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Temperature-dependent nonlinear screening of a proton in an electron gas

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Temperature-dependent local-density formalism is applied to the calculation of the screening density profile around a proton embedded in an electron gas. Characteristic quantities such as screening length, density at the proton site, and oscillations at low temperatures are studied. The total energy of the impurity and the entropy are computed and the existence of a bound state discussed. Comparisons are made with other linear and nonlinear theories, particularly the random-phase linear-response theory.

I. INTRODUCTION

The recent development of diagnostic techniques for laser produced plasmas has stimulated theoretical studies of the electronic structure of impurities embedded in an electron gas. As these techniques rest on the modifications of the impurity electronic properties with density and temperature, an accurate knowledge of the dependence of screening effects on the plasma parameters is of crucial importance.

The well-known Debye model gives a simple description of the linear screening of a point charge in a classical (high-temperature, low-density) plasma. Such an approach is easily extended to all densities by using the linearized Thomas-Fermi (TF) theory, which takes into account the degeneracy effects.

A complete treatment of the linear response of an electron gas at any temperature and density, in the random-phase approximation (RPA), has been performed by Gouedard and Deutsch.[1] These authors have shown how the Debye model is recovered from the RPA linear theory in the classical regime. At low temperatures and metallic densities, they pointed out that the electron density exhibits Friedel oscillations, a well-known phenomenon in solid-state physics.[2] The parameters which determine the transition between the two regimes were defined, leading to a good understanding of the physics of screening. The binding energy of a ground-state electron in the potential of a proton deduced from this linear theory has been calculated by Gupta and Rajagopal for various densities and temperatures.[3]

The same model of an electron gas neutralized by a positive background simulating the ionic charges (jellium) has been extensively used in solid-state physics, at zero temperature. The screening of an impurity in the jellium has been numerically studied in great detail, especially in the case of a proton.[4–15] The comparison of quantum-mechanical nonlinear calculations in the local-density formalism (LDF) with the results of the linear RPA approximation has revealed the importance of nonlinear effects, for instance: strong enhancement of the electron density at the nucleus and phase effects in the asymptotic form of the density.[6] We thought that a similar comparison between linear and nonlinear screening of a proton at any temperature would be useful.

In this paper, we present the numerical results of complete nonlinear quantum-mechanical calculations of the screening of a proton in a dense electron gas at various temperatures. The exchange-and-correlation effects are taken into account within the temperature-dependent local-density formalism proposed by Mermin.[16] Comparison is made with TF and linear RPA theories. In Sec. II we describe the theoretical model; the equations to be solved are presented and the expressions of thermodynamic quantities of interest are given. The numerical results are reported and discussed in Sec. III.

II. THEORY

Following the zero-temperature approach of Hohenberg and Kohn[17] and Kohn and Sham,[18] for the ground-state properties of an electron gas in an external potential $v(\vec{r})$, Mermin showed that[16]: (i) the free energy F of an inhomogeneous electron gas in thermal equilibrium is a unique functional $F[n]$ of the one-electron density $n(\vec{r})$; and (ii) the grand potential

$$\Omega[n]=F[n]-\mu\int n\,d\vec{r} \tag{1}$$

is minimum for the equilibrium density $n(\vec{r})$. The free energy is defined by

$$F[n]=F_s[n]+\tfrac{1}{2}\int n(\vec{r}_1)\frac{1}{r_{12}}n(\vec{r}_2)\,d\vec{r}_1\,d\vec{r}_2 +F_{\text{xc}}[n]+\int v(\vec{r})n(\vec{r})\,d\vec{r}\,, \tag{2}$$

where $F_s[n]$ is the kinetic free energy of noninteracting electrons with density $n(\vec{r})$ and $F_{\text{xc}}[n]$ is the exchange-and-correlation contribution to the free energy. With a local approximation

$$F_{\text{xc}}[n]=\int \mathcal{F}_{\text{xc}}[n(\vec{r})]\,d\vec{r}\,, \tag{3}$$

where $\mathcal{F}_{\text{xc}}(n)$ is a *scalar* function of the density (the dependence of $\mathcal{F}_{\text{xc}}$ on the temperature T is not written explicitly), the minimum property of Ω leads to the functional equation

$$\frac{\delta F_s[n]}{\delta n(\vec{r})}+V(\vec{r})-\mu=0\,, \tag{4}$$

$$V(\vec{r})=v(\vec{r})+\int n(\vec{r}\,')\frac{1}{|\vec{r}-\vec{r}\,'|}\,d\vec{r}\,'+\frac{d\mathcal{F}_{\text{xc}}(n)}{dn}\,, \tag{5}$$

where μ is the chemical potential. $V(\vec{r})$ defined by Eq. (5) is an effective potential, including the exchange-and-correlation potential

$$V_{\text{xc}}(n(\vec{r}))=\frac{d\mathcal{F}_{\text{xc}}(n)}{dn}\,. \tag{6}$$

Equation (4) is equivalent to the equation for noninteracting electrons in the effective potential $V(\vec{r})$, so that its solution is given by the following system:

$$(-\tfrac{1}{2}\Delta+V)\psi_i=\epsilon_i\psi_i\,, \tag{7}$$

$$n=\sum_i f(\epsilon_i)\psi_i^*\psi_i\,, \tag{8}$$

where $f(\epsilon_i)$ is the Fermi-statistics occupation number

$$f(\epsilon_i)=\{1+\exp[\beta(\epsilon_i-\mu)]\}^{-1}\,, \tag{9}$$

depending on the temperature ($\beta^{-1}=k_BT$) and the chemical potential fixed by the total number of electrons. For a proton ($Z=1$) embedded in a jellium at density n_0, the external potential is

$$v(r)=-\frac{Z}{r}-\int n_0\frac{1}{|\vec{r}-\vec{r}\,'|}\,d\vec{r}\,'\,,$$

so that the effective potential [Eq. (5)] is

$$V(r)=-\frac{Z}{r}+\int[n(r')-n_0]\frac{1}{|\vec{r}-\vec{r}\,'|}\,d\vec{r}\,' +V_{\text{xc}}(n)\,. \tag{10}$$

At large radii, the displaced electron charge vanishes, and the Coulomb part of $V(r)$ also vanishes due to the perfect screening of the proton, so that the asymptotic value of $V(r)$ is $V_{\text{xc}0}=V_{\text{xc}}(n_0)$. Applying Eq. (4) at large r gives

$$\frac{\delta F_s[n_0]}{\delta n_0}=\mu-V_{\text{xc}0}=\bar{\mu}\,,$$

or, equivalently

$$n_0=\frac{\sqrt{2}}{\pi^2}\beta^{-3/2}I_{1/2}(\beta\bar{\mu})\,, \tag{11}$$

where the standard definition of the Fermi functions has been used:

$$I_\alpha(\eta)=\int_0^\infty\frac{y^\alpha}{1+e^{y-\eta}}\,dy\,. \tag{12}$$

It is convenient to define a new potential

$$\bar{V}(r)=V(r)-V_{\text{xc}0}\,, \tag{13}$$

which goes to zero at infinity, and new eigenvalues of Eq. (7):

$$\bar{\epsilon}_i=\epsilon_i-V_{\text{xc}0}\,. \tag{14}$$

The potential $\bar{V}(r)$ may have bound states $\bar{\epsilon}_b$. The treatment of the delocalized states proposed by Friedel for impurities at zero temperature[2] can be applied in the nonzero case too. The eigenfunctions ψ_{klm} of Eq. (7) for energy $\bar{\epsilon}_k=\frac{1}{2}k^2$, satisfying the boundary condition $\psi_{klm}=0$ at a very large radius R, and normalized within the sphere $r\le R$, are

$$\psi_{klm}(\vec{r})=A_{klm}\varphi_{kl}(r)Y_{lm}(\hat{r})\,, \tag{15}$$

where φ_{kl} has the asymptotic form

$$\varphi_{kl}(r)\rightarrow\frac{1}{r}\sin\left[kr-l\frac{\pi}{2}+\eta_l\right]\,, \tag{16}$$

$\eta_l(k)$ being the phase shifts in the potential $\bar{V}(r)$. A straight-forward derivation gives, for the density defined in Eq. (8),

$$n(r)-n_0=\sum_b f(\bar{\epsilon}_b)\psi_b^*\psi_b+\frac{1}{\pi^2}\int_0^\infty f(\bar{\epsilon}_k)\,dk\sum_l(2l+1)[\varphi_{kl}^2-k^2j_l^2(kr)]\;. \tag{17}$$

The density of states in the continuum is modified by the potential $\bar{V}(r)$ and becomes

$$\rho(k)=\rho_0(k)+\frac{2}{\pi}\sum_l(2l+1)\frac{d\eta_l}{dk}\;, \tag{18}$$

where $\rho_0(k)$ is the density of states per unit of wave vector in the unperturbed electron gas. The following generalized Friedel sum rule expresses the total screening of the point charge by the displaced density:

$$Z=\sum_b f(\bar{\epsilon}_b)+\frac{2}{\pi}\int_0^\infty f(\bar{\epsilon}_k)dk\sum_l(2l+1)\frac{d\eta_l}{dk}\;. \tag{19}$$

The first right-hand side term is the amount of bound charge Z_b; an integration by parts gives, with the convention $\eta_l(0)=0$:

$$Z_f=Z-Z_b=\beta\frac{2}{\pi}\int_0^\infty kf(\bar{\epsilon}_k)[1-f(\bar{\epsilon}_k)]\sum_l(2l+1)\eta_l\,dk\;. \tag{20}$$

The thermodynamic quantities are easily calculated in that model. Their modification from the perfect jellium to the perturbed system are

(i) Entropy:

$$\Delta S=S[n]-S[n_0]=\Delta S_b+\Delta S_f+\Delta S_{\text{xc}}\;, \tag{21}$$

$$\Delta S_b=-\sum_b[f_b\ln f_b+(1-f_b)\ln(1-f_b)]\;, \tag{22}$$

where we now use for brevity the notation $f_b=f(\bar{\epsilon}_b)$. ΔS_b is the contribution of the bound states. The continuous spectrum gives

$$\Delta S_f=\beta^2\frac{2}{\pi}\int_0^\infty kf_k(1-f_k)(\tfrac{1}{2}k^2-\bar{\mu})\times\sum_l(2l+1)\eta_l\,dk\;, \qquad (23$$

with $f_k=f(\frac{1}{2}k^2)$. The term due to exchange and correlation is

$$\Delta S_{\text{xc}}=\beta^2\frac{\partial}{\partial\beta}[F_{\text{xc}}(n)-F_{\text{xc}}(n_0)]\;. \tag{24}$$

The approximation used for F_{xc} will be defined below.

(ii) Free energy:

$$\begin{aligned}\Delta F&=F[n]-F[n_0]\\&=Z\mu+\Delta F_b+\Delta F_1+\Delta F_2+\Delta F_3\;,\end{aligned} \tag{25}$$

$$\Delta F_b=\sum_b f_b(\bar{\epsilon}_b-\bar{\mu})-T\Delta S_b\;, \tag{26}$$

$$\Delta F_1=-\frac{2}{\pi}\int_0^\infty kf_k\sum_l(2l+1)\eta_l\,dk\;, \tag{27}$$

$$\begin{aligned}\Delta F_2=&-\tfrac{1}{2}\int\frac{Z}{r}(n-n_0)d\vec{r}\\&-\tfrac{1}{2}\int(n+n_0)\bar{V}_c(r)d\vec{r}\;,\end{aligned} \tag{28}$$

$$\begin{aligned}\Delta F_3=&F_{\text{xc}}(n)-F_{\text{xc}}(n_0)\\&-\int[nV_{\text{xc}}(n)-n_0V_{\text{xc}0}]d\vec{r}\;.\end{aligned} \tag{29}$$

In Eq. (28), $\bar{V}_c=\bar{V}-[V_{\text{xc}}(n)-V_{\text{xc}0}]$ is the Coulomb part of $\bar{V}$.

For the exchange-and-correlation free energy we have used the results of Gupta and Rajagopal[19] who proposed a local-density functional for a wide range of densities and temperatures, based on the first-order exchange and sum of ring diagrams for the interacting electron gas. We have performed an analytical fit of their values of the ratio $F_{\text{xc}}(n,T)/F_{\text{xc}}(n,0)$. The Kohn-Sham-Wigner exchange-and-correlation functional has been taken for $F_{\text{xc}}(n,0)$.

At this point, we should mention that the model described here has several features in common with the self-consistent model for condensed matter proposed by Liberman.[20] Liberman assumes that the ions surrounding a particular atom in a condensed material may be replaced by a positive charge distribution which is constant outside of a sphere containing the atom and zero inside. Liberman's model leads to the same kind of equations as the present single-impurity model, but with the additional constraint of having the right number of electrons inside the Wigner-Seitz sphere where the central atom is located. As further simplifications have been made by Liberman, such as replacing the electron density outside the cavity with its volume average and including exchange at any temperature by means of the $n^{1/3}$ Kohn-Sham potential, the physical meaning of the results is very different, but the numerical techniques are similar.

As demonstrated in Ref. 1 within linear response, Thomas-Fermi theory gives the correct asymptotic limit for the impurity problem. In Sec. III we shall naturally compare our results with those obtained in TF theory, including the same exchange-and-correlation contribution as in the quantum model. In the TF case, the displaced density is[21]

$$n(r)-n_0=\frac{\sqrt{2}}{\pi^2}\beta^{-3/2}[I_{1/2}(\beta(\bar{\mu}-\bar{V})) -I_{1/2}(\beta\bar{\mu})]\,. \qquad (30)$$

In the TF entropy, $\Delta S_b=0$ and

$$\Delta S_f=\frac{5}{3}\frac{\sqrt{2}}{\pi^2}\beta^{-3/2}\int d\vec{r}[I_{3/2}(\beta(\bar{\mu}-\bar{V}))-I_{3/2}(\beta\bar{\mu})] -\beta\int d\vec{r}\,n(\bar{\mu}-\bar{V})\,. \qquad (31)$$

In the free-energy expression, ΔF_2 and ΔF_3 [Eqs. (28) and (29)] remain valid, but $\Delta F_b=0$ and ΔF_1 must be replaced with

$$\Delta F_1=-\frac{2}{3}\frac{\sqrt{2}}{\pi^2}\beta^{-5/2} \times\int d\vec{r}[I_{3/2}(\beta(\bar{\mu}-\bar{V})) -I_{3/2}(\beta\bar{\mu})]\,. \qquad (32)$$

The linear-response density profile, which will be used for various comparisons is defined by

$$n-n_0=(2\pi)^{-3}\int d\vec{q}\,\frac{\sin qr}{qr}\left[-\frac{4\pi Z}{q^2}\right]\frac{\pi_0(q)}{\epsilon(q)}\,, \qquad (33)$$

where $\pi_0(q)$ is the RPA noninteracting electron polarizability

$$\pi_0(q)=PP\frac{1}{\pi^2 q}\int_0^\infty kf_k\ln\left|\frac{q-2k}{q+2k}\right|dk\,, \qquad (34)$$

and $\epsilon(q)$ the interacting static dielectric constant

$$\epsilon(q)=1-\left[\frac{4\pi}{q^2}+X(q)\right]\pi_0(q)\,, \qquad (35)$$

$X(q)$ being the temperature-dependent local field factor consistent with the exchange-and-correlation functional:

$$X(q)=\frac{dV_{\mathrm{xc}}(n_0)}{dn_0}\,. \qquad (36)$$

A numerical procedure due to Pelissier[22] has been used to compute $\pi_0(q)$.

An interesting quantity measuring the extent of the screening charge around the impurity is the screening constant k. In the linearized TF approximation, the density is given by

$$n-n_0=\frac{Zk_{\mathrm{TLF}}^2}{4\pi r}e^{-k_{\mathrm{TFL}}r}\,, \qquad (37)$$

$$k_{\mathrm{TFL}}^2=\frac{2\sqrt{2}}{\pi}\beta^{-1/2}I_{-1/2}(\beta\bar{\mu})\,. \qquad (38)$$

With $n-n_0$ given by Eq. (37), the integrated displaced charge inside a sphere of radius $R_0=2/k_{\mathrm{TFL}}$ is

$$Q=0.594Z=\int_0^{R_0}(n-n_0)4\pi r^2\,dr\,. \qquad (39)$$

Now, for any density we calculate R_0 satisfying Eq. (39) and define the screening constant by $k=2/R_0$.

III. NUMERICAL RESULTS AND DISCUSSION

Self-consistent calculations of a hydrogen impurity in jellium have been performed for three values of the density parameter $r_s=[3/(4\pi n_0)]^{1/3}$ = 1, 2, and 4. In order to explore the degenerate and nondegenerate regions, three temperatures scaled on the Fermi temperature $T_F[k_BT_F=\frac{1}{2}(3\pi^2n_0)^{2/3}]$: $T/T_F=0.5$, 1.0, 2.0 have been selected. The parameters corresponding to these calculations are summarized in Table I.

The thermodynamic quantities are reported in Table II. The impurity energy is $\Delta E=\Delta F+T\Delta S$ with ΔF and ΔS given in Eqs. (21)–(29). We first notice a good agreement at $T=0$ between our values $\Delta\Omega=\Delta E-Z\mu=-0.696$, -0.534, -0.464 a.u. at $r_s=1$, 2, and 4, respectively, and the results of Zaremba *et al.*,[8] who found $\Delta\Omega=-0.692$, -0.537, -0.469 a.u. The TF values for ΔE are always lower (as for free atoms) because the potential energy is larger in magnitude due to the infinite electron charge at the proton. The increase

TABLE I. Parameters for the nonzero-temperature calculations. Three densities of the electron gas have been studied, corresponding to the values $r_s=1$, 2, and 4. ($n_0=1$ a.u. is equivalent to 6.75×10^{24} e cm^{-3}.) At each density, three temperatures $T/T_F=0.5$, 1.0, and 2.0 are considered (1 a.u. of temperature $=3.16\times10^5$ K). $\bar{\mu}$ is the chemical potential measured with respect to the exchange-and-correlation potential $V_{\text{xc}0}$; $\bar{\mu}/T$ is a function of T/T_F only.

r_s	n_0 (a.u.)	T_F (a.u.)	$t=T/T_F$	$\bar{\mu}$ (a.u.)
1.0	0.239	1.842	0.5	1.369
1.0	0.239	1.842	1.0	−0.0395
1.0	0.239	1.842	2.0	−4.533
2.0	0.0298	0.4604	0.5	0.3421
2.0	0.0298	0.4604	1.0	−0.0099
2.0	0.0298	0.4604	2.0	−1.133
4.0	0.00373	0.1151	0.5	0.0855
4.0	0.00373	0.1151	1.0	−0.0025
4.0	0.00373	0.1151	2.0	−0.2833

of ΔE with temperature, which is proportional to the extra density of states at the Fermi level $\epsilon=\mu_0$ (at least at low T), is faster for the high densities. This increase is in general slightly underestimated by the TF model, but nevertheless the agreement between LDF and TF is satisfactory for the thermal part of ΔE. The entropies are very comparable too, except at low temperature and low density ($T/T_F=0.5$, $r_s=4$). The eigenvalue ϵ_{1S} [Eq. (7)] exists at $T=0$ for $r_s\geq2$ and decreases when T increases. In the range of parameters studied here, we never found a second bound state. But other bound states are expected to appear at higher temperatures.

Table III is concerned with the structure of the displaced density. The screening constant k_{TFL} [Eq. (38)] obtained in the linearized TF approximation is tabulated first. The ratio of the screening constant k, defined in Eq. (39), to k_{TFL} is then given for three models: the present local-density functional (LDF) model, the linear-response (LR) model, and the nonlinearized TF model with exchange and correlation. This ratio is always larger than one in the LDF calculation: this means that the use of the standard k_{TFL} may be a rather poor approximation, particularly at $r_s>2$. The extent of the screening charge is considerably smaller than indicated by k_{TFL}; as could be expected, the

TABLE II. Results for internal energy ΔE, entropy ΔS, and eigenvalue $\bar{\epsilon}$ with 1s symmetry, as obtained in the local-density functional formalism (LDF). The values of ΔE and ΔS calculated in the Thomas-Fermi model (with the same exchange-and-correlation functional) are shown for comparison. All values in atomic units.

		LDF			TF	
r_s	T/T_F	ΔE	ΔS	$\bar{\epsilon}_{1s}$	ΔE	ΔS
1.0	0.0	0.483	0.0	. . .	0.070	0.0
1.0	0.5	0.974	0.898	. . .	0.534	0.882
1.0	1.0	2.055	1.678	−0.0006	1.659	1.710
1.0	2.0	4.733	2.462	−0.036	4.365	2.725
2.0	0.0	−0.427	0.0	−0.00004	−0.898	0.0
2.0	0.5	−0.321	0.658	−0.006	−0.804	0.681
2.0	1.0	−0.019	1.542	−0.037	−0.548	1.430
2.0	2.0	0.713	2.535	−0.105	0.159	2.478
4.0	0.0	−0.543	0.0	−0.010	−1.061	0.0
4.0	0.5	−0.531	0.053	−0.023	−1.046	0.388
4.0	1.0	−0.460	0.879	−0.063	−0.998	0.942
4.0	2.0	−0.253	2.088	−0.148	−0.843	1.857

TABLE III. Comparison between the displaced electron density at the proton in the present local-density functional formalism (LDF) and in the linear-response theory (LR). $n(0)-n_0$ is infinite in the TF model. The screening constants, measured in units of k_{TFL} (screening constant of the *linearized* TF model), as obtained in the LDF, LR, and TF models, are also compared. All values are in atomic units.

			LDF		LR		TF
r_s	T/T_F	k_{TFL}	$n(0)-n_0$	k/k_{TFL}	$n(0)-n_0$	k/k_{TFL}	k/k_{TFL}
1.0	0.0	1.563	0.966	1.245	0.402	1.123	1.164
1.0	0.5	1.380	0.841	1.176	0.365	1.067	1.177
1.0	1.0	1.137	0.682	1.122	0.320	1.044	1.144
1.0	2.0	0.863	0.486	1.075	0.259	1.027	1.080
2.0	0.0	1.105	0.478	1.496	0.093	1.094	1.386
2.0	0.5	0.976	0.428	1.490	0.086	1.093	1.446
2.0	1.0	0.804	0.349	1.385	0.077	1.088	1.411
2.0	2.0	0.610	0.235	1.195	0.064	1.057	1.250
4.0	0.0	0.782	0.346	1.904	0.022	1.031	1.858
4.0	0.5	0.690	0.338	2.066	0.021	1.083	2.056
4.0	1.0	0.568	0.306	2.228	0.019	1.147	2.237
4.0	2.0	0.432	0.222	1.942	0.016	1.133	1.943

discrepancy decreases when density and temperature increase. This shortcoming is clearly a consequence of linearization since the values k/k_{TFL} calculated in the nonlinear TF model are very close to the LDF values. The ratio k/k_{TFL} obtained in LR is always close to one (maximum deviation: 15%) and considerably too low at $r_s=4$. We conclude that the RPA linear response does not improve significantly the linear TF screening length and may be relevant at high densities only.

The comparison of the electron densities at the proton site, obtained in LDF and LR [TF has not to be considered since it gives an infinite $n(0)$] is shown in Table III. At zero temperature, the LDF value of $n(0)-n_0$ is much larger than the LR value. The ratio increases from 2.4 at $r_s=1$ to 15.7 at $r_s=4$. In both models, the charge at the proton decreases when T increases, the screening cloud being more and more spread out. The ratio of the LDF and LR values is slightly smaller at $T/T_F=2$: it goes from 1.9 at $r_s=1$ to 13.9 at $r_s=4$. The main features of the displaced charge are very poorly accounted for by LR, particularly at $r_s=2$ and 4.

A different aspect of the screening-charge profile is the possible existence of Friedel oscillations. In Table IV we give the first node and the first minimum of $n(r)-n_0$, where they do exist. We see that the oscillations exist or do not exist, in LDF and LR, for the same values of the parameters. The first node is always farther from the proton in the LR calculation, indicating a significant difference in the phases given by the two models. Gouedard and Deutsch[1] have shown that,

TABLE IV. Oscillations of the displaced electron density when observed. The first node of $n-n_0$ is r_N (a.u.). The first minimum of the displaced density is shown in the column $(n-n_0)/n_0$. Oscillations have disappeared for the other values of T/T_F. The last column gives the ratio of the damping constant of the Friedel oscillations at low temperatures to the TF screening constant, as derived in linear theory.

		LDF		LR		
r_s	T/T_F	r_N	$(n-n_0)/n_0$	r_N	$(n-n_0)/n_0$	$k_{\mathrm{LR}}/k_{\mathrm{TFL}}$
1.0	0.0	2.88	-0.84×10^{-3}	3.13	-0.67×10^{-3}	0.0
2.0	0.0	2.37	-0.18×10^{-1}	3.01	-0.14×10^{-1}	0.0
	0.5	10.7	-0.87×10^{-7}	11.5	-0.19×10^{-6}	1.39
4.0	0.0	3.30	-0.19	4.90	-0.10	0.0
	0.5	3.48	-0.78×10^{-1}	5.33	-0.26×10^{-1}	0.98
	1.0	5.56	-0.54×10^{-3}	8.41	-0.21×10^{-3}	2.12

in linear RPA theory, the effect of low temperatures is to damp the $T=0$ density with a factor $\exp(-k_{\rm LR}r)$. The screening constant $k_{\rm LR}$ is twice the imaginary part of the smallest pole of the Fermi statistics occupation number f_k

$$k_{\rm LR}=k_F\{2[-\gamma+(\gamma^2+\pi^2t^2)^{1/2}]\}^{1/2}\ , \qquad (40)$$

with $\gamma=\bar{\mu}/T_F$, $t=T/T_F$, and k_F being the Fermi momentum. Gouedard and Deutsh concluded that the condition $k_{\rm TFL}\leq k_{\rm LR}$ defines the TF regime, the Friedel-type behavior corresponding to the opposite inequality. The ratio $\tau=k_{\rm LR}/k_{\rm TFL}$ is given in Table IV. We see that oscillations are still present for $\tau>1$, particularly for the lowest density, indicating that $\tau=1$ is not a rigorous criterion for the vanishing of the Friedel oscillations.

We have presented a temperature-dependent nonlinear calculation of the screening of a proton in an electron gas at various densities, within the framework of LDF formalism, including exchange-and-correlation effects. Connection has been made with (i) complete TF theory, (ii) linear-response theory in RPA approximation, and (iii) linearized TF theory. The important effects of nonlinearity on the displaced density at the proton position, screening length, and phase of oscillations have been pointed out. The model used here can be easily applied to calculations of higher-Z impurities in an electron gas, which are needed for plasma diagnostics.

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