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Nonlinear additives to the Brooks-Herring screened potential

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***Abstract*—In the present work we calculate the Nonlinear additives to the Brooks-Herring electrostatic screened potential. We also calculate the corresponding additives to the ionized impurity scattering mobility in n-GaAs over a wide range of doping levels and temperatures. It is demonstrated that the additives to the mobility changes its value up to 50%. The most dramatically mobility is changed near the Mott transition, when the doping level is about 10^{14}-$2x10^{16}$ cm^{-3} and temperature is below 50 K. Also, the results allow us to conclude that the Nonlinear additives break the cross section symmetry with respect to the sign of the charge of the scattering center.**

Keywords—ionized impurity scattering mobility; Brooks-Herring approach; screened potential; Nonlinear additives; n-GaAs;

I. INTRODUCTION

The scattering of electrons by ionized impurities in solids has been studied for more than half a century. The problem is related to the nature of long-range action of the electrostatic potential, which complicates the reduction of the many-body problem to the problem of two bodies. The basic idea for solving the problem is to perform statistical averaging of the field source over the all charged particles. Thus averaging leaves only effective near-field, while the far-field averages to zero. It was suggested many different theoretical models during the last 70 years. The most famous of them are the Conwel and Weisskopf model [1], models that reduce the problem to the third body exclusion method [2-4], model of the partial-wave phase-shift [5-9] and Brooks-Herring model [10, 11]. The Conwel and Weisskopf model was a simple attempt to avoid divergence in collusion integral by using cutoff parameter therefore it is not quite consistent.

The idea of third body exclusion methods is that the particle scattered by a given center must not be scattered by another one. On our opinion, the cross section must not be subjected by this additional condition because it follows from the Boltzmann kinetic equation.

The model of the partial-wave phase-shift has been developed for the case of extremely high carrier concentrations that is realized in metallic alloys. The method usually includes the density functional formalism or the random phase approximation that are more general than the Thomas-Fermi approximation. On the other hand, the basic equation for the partial-wave phase-shift method is the Friedel sum rule. The latter is the sequence of the semiclassical approach for the radial wave functions [6]. Therefore the approach is valid only when the scattered particle wavelength is much shorter than the average distance between impurities that is incorrect for most cases of doped semiconductors. Also, it has to be emphasized, that the quantum peculiarities of the screening appear only on the distances in order of lattice constant, and so they are not essential for the particles near thermal equilibrium state [12].

Given the above, the Brooks-Herring model is the most consistent for low and moderate carrier concentrations (criterion can be found in .9, Ref. [13]).

The validity of the Brooks-Herring approach was discussed several times [13-15], but to the best of our knowledge this investigation mathematically not rigorous or just comparable. Moreover, previous authors consider only limiting cases of non-degenerate or degenerate electron gases.

It is well known that Brooks-Herring screened potential $\phi_{BH}(r) \propto \exp(-r/\lambda)/r$ can be obtained as the solution of the Poisson equation with linearized right-hand side. The parameter λ is named screening length. The main issues that arise in this model is the validity of the expansion of the right-hand side of Poisson's equation in power series and accuracy which implements a linear term of the expansion.

To the best of our knowledge, the nonlinear Poisson equation for the ionized impurity potential firstly was considered by Csavtnszky [16] and Adawi [17]. The corresponding mobility was calculated by Chattopadhyay [18]. But the obtained results are not realistic because of the incorrect boundary conditions.

In the present investigations, we obtain the approximate solution of Poisson's equation that contains the following nonlinear terms of the expansion. As an example, the calculation of the ionized impurity scattering mobility is performed for n-GaAs parameters. The results of the calculation give an opportunity to determine which areas and with what precision Brooks-Herring approach is valid. In addition, the results also provide an opportunity to

assess the accuracy of the formulas for mobility with the following nonlinear terms. The mobility is calculated in the framework of semiclassical Boltzmann equation with the first-order Born approximation. The validity of the approximation is well analyzed in Ref. [19], Chapter 11 pp. 190-197 and Chapter 15 pg. 253.

II. SCREENED POTENTIAL

The Poisson equation for the screened potential has the form

$$\Delta\phi(\mathbf{r}) = -\frac{4\pi e}{\epsilon}\left\{n[\zeta - e\phi(\mathbf{r}), T] - n[\zeta, T]\right\}, \tag{1}$$

where $n(\zeta,T) = 2[mT/(2\pi\hbar^2)]^{3/2}\mathcal{F}_{1/2}(\zeta/T)$ is the electron concentration as the function of temperature T and chemical potential ζ, $\mathcal{F}_{1/2}(x)$ is the Fermi-Dirac integral [20], m is the effective mass, ϵ is the static dielectric constant and $e = -|e|$ is the electron charge. The boundary conditions to the (1) are discussed below.

We will restrict the investigation to the centrally symmetric case for the bulk semiconductor electron gas ($\phi(\mathbf{r}) \equiv \phi(r)$). Leaving only the first non-zero term of the right-hand side power-series expansion, one can obtain the Brooks-Herring approach for the screened potential $\phi_{BH}(r)$ with the screening length λ:

$$\lambda^{-2} = \frac{4\pi e^2}{\epsilon}\frac{\partial n(\zeta,T)}{\partial\zeta}. \tag{2}$$

Below we use dimensionless coordinate $x = r/\lambda$ and potential $\phi(r) = \varphi(x)Z|e|/\epsilon\lambda$, where Z is the charge of the scattering center in $|e|$ units. Proceeding the expansion of the right-hand side of (1) one obtains:

$$\frac{d^2\varphi(x)}{dx^2} + \frac{2}{x}\frac{d\varphi(x)}{dx} - \varphi(x) = \sum_{l=2}^{L}\gamma_l\varphi(x)^l + R_L(x),$$
$$\gamma_l = \frac{1}{l!}\frac{\frac{\partial^l n(\zeta,T)}{\partial\zeta^l}}{\frac{\partial n(\zeta,T)}{\partial\zeta}}\left[\frac{Ze^2}{\epsilon\lambda}\right]^{l-1}, \tag{3}$$
$$R_L(x) = \frac{1}{(L+1)!}\frac{\frac{\partial^{L+1}n[\zeta+e\xi\phi(x),T]}{\partial\zeta^L}}{\frac{\partial n(\zeta,T)}{\partial\zeta}}\left[\frac{Ze^2}{\epsilon\lambda}\right]^L, \qquad 0<\xi<1;$$

where we use the remainder term in the Lagrange form [21]. Note that since the functions $\partial^{L+1}n(\zeta,T)/\partial\zeta^{L+1}$ have a maximum in the region $\zeta \in (-T,\ T)$, in the degenerate case strict inequality holds $|R_L(x)| < |\gamma_{L+1}\phi(x)^{L+1}|$, whereas in the case of Boltzmann electron gas we can speak only about the order of magnitude $|R_L(x)| \sim |\gamma_{L+1}\varphi(x)^{L+1}|$. We proceed the consideration, omitting the remainder term $R_L(x)$ and supposing that tolerance is estimated by the value $|\gamma_{L+1}\varphi(x)^{L+1}|$.

Supposing that $\{\gamma_l\}$ are small parameters one can replace $\sum_{l=2}^{L}\gamma_l\varphi(x)^l$ with $\sum_{l=2}^{L}\gamma_l\varphi_{BH}(x)^l$ in the right-hand side of (3), where $\varphi_{BH}(x) = \exp(-x)/x$ is the dimensionless Brooks-Herring potential. The approach is invalid for $x \to 0$ because one cannot treat terms as a small values in right-hand side of (3).

Therefore we subject the approximate solution to the conditions $[\varphi(x)/\varphi_{BH}(x)]_{x\to\infty} = 1$ and $[\varphi'(x)/\varphi'_{BH}(x)]_{x\to\infty} = 1$. The first approach has form

$$\varphi(x) \simeq \varphi_1^L(x,1,1), \tag{4}$$

Where

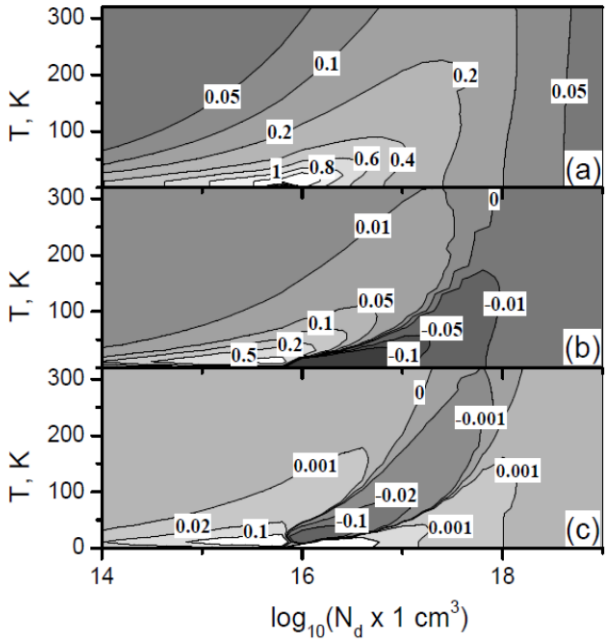

Fig. 1. Contour plots of the coefficients $\{\gamma_l\}$, versus temperature T and donor concentration N_d (logarithmic scale) for bulk GaAs. Frames a-c correspond to γ_{2-4}, $Z = 1$.

$$\varphi_1^L(x,\alpha_0,\beta_0) = \frac{\exp(-x)}{x}$$
$$+\sum_{l=2}^{L}\frac{\gamma_l\beta_0^l}{2x}\int_x^\infty\frac{\{\exp[-x-x'(\alpha_0 l-1)] - \exp[x-x'(\alpha_0 l+1)]\}}{x'^{l-1}}dx', \tag{5}$$

at that the upper index L identifies the number of taken into account nonlinear terms and the lower index identifies the number of iterations was done. It is easy to see that for $L > 2$ iteration procedure is divergent for $x \to 0$. On the other hand, relaxation processes are introduced through the Fourier components $\Phi(q)$ of the potential in the Born approximation, and the divergence became are not essential for if q is finite. Indeed, the necessary condition for the existence of the integral is that the small region of integration gives a small contribution to the integral. For small q, one can estimate, that the region where $|\varphi_1^L(x,1,1) - \varphi_{BH}(x)| > \varphi_{BH}(x)$ is $x \lesssim \exp(-1/|\gamma_3|)$, for $L = 3$. Hence, the corresponding contribution to the Furrier components $\Phi(q)$ has an order of $|\gamma_3|\exp(-1/|\gamma_3|)$. Similarly, one can estimate that for $L = 4$ this value has an order of $\gamma_4^2 + |\gamma_3|\exp(-1/|\gamma_3|)$. The Fourier transformation of the (4) is possible for $L \leq 4$ and has the next form

$$\Phi_1^L(q,\alpha_0,\beta_0)=\frac{4\pi}{q^2+1}+\sum_{l=2}^{L}\gamma_l\beta_0^l F_l(q,\alpha_0), \tag{6}$$

where $q=\mathfrak{q}\lambda$ and $\mathfrak{q}$ is the wave-vector transfer value. To obtain usual dimension one has to multiply the Fourier component by the factor $Z|e|\lambda^2/\epsilon$. The coefficients $F_l(q,\alpha_0)$ are defined as the next

$$F_l(q,\alpha_0)=\frac{4\pi}{q}$$
$$\times\begin{cases}\frac{1}{1+q^2}\left[q\ln\left(\frac{2\alpha_0+1}{2\alpha_0-1}\right)-2\arctan\left(\frac{q}{2\alpha_0}\right)\right], & l=2;\\ \frac{1}{1+q^2}\left\{6\alpha_0\arctan\left(\frac{q}{3\alpha_0}\right)\right. & \\ \quad\left.+q\ln|9\alpha_0^2+q^2|-q\ln\left[\frac{(3\alpha_0+1)^{3\alpha_0+1}}{(3\alpha_0-1)^{3\alpha_0-1}}\right]\right\}, & l=3;\\ \arctan\left(\frac{q}{4\alpha_0}\right)\left(\frac{q^2-16\alpha_0^2}{1+q^2}\right) & \\ +\frac{q}{1+q^2}\left\{\frac{1}{2}\ln\left[\frac{(4\alpha_0+1)^{(4\alpha_0+1)^2}}{(4\alpha_0-1)^{(4\alpha_0-1)^2}}\right]-4\alpha_0\ln|16\alpha_0^2+q^2|\right\}, & l=4;\end{cases} \tag{7}$$

One can see from (7) that for any $q<q_{max}$ coefficients $|F_l(q,\alpha_0)|<const(q_{max})$. Therefore, if γ_l are small enough, then (6) and (7) with $\beta_0=1$ and $\alpha_0=1$ give the valid Fourier components of the screened potential. Next, we consider bulk GaAs as an example. To calculate $\{\gamma_l\}$ we need the equation of electroneutrality

$$n(\zeta,T)=\begin{cases}N_d/\{\exp[(\zeta-E_d)/T]+1\}, & N_d<10^{16}\mathrm{cm}^{-3};\\ N_d, & N_d\geq 10^{16}\mathrm{cm}^{-3};\end{cases} \tag{8}$$

where N_d is the donor concentration and E_d is the donor energy level. In the latter formula we suppose that donor concentration higher than 10^{16} cm^{-3} leads to the Mott transition in bulk GaAs (see for example pg. 41, Fig. 21 in Ref. [22]). Figs. 1 (a-c) demonstrate coefficients γ_{2-4} for n-GaAs parameters [23] versus temperature T and donor concentration N_d as the contours of equivalent values. The calculations performed for $Z=1$. Obviously, in the case $Z=-1$ (acceptors) $\gamma_{2,4}$ change their signs to opposite [see (3)]. Therefore, screened potential loses its symmetry relative to the sign of the centers charge, when the nonlinear terms are taken into account.

It was supposed that the system is quasiequilibrium, hence the concentration is determined by the Fermi-Dirac statistics and the chemical potential satisfies the condition of electroneutrality (7). In the case of a non-equilibrium process the explicit dependence of the distribution function on the ionized impurity potential is very specific, therefore generalization of the result obtained is complicated. Nevertheless, there are cases when electron-electron interaction is dominant and the distribution function can be approached with the Fermi function $F_F(\zeta_e,T_e)$, where the electron temperature T_e and the chemical potential ζ_e are defined by the energy and concentration balance equations (see for example Ref. [24] Chapter 2, pp. 79-87 and Chapter 7, pp. 299-309). In this case the (1-3) are correct if one replaces (ζ,T) with (ζ_e,T_e) and (8) with the balance equations for T_e and ζ_e.

III. ADDITIVES TO MOBILITY

In the present section we calculate the nonlinear additives to the ionized impurity scattering mobility in n-GaAs [23].

The transport time for the electron-impurity scattering can be calculated according to the formula [13, 20]

$$\tau_L^{-1}(E)=\frac{N_d(Ze^2)^2}{8\pi\sqrt{2m}\epsilon^2E^{3/2}}\int_0^{2\sqrt{2mE}\lambda/\hbar}dqq^3|\Phi_1^L(q,1,1)|^2, \tag{9}$$

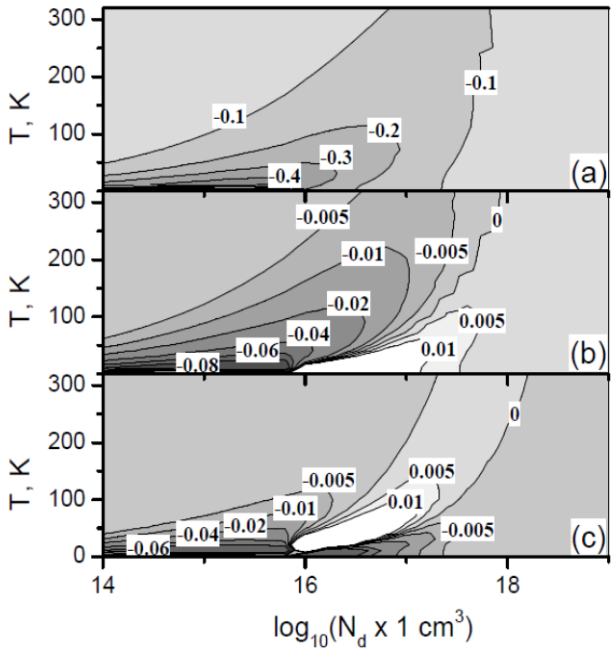

Fig. 2. Contour plots of the relative additives to the mobility in bulk GaAs versus temperature T and donor concentration N_d (logarithmic scale). Frames a-c correspond to Υ_{2-4}

where E is the electron energy and $\Phi_1^L(q,1,1)$ is defined by the formulas (6), and (7) with $\alpha_0=1$ and $\beta_0=1$. The low-field mobility of the electron gas can be introduced in the form [20]:

$$\mu_{imp}^L=\frac{16\pi\sqrt{2m}T^{3/2}|e|}{3n(\zeta,T)(2\pi\hbar)^3}\int_0^\infty dzz^{3/2}\tau_L(zT)\frac{\exp(z-\zeta/T)}{[\exp(z-\zeta/T)+1]^2}. \tag{10}$$

To demonstrate the influence of the nonlinear additives on mobility we introduce the next dimensionless parameter

$$\Upsilon_L=\frac{\mu_{imp}^L-\mu_{imp}^{L-1}}{\mu_{imp}^1}, \tag{11}$$

where μ_{imp}^1 is the mobility calculated in the Brooks-Herring approach. The parameters $\{\Upsilon_L\}$ may be treated as the relative mobility changes due to the L-th nonlinear term. The results of calculation for GaAs parameters one can see in Fig. 2 (a-c). It is easy to see that outside the region $T<50K$, $N_d\in(10^{14}$ cm^{-3}; 2x10^{16} cm^{-3}) nonlinear additives change the mobility

no more then 20%. Whereas, inside the region $T < 50K$, $N_d \in$ (10^{14} cm^{-3}; 2x10^{16} cm^{-3}) the changes in mobility with the addition of the quadratic term Υ_2 is very significant see [Fig. 2 (a)]. On the other hand, with increasing amounts of nonlinear terms from $L = 2$ to $L = 4$, the mobility does not change substantially [see Figs. 2 (b) and (c)]. Correspondingly, one may expect that for $L = 2$ the mean inaccuracy of the formulas (6) and (7) caused by the power-series cutoff at most 10% in the low temperature region and below 5% for $T > 50K$ [see Fig. 1(b)]. In the case $L = 3$ inaccuracy decreases even further [see Fig. 2(c)].

IV. LONG-WAVE LIMIT

Considering (6) and (7), one can see that for $q \ll 1$ Fourier components in (6) can be rewritten as

$$\beta_1 - \beta_1\alpha_1^2 q^2 = 1 + \sum_{l=2}^{L} \frac{\gamma_l \beta_0^l}{4\pi} F_l(0,\alpha_0) - \left[1 - \sum_{l=2}^{L} \frac{\gamma_l \beta_0^l}{8\pi} \frac{\partial^2 F_l(q,\alpha_0)}{\partial q^2}\bigg|_{q=0}\right] q^2 + O_1(q^4), \tag{12}$$

where we suppose that $\Phi_1^L(q,\alpha_1,\beta_1) = 4\pi\beta_1/(1+\alpha_1^2 q^2) + O_2(q^4) = 4\pi\beta_1(1-\alpha_1^2 q^2) + O_3(q^4)$ and the functions $O_{1-3}(x)$ describe small values in order of the argument. It is easy examining that functions $\Phi_k^L(q,\alpha_k,\beta_k) \simeq 4\pi\beta_k/(1+\alpha_k^2 q^2)$ conserve this form for arbitrary number of iterations *k*. Neglecting the small values $O_{1-3}(q^4)$ and supposing that the number of convergent iterations is infinite, one could obtain the algebraic system of equations for the parameters $\alpha = \alpha_{N\to\infty}$ and $\beta = \beta_{N\to\infty}$:

$$\begin{cases} \sum_{l=2}^{L} \gamma_l \beta^l a_l(\alpha) - \beta + 1 = 0; \\ \sum_{l=2}^{L} \gamma_l \beta^l b_l(\alpha) + \alpha^2\beta - 1 = 0; \end{cases} \tag{13}$$

where the coefficients $a_{2.3.4}(\alpha) = F_{2.3.4}(0,\alpha)/4\pi$ are defined by the equality

$$a_l(\alpha) = \begin{cases} \ln\left(\frac{2\alpha+1}{2\alpha-1}\right) - \frac{1}{\alpha}, & l = 2; \\ 2 + 2\ln|3\alpha| - \ln\left[\frac{(3\alpha+1)^{3\alpha+1}}{(3\alpha-1)^{3\alpha-1}}\right], & l = 3; \\ -4\alpha - 8\alpha\ln|4\alpha| + \frac{1}{2}\ln\left[\frac{(4\alpha+1)^{(4\alpha+1)^2}}{(4\alpha-1)^{(4\alpha-1)^2}}\right], & l = 4; \end{cases} \tag{14}$$

and the coefficients $b_{2,3,4}(\alpha) = (8\pi)^{-1}\,\partial^2 F_{2.3.4}(q,\alpha)/\partial q^2|_{q=0}$ are defined by the next equality

$$b_l(\alpha) = \begin{cases} \frac{1}{12\alpha^3} + \frac{1}{\alpha} - \ln\left(\frac{2\alpha+1}{2\alpha-1}\right), & l = 2; \\ \frac{1}{27\alpha^2} + \ln\left[\frac{(3\alpha+1)^{3\alpha+1}}{(3\alpha-1)^{3\alpha-1}}\right] - 2 - 2\ln|3\alpha|, & l = 3; \\ \frac{1}{12\alpha} - \frac{1}{2}\ln\left[\frac{(4\alpha+1)^{(4\alpha+1)^2}}{(4\alpha-1)^{(4\alpha-1)^2}}\right] + 4\alpha + 4\alpha\ln|16\alpha^2|, & l = 4. \end{cases} \tag{15}$$

If the algebraic system (13) with given L and coefficients (14), (15) has real positive solutions then the iteration procedure is supposed to be convergent. Choosing the solution that is closest to the pair $\alpha = 1$ and $\beta = 1$ one can use the Fourier components

$$\Phi_{N\to\infty}^L(q) \approx \frac{4\pi\beta}{1+\alpha^2 q^2}, \qquad q \ll 1. \tag{16}$$

The latter approach valid for processes with a small wave-vector transfer q, but for arbitrary $\gamma_{2.3.4}$ that provide eqs. (13)-(15) with real positive roots. To analyze the system we consider limiting case $q \to 0$ and put $L = 2$. Under such conditions we obtain $\alpha = 1$ and only one equation $0.1\gamma_2\beta^2 - \beta + 1 = 0$. The real root $\beta = 5[1 - \sqrt{1 - 0.4\gamma_2}]/\gamma_2$ that satisfies the mentioned above conditions exists only if $\gamma_2 < 2.5$. Note, that in the case $Z < 0$ the latter inequality is always satisfied. On the other hand, in the case $Z > 2$ it fails in the low temperature region [see Fig. 1(a)]. The linearization of the system (14) leads to the approximate solution $\alpha \simeq 1 - 0.04\gamma_2$ and $\beta \simeq 1 + 0.1\gamma_2$. Therefore, one can expect that if $Z > 0$ then $\alpha < 1$ and $\beta > 1$, whereas if $Z < 0$ then $\alpha > 1$ and $\beta < 1$. One also can estimate that inaccuracy of the first iteration, considered in Sec. III is about $0.1\gamma_2 \lesssim 10\%$ for slow particles [see Fig. 1(a)]. The physical interpretation of the approach (13)-(16) is simple: the Brooks-Herring screened potential remains valid for slow particles, but the screening length became in α times larger and the charge of the ionized impurity became β/α^2 times larger.

V. CONCLUSION

The validity of the results obtained is restricted to the conditions for the Born and the effective mass approximations.

The latter supposes $\lambda \gg l_c$ (l_c is the lattice constant) that is well satisfied for the considered doping levels, whereas Born approximation is questionable for some regions of parameters. We also omit consideration of the nonparabolicity effect that is not essential for the investigation performed.

The main theoretical results are next: (i) the screened potential loses its symmetry relative to the sign of the scattering centers charge, when the nonlinear terms are taken into account; (ii) in the region $T < 50K$, $N_d \in$ (10^{14}; 2x10^{16}) cm^{-3} the nonlinear terms changes the ionized impurity scattering mobility up to 50% in n-GaAs;(iii) the Brooks-Herring screened potential is valid in low temperature region under the condition $q \equiv q\lambda \ll 1$, but with the different screening length $\lambda' = \alpha\lambda$ and the different charge of the scattering center $Z' = \beta Z|e|/\alpha^2$, where $\alpha \simeq 1 - 0.04\gamma_2$, $\beta \simeq 1 + 0.1\gamma_2$ and $\gamma_2 = (Ze^2/2\epsilon\lambda)\,[\partial^2 n(\zeta,T)/\partial\zeta^2]\,[\partial n(\zeta,T)/\partial\zeta]^{-1}$.

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