], \tag{A1}$$

from which all possible moments of the potential fluctuations are deduced, because $\langle V^k(\mathbf{r})\rangle = \int_{-\infty}^{\infty} V^k P(V)dV = i^k\phi^{(k)}(0)$. Differentiating (A1) yields

$$\frac{d\phi(t)}{dt}=-in\int d\mathbf{R}\,v(\mathbf{R})[e^{-iv(\mathbf{R})t}\phi(t)], \tag{A2}$$

and after taking the inverse Fourier transform of (A2), we obtain an integral equation for $P(V)$,

$$n\int d\mathbf{R}\,v(\mathbf{R})P(V-v(\mathbf{R}))=VP(V), \tag{A3}$$

which first appeared in one dimension in the work of Lax and Philips.[19]

Here we are mainly interested in asymptotic forms of $P(V)$. One observes that $\lim_{n\to 0}P(V)=\delta(V)$. The HDL is somewhat more complicated.[17] Expanding the argument of (A1) in a power series, we obtain

$$\phi(t)=\exp\left[\sum_{m=1}^{\infty} b_m\frac{(-it)^m}{m!}\right], \tag{A4}$$

where b_m is the mth semi-invariant of $P(V)$,

$$b_m=n\int d\mathbf{R}\,v^m(\mathbf{R}). \tag{A5}$$

Defining

$$\sigma^2=b_2,\quad x=\frac{b_1-V}{\sigma}, \tag{A6}$$

we can write $P(V)$ as

$$P(V)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\left[-ix\sigma t-\frac{\sigma^2}{2}t^2\right]\times\exp\left[\sum_{m=3}^{\infty} b_m\frac{(-it)^m}{m!}\right]dt. \tag{A7}$$

If all semi-invariants exist, then $\phi(t)$ is an integral complex function, which can be expanded as a power series in t, converging for all finite t. Thus, we can write

$$\exp\left[\sum_{m=3}^{\infty} b_m\frac{(-it)^m}{m!}\right]=\sum_{k=0}^{\infty} c_k(it\sigma)^k. \tag{A8}$$

The remaining integral in (A7) can be done and written as a function of Hermite polynomials H_m of order m,[33]

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp\left(-ix\sigma t-\frac{\sigma^2}{2}t^2\right)(it\sigma)^k dt = \frac{1}{\sqrt{2\pi}\sigma}(-1)^k\frac{d^k}{dx^k}[\exp(-x^2/2)] = \frac{1}{\sqrt{2\pi}\sigma}2^{-k/2}H_k\left[\frac{x}{\sqrt{2}}\right]\exp(-x^2/2).$$

We finally obtain

$$P(V)=\frac{\exp(-x^2/2)}{\sqrt{2\pi}\sigma}\left[1+\sum_{k=3}^{\infty}\frac{c_k}{2^{k/2}}H_k\left[\frac{x}{\sqrt{2}}\right]\right], \tag{A9}$$

where the coefficients c_k can be extracted from (A8). Listed to order ten, we have

$$c_0=1\ ,$$
$$c_1=c_2=0\ ,$$
$$c_3=-\frac{b_3}{3!\sigma^3}\ ,$$
$$c_4=\frac{b_4}{4!\sigma^4}\ ,$$
$$c_5=-\frac{b_5}{5!\sigma^5}\ ,$$
$$c_6=\frac{1}{\sigma^6}\left[\frac{b_6}{6!}+\frac{b_3^2}{2(3!)^2}\right]\ ,$$
$$c_7=-\frac{1}{\sigma^7}\left[\frac{b_7}{7!}+\frac{b_3b_4}{3!4!}\right]\ ,$$
$$c_8=\frac{1}{\sigma^8}\left[\frac{b_8}{8!}+\frac{b_3b_5}{3!5!}+\frac{b_4^2}{2(4!)^2}\right]\ ,$$
$$c_9=-\frac{1}{\sigma^9}\left[\frac{b_9}{9!}+\frac{b_3b_6}{3!6!}+\frac{b_4b_5}{4!5!}+\frac{b_3^3}{(3!)^4}\right]\ ,$$
$$c_{10}=\frac{1}{\sigma^{10}}\left[\frac{b_{10}}{10!}+\frac{b_3b_7}{3!7!}+\frac{b_4b_6}{4!6!}+\frac{b_5^2}{2(5!)^2}+\frac{b_3^2b_4}{2(3!)^2 4!}\right]\ .$$

The shift b_1 results from the average potential of the charged impurities. Due to charge neutrality, however, this energy shift is exactly compensated by the potential energy of the electrons, and will be disregarded further.

In order to evaluate $P(V)$ in the HDL where n approaches infinity, we find after regrouping the terms in (A9) in increasing negative powers of n_d for the different dimensions, taking into account that inverse Thomas-Fermi screening length $\kappa_d\sim O(n_d^{1/2-1/d})$,

$$P(V)\sim\frac{\exp(-x^2/2)}{\sqrt{2\pi}\sigma}(1+A_1+A_2+A_3+A_4)\ , \tag{A10}$$

where

$$A_1=-\frac{b_3}{3!\sigma^3 2^{3/2}}H_3\left[\frac{x}{\sqrt{2}}\right]\ ,$$
$$A_2=\frac{b_4}{4!4\sigma^4}H_4\left[\frac{x}{\sqrt{2}}\right]+\frac{b_3^2}{2^4\sigma^6(3!)^2}H_6\left[\frac{x}{\sqrt{2}}\right]\ ,$$
$$A_3=-\frac{b_5}{5!\sigma^5 2^{5/2}}H_5\left[\frac{x}{\sqrt{2}}\right]-\frac{b_3b_4}{3!4!\sigma^7 2^{7/2}}H_7\left[\frac{x}{\sqrt{2}}\right]-\frac{b_3^3}{(3!)^4\sigma^9 2^{9/2}}H_9\left[\frac{x}{\sqrt{2}}\right]\ ,$$
$$A_4=\frac{b_6}{6!8\sigma^6}H_6\left[\frac{x}{\sqrt{2}}\right]+\frac{1}{16\sigma^8}\left[\frac{b_3b_5}{3!5!}+\frac{b_4^2}{2(4!)^2}\right]H_8\left[\frac{x}{\sqrt{2}}\right]+\frac{b_3^2b_4}{2(3!)^2 4!32\sigma^{10}}H_{10}\left[\frac{x}{\sqrt{2}}\right]+\frac{b_3^4}{(3!)^4 4!64\sigma^{12}}H_{12}\left[\frac{x}{\sqrt{2}}\right]\ ,$$

and

$$A_m\sim O(n_d^{-mp})\ , \tag{A11}$$

with $p=1-d/4$. If we put $n_d=L^{-d}$, where L is a unit length, it follows from (A10) and (A11) that the second dimension converges most rapidly. The distribution function $P(V)$ clearly converges to a Gaussian

$$P(V)=\frac{1}{\sqrt{2\pi}\sigma}\exp\left[-\frac{V_2}{2\sigma^2}\right] \tag{A12}$$

in the HDL, as it should, by virtue of the central-limit theory.

APPENDIX B: HDL INVERSE SCREENING LENGTH

We will prove that the inverse screening length κ_s calculated self-consistently will tend to κ_n calculated non-self-consistently. Consider the difference ΔK between

$$\kappa_s^2=-\frac{e^2}{\epsilon_d}\int_{-\infty}^{\infty}\rho(E)\frac{df_{\rm FD}(E-E_F)}{dE}dE \tag{B1}$$

and

$$\kappa_n^2=-\frac{e^2}{\epsilon_d}\int_{\rho_0^{-1}(0)}^{\infty}\rho_0(E)\frac{df_{\rm FD}(E-E_{Fo})}{dE}dE\ . \tag{B2}$$

Applying (2.1) and developing $[df_{\rm FD}(E-E_F)]/dE$ around $(E-E_{Fo})$ to first order, since $\Delta E_F=(E_{Fo}-E_F)$ is small (B1) reads

$$\kappa_s^2=-\int_{-\infty}^{\rho_0^{-1}(0)}\int_{\rho_0^{-1}(0)}^{\infty}\rho_0(\nu)P(E-\nu)d\nu\frac{df_{\rm FD}(E-E_F)}{dE}dE+\int_{\rho_0^{-1}(0)}^{\infty}\int_{\rho_0^{-1}(0)}^{\infty}\rho_0(\nu)P(E-\nu)d\nu\left[-\frac{df_{\rm FD}(E-E_{Fo})}{dE}-\frac{df_{\rm FD}^2(E-E_{Fo})}{dE^2}\Delta E_F\right]dE\ . \tag{B3}$$

The first integral becomes negligibly small in the HDL, where $E_F\gg 0$, and hence

$$\Delta K=-\frac{e^2}{\epsilon_d}\int_{\rho_0^{-1}(0)}^{\infty}\left[\int_{\rho_0^{-1}(0)}^{\infty}\rho_0(\nu)P(E-\nu)d\nu-\rho_0(E)\right]\frac{df_{\rm FD}(E-E_F)}{dE}dE-\frac{e^2}{\epsilon_d}\Delta E_F\int_{\rho_0^{-1}(0)}^{\infty}\int_{\rho_0^{-1}(0)}^{\infty}\rho_0(\nu)P(E-\nu)d\nu\frac{df_{\rm FD}^2(E-E_{Fo})}{dE^2}dE\ . \tag{B4}$$

The approximation (5.4) reduces (B4) to

$$\Delta K = -\frac{e^2}{\epsilon_d}\Delta E_F \int_{\rho_0^{-1}(0)}^{\infty} \rho_0(E)\frac{df_{\rm FD}^2(E-E_{Fo})}{dE^2}dE \ , \tag{B5}$$

which is very small. Indeed, both ΔE_F and the integral are small because $[df_{\rm FD}^2(E-F_{Fo})]/dE^2$ is a rapidly decreasing odd function around E_{Fo}, multiplied by a slowly varying function around E_{Fo}, and integrated over a range sufficiently far extended around E_{Fo}. This completes the proof.

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