Temperature-dependent screened potential in the Thomas Fermi approximation for 1D, 2D and 3D systems

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Recibido el 24 de septiembre de 1997; aceptado el 2 de julio de 1998

Within the Thomas Fermi approximation (TFA) we use a generalized approach to derive the dielectric function and screened potential for 1D, 2D and 3D systems. For all dimensions we present the asymptotic behavior of the temperature-dependent screened Coulomb potential in terms of the corresponding TFA screening parameters.

Keywords:

Dentro de la aproximación de Thomas-Fermi (ATF) usamos un formalismo generalizado para derivar una función dieléctrica y el potencial apantallado para sistemas en 1D, 2D y 3D. Para todas las dimensiones presentamos el comportamiento asintótico del potencial de Coulomb apantallado en todas las dimensiones en términos de los correspondientes parámetros de apantallamiento de la ATF.

Descriptores:

PACS: 73.20.Dx; 78.20. Ci

1. Introduction

One of the most important many-body effects is the so-called screening or shielding effect which reduces the strength of a given interaction due to the presence of mobile charged carriers. We are interested in studying the screening effects of these carriers when they are very mobile; that is, when they can be considered as quasi-free carriers. It is important to mention that the total medium to be studied is neutrally charged, that is, the total charge density of the quasi-free carriers has to be balanced by an opposite charge density. In real systems the electronic density can be balanced by an opposite charge distribution made of a lattice of shielded nuclei (crystal) or free ions (plasma). Clearly, since electrons (quasi-free carriers) are the lighter particles, their contribution to screening is generally more important.

Quasi-free carriers can be generated by a variety of processes. For instance, they can be produced by modulation-doping or optically by intense illumination of a nominally undoped system. The way these carriers screen the bare Coulomb potential depends on the dimensionality of the system. When the dimensionality of the system is lowered, the screening effects decrease. That is, the influence of screening in 2D is considerably weaker than in 3D and this trend continues if one passes from 2D quantum wells to quasi-one-dimensional quantum wires. This occurs because, if we assume that the quasi-free-carriers are confined in low dimensional systems (2D or 1D), screening between any two charges occurs mainly inside the system-corresponding to field lines inside the material-whereas the field lines that abandon the system are not directly affected by those charges. Clearly, screening is not decreased in this way in a bulk material (3D) since all field lines are screened by the charge carriers. It might be for this reason (weak screening in 1D) that the behavior in real space of screened Coulomb potential in quantum wires has not been investigated in detail. Therefore, the purpose of this paper is to derive expressions for the small wavevector dielectric function and for the long range screened Coulomb potential for 1D, 2D and 3D systems. We resort to the well known Thomas-Fermi approximation (TFA) which provides a simple model for screening and has been extensively used for 2D [1–3] and 3D [4]. An advantage of the TFA screening model is that it generally allows to include in a relatively simple way the dependence on the temperature and on the electron density, unlike more sophisticated models such as RPA. However, it is well known that TFA has an important disavantadge; it cannot reproduce Friedel oscillations of degenerate systems at low temperatures that arise from the abrupt change in screening at a wave vector of $k = 2k_f$ where k_f is the carrier wave vector at the Fermi surface. These oscillations occur in 3D [5], 2D [6] and 1D [7] systems, dominate the long-range behavior of the screened potential and they tend to disappear when the carrier occupation probability becomes a smooth function of the wave vector k, that is, when the temperature increases sufficiently.

Previous important works on 3D Thomas-Fermi screening models are those of Calles *et al.* [8] and Shivamoggi and Mulser [9]. In the former treatment of screening [8] the well-

known results of the Hartree-Fock free electron-theory where incorporated in a simple way as a correction of the screening parameter to obtain that screening is not as strong as estimated in the original free electron approximation. In the latter treatment [9] thermal, relativistic and very strong magnetic field effects were investigated, as well as the motion of the test charge. However in latter reference thermal effects were taken into account only for very small temperatures, but fortunately as we will discuss later, there exist a complementary calculation [10] that extends the results to higher temperatures.

The way these carriers screen the bare Coulomb potential depends on the dimensionality of the system. When the dimensionality of the system is lowered, the screening effects decrease. That is, the influence of screening in 2D is considerably weaker than in 3D and this trend continues if one passes from 2D quantum wells to quasi-one-dimensional quantum wires. This occurs because, if we assume that the quasi-free-carriers are confined in low dimensional systems (2D or 1D), screening between any two charges occurs mainly inside the system-corresponding to field lines *inside* the material-whereas the field lines that abandon the system are not directly affected by those charges. Clearly, screening is not decreased in this way in a bulk material (3D) since all field lines are screened by the charge carriers. It might be for this reason-weak screening in 1D-that the behavior in real space of screened Coulomb potential in quantum wires has not been investigated in detail. Therefore, one the purposes of this paper is to derive expressions for the small wavevector dielectric function and for the long range screened Coulomb potential. We resort to the well known Thomas-Fermi approximation (TFA) which provides a simple model for screening and has been extensively used for 2D [1–3] and 3D [4]. An advantage of the TFA screening model is that it generally allows to include in a relatively simple way the dependence on the temperature and on the electron density, unlike more sophisticated models such as RPA (Random Phase Approximation) [11]. However, it is well known that TFA has an important disavantadge; it cannot reproduce Friedel oscillations of degenerated systems at low temperatures that arise from the abrupt change in screening at a wave vector of $k = 2k_f$ where k_f is the carrier wave vector at the Fermi surface. These oscillations occur in 3D [5], 2D [6] and 1D [7] systems, dominate the long-range behavior of the screened potential and they tend to disappear when the carrier occupation probability becomes a smooth function of the wave vector k, that is, when the temperature increases sufficiently. In contrast to metals, for which the intrinsic energy scales are usually much larger than the temperature, in low dimensional semiconductor structures the experimental temperature can be compared to the intrinsic energies. For example, for a quasi-one-dimensional semiconductor quantum wire (QW) to be in the quantum limit, the doping must be necessary low and hence the Fermi energy is also small, where by quantum limit we mean that electrons are confined to the lowest subband of a QW. For a semiconductor QW, some of their many-body properties have been discussed, for example, in the extensive work of Hu and Das Sarma [12, 13] and the references quoted therein. These properties can manifest as lattice Peierls distortion, disorder-induced Anderson localization, hole screening effects, plasma effects and impurity scattering, the last two of them being the most important ones for actual semiconductor QWs [12, 13]. Because the plasmon dispersion in a QW goes to zero as the momentum q gets small, dynamical effects are expected to be important for small q. In fact, Hu and Das Sarma have argued that for 1D systems low-energy virtual plasmon excitations can be crucial in dynamical screening since they cause the Fermi surface to disappear (in the sense that elementary excitations are very different from those of the noninteracting systems), but when impurity scattering is included, the Fermi surface reappears because these plasmons are damped by impurity scattering, which is consistent with Raman scattering and photoluminescence experiments since these experiments are explained successfully on the basis of standard Fermi-liquid theory [12, 13]. Therefore, in the light of these results, it seems that our static screening theory-which does not include plasma effects- can be safely applied to most semiconductor QWs, but it should not be applied to very clean QWs (where by clean we mean that it lacks impurity scattering).

In spite of all work done on TFA models, it seems that it lacks a unified approach valid for all dimensions, so the motivation of this work is to develop the main TFA concepts in a general way. The paper is structured as follows; in Sect. 2 we derive, for all dimensions, general expressions for the Fourier transforms of the screened potentials and corresponding dielectric functions. In Sect. 3 we develop the TFA approach for these quantities, in Sect. 4 we present analytical expressions for the temperature dependence of the TFA screening parameters, and in Sect. 5 we present the asymptotic behavior of the potentials in terms of the TFA screening parameter.

2. Dielectric function

We will consider only the presence of a periodic background potential through an effective mass m^*. If we have a positively charged particle placed at a given position in a electron gas and rigidly held there, it will attract electrons, creating a surplus of negative charge in its neighborhood, which reduces or screens its field. Let us introduce two electrostatic potentials. The first, $\phi^{\rm ext}$, arises only from the positively charged particles so that it satisfies the Poisson equation given by

$$-\nabla^2\phi^{\rm ext} = \frac{4\pi}{\kappa}\rho^{\rm ext}(\vec{r}), \tag{1}$$

where $\rho^{\rm ext}$ is the quasi-free particle charge density and κ is the constant of the medium or media that contains the system. For 1D and 2D systems, this macroscopic constant accounts for the dielectric function of the media that surrounds the corresponding low dimensional system while for a 3D system this constant can represent the contribution to the dielectric

constant of the bounded charges. With κ defined in this way we will be able to apply our generalized TFA approach to all dimensions. The second, ϕ, is the full physical potential produced by both the positive charged particle and the cloud of screening electrons, it satisfies

$$-\nabla^2\phi = \frac{4\pi}{\kappa}\rho(\vec{r}), \tag{2}$$

where ρ is the full density,

$$\rho(\vec{r}) = \rho^{\rm ext}(\vec{r}) + \rho^{\rm ind}(\vec{r}) \tag{3}$$

and $\rho^{\rm ind}$ is the charge density induced in the electron gas by the presence of the external particle.

In a static model, since the external charge has electrostatic influence over a finite vicinity which surrounds it, ϕ has to have a nonlocal relation with $\phi^{\rm ext}$ given by

$$\phi^{\rm ext}(\vec{r}_J) = \int d\vec{r}'_J \frac{\epsilon(|\vec{r}_J - \vec{r}'_J|)}{\kappa}\phi(\vec{r}'_J), \tag{4}$$

where J indicates the dimensionality of the homogeneous system. The corresponding Fourier transforms satisfies

$$\phi(q_J) = \frac{\kappa\phi^{\rm ext}(q_J)}{\epsilon^{J\rm D}(q_J)}, \tag{5}$$

where $\epsilon^{J\rm D}(q_J)$ is the absolute value of the J-dimensional wave vector dependent dielectric constant of the J-dimensional system.

The most natural quantity to be calculated is not the dielectric constant but the charge density $\rho^{\rm ind}$ induced in the electron gas by the total potential ϕ. When $\rho^{\rm ind}$ and ϕ are linearly related (for sufficiently weak ϕ), then their Fourier transform satisfies

$$\rho^{\rm ind}(q_J) = \chi(q_J)\phi(q_J). \tag{6}$$

We can relate ϵ to χ by taking the Fourier transforms of the Poisson Eqs. (1) and (2). Since these transforms depend on the dimensionality of the system involved, we perform for the z oriented 1D, x-y oriented 2D and the 3D systems the z-Fourier, x-y-Fourier and 3D Fourier transform, respectively, to yield

$$\left(q_z^2 - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2}\right)\phi(x,y,q_z) = \frac{4\pi}{\kappa}\rho(x,y,q_z), \tag{7}$$

$$\left(q_x^2 + q_y^2 - \frac{d^2}{dz^2}\right)\phi(q_x,q_y,z) = \frac{4\pi}{\kappa}\rho(q_x,q_y,z), \tag{8}$$

$$\left(q_x^2 + q_y^2 + q_z^2\right)\phi(q_x,q_y,q_z) = \frac{4\pi}{\kappa}\rho(q_x,q_y,q_z), \tag{9}$$

where ρ and ϕ have hybrid arguments (in real and Fourier spaces). We solve Eqs. (7) and (8) for $\phi(x,y,q_z)$ and $\phi(q_x,q_y,z)$ by using the corresponding Green function of each inhomogeneous Hemholtz equation [14], we find respectively

$$\phi(r,\theta,q_z) = \frac{2}{\kappa}\int K_0[q_z s(r,r',\theta)]\rho(r',\theta',q_z)r'dr'd\theta', \tag{10}$$

$$\phi(q_x,q_y,z) = \frac{2\pi}{\kappa\sqrt{q_x^2+q_y^2}}\int \rho(q_x,q_y,z') \times e^{-\sqrt{q_x^2+q_y^2}|z-z'|}dz', \tag{11}$$

where $K_0[q_z s(r,r',\theta)]$ is the modified Bessel function of second class and $s(r,r',\theta) = \sqrt{r^2+(r')^2-2rr'\cos\theta}$. The solution of Eq. (9) is just algebraic.

Finally, since the 1D and 2D potentials can be calculated as $\phi_{1\rm D}(q_z) = \lim_{q_z a\to 0}\phi(r,\theta,q_z)$, $\phi_{2\rm D}(q_x,q_y) = \lim_{z\to z'}\phi(q_x,q_y,z)$, respectively, where a is the radius of the cylindrical section of the wire (or yields the order of magnitude of the cross section of the wire for other noncircular sections) and we have that [16] $K_0(q_z s(r,r',\theta)) \approx -\ln(q_z a/2) - \ln[s(r,r',\theta)/a] - \gamma \approx -\ln(q_z a/2) \approx -\ln(q_z a)$ for very small values of $q_z a$, thus we arrive at

$$\phi_{1\rm D}(q_z) = -\frac{2}{\kappa}\ln(q_z a)\,\rho_{1\rm D}, \tag{12}$$

$$\phi_{2\rm D}(q_x,q_y) = \frac{2\pi}{\kappa}\frac{\rho_{2\rm D}}{\sqrt{q_x^2+q_y^2}}, \tag{13}$$

where $\rho_{1\rm D} = \int \rho r'dr'd\theta'$ and $\rho_{2\rm D} = \int \rho dz'$ are respectively, the 1D and 2D charge density. By performing the same treatment for $\phi^{\rm ext}$ on each dimension we obtain

$$\phi^{\rm ext}_{1\rm D}(q_z) = -\frac{2}{\kappa}\ln(q_z a)\,\rho^{\rm ext}_{1\rm D}, \tag{14}$$

$$\phi^{\rm ext}_{2\rm D}(q_x,q_y) = \frac{2\pi}{\kappa}\frac{\rho^{\rm ext}_{2\rm D}}{\sqrt{q_x^2+q_y^2}}, \tag{15}$$

$$\phi^{\rm ext}_{3\rm D}(q_x,q_y,q_z) = \frac{4\pi}{\kappa}\frac{\rho^{\rm ext}_{3\rm D}}{q_x^2+q_y^2+q_z^2}. \tag{16}$$

Together with Eq. (3) for 1D, 2D and 3D densities and Eq. (6) these give

$$\phi_{1\rm D} = \frac{\phi^{\rm ext}_{1\rm D}}{1 + 2\ln(q_z a)\dfrac{\chi(q_z)}{\kappa}}, \tag{17}$$

$$\phi_{2\rm D} = \frac{\phi^{\rm ext}_{2\rm D}}{1 - \dfrac{\chi\left(\sqrt{q_x^2+q_y^2}\right)}{\kappa}\dfrac{2\pi}{\sqrt{q_x^2+q_y^2}}}, \tag{18}$$

$$\phi_{3\rm D} = \frac{\phi^{\rm ext}_{3\rm D}}{1 - \dfrac{\chi\left(\sqrt{q_x^2+q_y^2+q_z^2}\right)}{\kappa}\dfrac{4\pi}{q_x^2+q_y^2+q_z^2}}. \tag{19}$$

By comparing this with Eq. (5) leads to the relation

$$\frac{\epsilon^{1D}(q)}{\kappa} = 1 + 2\ln(q_z a)\,\frac{\chi(q_z)}{\kappa}, \tag{20}$$

$$\frac{\epsilon^{2D}(q)}{\kappa} = 1 - \frac{\chi(\sqrt{q_x^2+q_y^2})}{\kappa}\,\frac{2\pi}{\sqrt{q_x^2+q_y^2}}, \tag{21}$$

$$\frac{\epsilon^{3D}(q)}{\kappa} = 1 - \frac{\chi(\sqrt{q_x^2+q_y^2+q_z^2})}{\kappa}\,\frac{4\pi}{q_x^2+q_y^2+q_z^2}. \tag{22}$$

Except for the assumption that the externally applied charge is weak enough to produce only a linear response in the electron gas, the foregoing analysis has been exact. The following step is to calculate χ by using the Thomas-Fermi method which has the advantage that it is applicable even when a linear relation between $\rho^{\rm ind}$ and ϕ does not hold but has the limitation that is reliable only for very slowly varying external potential.

3. TFA model

Let us consider ϕ as a slow varying function of $\vec{r}$ in the sense that the energy of a charge carrier which is under its influence is given by

$$E(\vec{k}) = \frac{\hbar^2 k^2}{2m} - e\phi, \tag{23}$$

thus the energy is modified from its free electron value by the total local potential. This only has sense in terms of wavepackets since we must require that $\phi(\vec{r})$ varies slowly on the scale of a Fermi wavelength. .

To calculate the charge density produced by these electrons we substitute Eq. (23) into the electronic number density, to find

$$n^J[\mu + e\phi(\vec{r})] = \frac{2}{(\pi)^J}\int d^J k \frac{1}{e^{\beta(\frac{\hbar^2 k^2}{2m} - e\phi - \mu)}+1}, \tag{24}$$

where J indicates the dimensionality of the system, the factor 2 accounts for the possible spin states, $\beta = 1/(\kappa_{\rm B}T)$ and a similar expression for the charge density of the positive background n_0 but with $\phi = 0$. Thus the induced charge density is given by

$$\rho^{\rm ind} = -e\{n[\mu + e\phi(\vec{r})] + n_0(\mu)\}, \tag{25}$$

which is the basic equation of the nonlinear Thomas-Fermi theory, e being the electron charge. If we expand Eq. (25) we obtain to leading order

$$\rho^{\rm ind} = -e^2\phi\frac{\partial n_0}{\partial \mu}. \tag{26}$$

Comparing the Fourier transform of Eq. (26) with Eq. (6) we find that

$$\chi(\vec{q}) = -e^2\frac{\partial n_0}{\partial \mu}, \tag{27}$$

where $\partial n_0/\partial\mu$ is independent of q. Substitution into Eq. (20) gives the Thomas-Fermi dielectric response function for all JD dimensions ($J = 1, 2, 3$).

$$\epsilon^{1D}(q_z) = \kappa - q_s^{1D}\ln(q_z a), \tag{28}$$

$$\epsilon^{2D}(q_x, q_y) = \kappa + \frac{q_s^{2D}}{\sqrt{q_x^2+q_y^2}}, \tag{29}$$

$$\epsilon^{3D}(q_x, q_y, q_z) = \kappa + \frac{(q_s^{3D})^2}{q_x^2+q_y^2+q_z^2}, \tag{30}$$

where we have introduced the Thomas-Fermi parameters $q_s^{1D} = 2e^2\partial n_0^{1D}/\partial\mu$, $q_s^{2D} = 2\pi e^2\partial n_0^{2D}/\partial\mu$ and $(q_s^{3D})^2 = 4\pi e^2\partial n_0^{3D}/\partial\mu$. Due to the fact that $n_0^J = [1/L]^J$ dimensions, q_s^{1J} is dimensionless and q_s^{2D}, q_s^{3D} have both dimensions of inverse of length; $1/L$.

Now, let us suppose that the external potential $\phi^{\rm ext}$ is that of a point charge, that is, $\phi = e/r$, thus its Fourier transform potential for the 1D, 2D and 3D cases respectively, are given by

$$\phi_{1D}^{\rm ext}(q_z) = \frac{-2e}{\kappa}\ln(q_z a), \tag{31}$$

$$\phi_{2D}^{\rm ext}(q_x, q_x) = \frac{2\pi e}{\kappa\sqrt{q_x^2+q_y^2}}, \tag{32}$$

$$\phi_{3D}^{\rm ext}(q_x, q_y, q_z) = \frac{4\pi e}{\kappa(q_x^2+q_y^2+q_z^2)}. \tag{33}$$

The total potential in the semiconductor will then be in each case

$$\phi_{1D}(q_z) = \frac{\phi^{\rm ext}(q_z)}{\epsilon^{1D}(q_z)} = \frac{-2e\ln(q_z a)}{1 - q_s^{1D}\ln(q_z a)}, \tag{34}$$

$$\phi_{2D}(q_x, q_y) = \frac{\phi^{\rm ext}(q_x, q_y)}{\epsilon^{2D}(q_x, q_y)} = \frac{2\pi e}{q_s^{2D} + \sqrt{q_x^2+q_y^2}}, \tag{35}$$

$$\phi_{3D}(q_x, q_y, q_z) = \frac{\phi^{\rm ext}(q_x, q_y, q_z)}{\epsilon^{3D}(q_x, q_y, q_z)} = \frac{4\pi e}{q_x^2+q_y^2+q_z^2+(q_s^{3D})^2}. \tag{36}$$

4. Temperature dependence of screening

TFA can be considered a useful and simple model of screening when the system does not exhibit Friedel oscillations, since these oscillations cannot be reproduced by TFA. As mentioned in Sect. 1, it is known [7] that in low-temperature 1D systems these oscillations also dominate, as in 3D and 2D systems, the long-range behavior of the screened Coulomb

potential. Since Friedel oscillations tend to disappear when the carrier occupation probability-the Fermi distribution- becomes a smooth function of the wave vector, then a necessary condition for the TFA to be able to yield a better description of the system-including screening effects-is to increase the temperature. Therefore, in order to present a complete one parameter-TFA theory it is important to be able to find the dependence of q_s^{3D} on the temperature. To do this, it is necessary to calculate $\partial n_0^{\text{3D}}/\partial\mu$.

For the 3D case the calculation of q_s^{3D} valid at very small temperatures was calculated by Shivamoggi [9] to obtain

$$\lambda_F^{-2} = \frac{2}{3}(q_s^{\text{3D}})^2 = \frac{4}{3\pi}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\mu}\left[1-\frac{\pi^2}{24}\left(\frac{KT}{\mu}\right)^2\right]e^2.$$

Joyce and Aguilera-Navarro [10, 15] complemented the calculation of Ref. 9 by extending their results to higher temperatures using a series representation of $n^{\text{3D}}(\mu)$ given by Eq. (24) and reversing it by using the rules of series reversion [16] which, up to third order in ν, led to the expression

$$\beta\mu \approx \ln\nu + \sum_{n=1}^{3} A_n\nu^n, \tag{37}$$

where $\nu = (4n)\left(\pi\beta\hbar^2/2m^*\right)^{3/2}$, $z = e^{\beta\mu}$, $A_1 = 0.353$, $A_2 = 4.9\times10^{-3}$ and $A_3 = 1.48\times10^{-4}$. Aguilera-Navarro [10] improved the convergence of this partial summation by using the Padé approximant $\nu d\beta\mu/d\nu \doteq [L/M](\nu)$, $L+M \leq 4$, where $[L/M]$ denotes the ratio of two polynomial of order L and M, respectively. The approximation with $L=2$ and $M=1$ gives the most accurate results. A final integration yields

$$\beta\mu = \ln\nu + K_1\ln(K_2\nu+1) + K_3\nu,$$

with $K_1 = 4.896$, $K_2 = 0.0450$ and $K_3 = 0.133$. This expression is exact in the classic limit and provides an excellent approximation for the range $-\infty < \mu\beta < 30$. From the latter equation $(q_s^{\text{3D}})^2 = (4\pi e^2)(\partial n_0^{\text{3D}}/\partial\mu)$ is given by

$$\frac{1}{(q_s^{\text{3D}})^2} = \frac{1}{4\pi e^2\beta n} + \frac{K_1\sqrt{\beta}}{4\pi e^2(K_2\nu+1)}\left(\frac{\pi\hbar^2}{2m^*}\right)^{3/2} + \frac{K_3\sqrt{\beta}}{4\pi e^2}\left(\frac{\pi\hbar^2}{2m^*}\right)^{3/2}$$

For a 2D system Eq. (24) yields

$$n^{\text{2D}} = \frac{1}{2\pi}\left(\frac{2m}{\hbar^2\beta}\right)\int_0^\infty dx\,\frac{1}{e^x e^{-\beta\mu}+1},$$

and using $t = e^x$ as an integration variable this expression becomes

$$n^{\text{2D}} = \frac{m}{\hbar^2\beta\pi}\ln\left(1+e^{\beta\mu}\right),$$

which leads to $\beta\mu = \ln\left(e^{\hbar^2\beta\pi n/m}-1\right)$, hence the exact expression for q_s^{2D} is given by

$$q_s^{\text{2D}} = \frac{2me^2}{\epsilon_0\hbar^2}\left(1-e^{-\hbar^2\beta\pi n/m}\right).$$

In the one-dimensional case q_s^{1D} can be calculated by using a similar procedure [17] to that used by Aguilera-Navarro [10] for q_s^{3D}, in which a series expansion of $n^{\text{1D}}(\mu)$ is performed as well as its series inversion. It leads to a partial summation of the form given by Eq. (37) where z is the same as before but $\nu = (n/2)\sqrt{\pi\beta\hbar^2/2m^*}$, $A_1 = -0.7071$, $A_2 = 0.1726$ and $A_3 = -0.7526$. Also a Padé approximant of the quality $\nu d(\beta\mu)/d\nu$ allows us to improve the convergence of this partial summation, that is [17]

$$\nu\frac{d\beta\mu}{d\nu} = 1 + K_1^1\nu + \frac{K_2^1\nu}{1+K_3^1\nu} + 2\pi\nu^2, \tag{38}$$

where the coefficients $K_1^1 = 14.91$, $K_2^1 = -15.61$ and $K_3^1 = -0.3802$. Here we have imposed the condition $\beta\mu \to \ln\nu$ as ν tends to zero which is required physically at low densities (classical limit) and, to have an approximation for $\nu[d(\beta\mu)/(d\nu)]$ valid for every value of μ, even for very low temperatures or high densities, we added to our Padé representation the asymptotic limit of $\beta\mu \to 2\pi\nu^2$ [18] valid for large values of ν.

It is interesting to remark that, in contrast to the approximation performed by Aguilera-Navarro [10] for the 3D case, the asymptotic behavior of μ is given by an integer power of ν in the 1D case allows us to match an *unique* expression for μ on its whole domain. Thus, by integrating Eq. (38) we find that μ is given by

$$\mu = \frac{\pi^2\hbar^2n^2}{8m^*} + K_1\frac{n\hbar}{2}\sqrt{\frac{\pi}{2m^*\beta}} + \frac{1}{\beta}\ln\left[\frac{n\hbar}{2}\sqrt{\frac{\pi\beta}{2m^*}}\right] + \frac{K_2}{\beta K_3}\ln\left[1+K_3\frac{n\hbar}{2}\sqrt{\frac{\pi\beta}{2m^*}}\right] + C, \tag{39}$$

where C is a numerical constant which can be found by integrating numerically $n(\mu)$. Since $q_s^{\text{1D}} = 2e^2\partial n_0/\partial\mu$, we have

$$\frac{1}{q_s^{\text{1D}}} = \frac{\pi^2\hbar^2n}{8m^*e^2} + K_1\frac{\hbar}{4e^2}\sqrt{\frac{\pi}{2m^*\beta}} + \frac{1}{2e^2n\beta} + K_2\frac{\frac{\hbar}{4e^2}\sqrt{\frac{\pi}{m^*\beta}}}{1+K_3\frac{n\hbar}{2}\sqrt{\frac{\pi\beta}{2m^*}}}. \tag{40}$$

5. Screened potential in real space

The Fourier transforms of last section can be inverted to give

$$\phi_{1D}(z) = -\frac{2e}{\kappa}\int_0^\infty \frac{dq_z}{2\pi}\, e^{iq_z x}\frac{\ln(q_z a)}{1 - q_s \ln(q_z a)}, \quad (41)$$

$$\phi_{2D}(x,y) = \frac{e}{\kappa}\int_0^\infty dq_r\, J_0(q\sqrt{x^2+y^2})\frac{q_2}{q_s^{2D}+q_2}, \quad (42)$$

$$\phi_{3D}(x,y,z) = \frac{e}{\pi\kappa}\int_0^\infty dq_3 \int_0^\pi d\theta_{q_3}\sin\theta_{q_3} \times \frac{e^{iq_3\cos(\theta_{q_3})\sqrt{x^2+y^2+z^2}}q_3^2}{q_3^2+(q_s^{3D})^2}, \quad (43)$$

where we have expressed the second and third integral in terms of cylindrical and spherical coordinates and we recall that q_J is magnitude of q in J dimensions. Here we have used the identity [19]

$$J_0\left(q_2\sqrt{x^2+y^2}\right) = \frac{1}{2\pi}\int_0^{2\pi} d\theta\, e^{iq_2\cos\theta\sqrt{x^2+y^2}}, \quad (44)$$

where $J_0(q_2\sqrt{x^2+y^2})$ denotes the Bessel function of first kind and zeroth order. We should mention that Eq. (41) does not converge formally for a real value of z, but we shall perform an analytical extrapolation by extending z to the complex domain and keeping just the real part of the resulting expression. For small values of q_s^{1D}, we can expand Eq. (41) in geometrical series and identify each of its terms [20] leading to

$$\phi_{1D}(z) = -\frac{e}{\kappa z} + \frac{e}{\kappa}\frac{q_s^{1D}}{\pi}\sum_{n=0}^{\infty}(q_s^{1D})^n\,\Re\left[\frac{\partial^{n+2}}{\partial\nu^{n+2}}\left(\frac{\Gamma(\nu)}{\mu^\nu}\right)\right]\Bigg|_{\nu=1,\mu=-iz}, \quad (45)$$

where Γ denotes the Gamma function [14] and $\Re$ indicates the real part of the quantity between brackets. By using Eq. [4.359 (1-5)] of Ref. [20] it is easy to show that Eq. (45) can be written explicitly up to order 4 in q_s as

$$\phi_{1D}(z) = -\frac{e}{\kappa z} + \frac{e}{\kappa}q_s^{1D}\frac{C+\ln z}{z} + \frac{e\,(q_s^{1D})^2}{\kappa z}\left\{\frac{\pi^2}{8} - \frac{3}{2}[C^2+\zeta(2,1)] + 3C\ln z - \frac{3}{2}\ln^2 z\right\} - \frac{e\,(q_s^{1D})^3}{\kappa z}\left\{2C^3 + \frac{\pi^2}{2}C - 6C\zeta(2,1) + 4\zeta(3,1) - \ln z\left[6C + C\frac{\pi^2}{2} + 6\zeta(2,1)\right] + 2C^2\ln^2 z - 2\ln^3 z\right\} + O\left[(q_s^{1D})^4\right] \quad (46)$$

Here $C \approx 0.577$ is the Euler's constant and $\zeta(j,k) = \sum_{l=0}^{\infty} 1/(l+k)^j$ is the Riemann's ζ function. Note that Eq. (46) does not depend on a, the radius of the wire, which means that these results are the same for any small a; Eq. (45) illustrates the limit behavior of ϕ, which reduces to the Coulomb potential when $q_s \to 0$, as it should be expected.

On the other hand, Eq. (42) can be rewritten as

$$\phi_{2D} = \frac{e}{\kappa\sqrt{x^2+y^2}} - \frac{1}{2}\frac{\pi e}{\kappa}q_s^{2D}\left[H_0\left(q_s^{2D}\sqrt{x^2+y^2}\right) - Y_0\left(q_s^{2D}\sqrt{x^2+y^2}\right)\right] \quad (47)$$

where $Y_0\left(q_s^{2D}\sqrt{x^2+y^2}\right)$ and $H_0\left(q_s^{2D}\sqrt{x^2+y^2}\right)$ are the Bessel function of second kind and the Struve function of argument $q_s^{2D}\sqrt{x^2+y^2}$ of order zero, respectively. By using their Taylor series and asymptotic expansion [19], up to the first nonvanishing orders in $1/q_s$ and q_s, we find that

$$\phi_{2D} \approx \frac{e}{\kappa\sqrt{x^2+y^2}} - \frac{\pi q_s^{2D}e}{\kappa}\left[1 - \ln\left(q_s^{2D}\frac{\sqrt{x^2+y^2}}{2}\right)\right], \quad (48)$$

$$\phi^{2D} \approx \frac{e}{\kappa(q_s^{2D})^2(x^2+y^2)^{\frac{3}{2}}}. \quad (49)$$

Finally, integration over theta in Eq. (43) can be readily done to give

$$\phi_{3D}(x,y,z) = \frac{e}{\pi\kappa}\frac{2}{\sqrt{x^2+y^2+z^2}}\int_0^\infty dq_3\frac{q_3\sin\left(q_3\sqrt{x^2+y^2+z^2}\right)}{q_3^2+(q_s^{3D})^2}. \quad (50)$$

This integral can be performed by interpreting it as the inverse sine transform of $q/[q^2 + (q_s^{3D})]^2$, which is just the imaginary part of the Fourier transform or the Sine transform of $(2e^{-q_s^{3D}|r|})/\pi$. This means that ϕ_{3D} is given by

$$\phi_{3D}(x,y,z) = \frac{e}{\kappa} \frac{\exp\left(-q_s^{3D}\sqrt{x^2+y^2+z^2}\right)}{\sqrt{x^2+y^2+z^2}}. \quad (51)$$

Let us compare the asymptotic behaviors for large q_s of the 3D [4], 2D [3] and 1D screened Coulomb systems which are proportional to $e^{-q_s^{3D}r}$, $1/(q_s^{2D})^2$ and $1/(q_s^{1D})$, respectively. From these expressions it can be seen that the potentials decrease more slowly as a function of q_s^{JD} when the dimensionality decreases. That is to say, by lowering the dimensionality the screening effect gets diminished. This result is reinforced by noting that the correcting terms to the Coulomb potential in Eq. (46) contain terms proportional to $1/z$ so that this potential still has a long range. In contrast, the 2D and 3D screened potentials have as first correcting terms those proportional to larger inverse powers of their respective variables, that is, $1/(x^2+y^2)$ and $1/(x^2+y^2+z^2)$.

Acknowledgments

We acknowledge partial support of DGAPA-UNAM and CONACyT-México through Grant Nos, IN-107796 and 3042P-E, respectively.

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