FREE ENERGY OF A SCREENED ION PAIR

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Abstract

We calculate the effect of weak electrostatic screening of ions in a plasma. The original calculation by Salpeter is based on a linearization of the Poisson-Boltzmann equation for the screened electrostatic potential. This approximation is valid where the potential is small, but is formally invalid in the vicinity of the ions where the solutions for the potential and the associated charge distribution diverge. In reality, quantum exclusion must prevent the divergence of the charge density of the screening cloud. Nevertheless, in the limit in which screening is weak, Salpeter's value for the total screening energy is essentially correct. Here we extend Salpeter's calculation to account approximately for both quantum-mechanical exclusion in the vicinity of the ions, using what we call the Poisson-Boltzmann-Fermi-Dirac approximation, and the polarization of the screening cloud. By matching the solution onto an expression for the two-center Poisson-Boltzmann charge distribution far from the ions we are able to construct a consistent solution over all space. We obtain the first-order term in the expansion of that solution, from which we calculate the free energy associated with the screened ion pair.

I. INTRODUCTION

Electrostatic screening is a significant phenomenon occuring in dense plasmas, and is particularly important in astrophysics. The accumulation of charge about ions can influence substantially the equation of state of stellar material; throughout much of the sun, for example, it provides the largest nonideal contribution aside from ionization. Screening also influences thermonuclear reaction rates, and must be accurately taken into account when calculating neutrino production rates in the solar core.

Nuclear reaction rates are enhanced by screening; the standard assumption, based on JWKB theory, is that the screened reaction rate during two-body interactions between heavy nuclei (ions) 1 and 2 in a plasma at temperature T is given by the unscreened rate multiplied by an enhancement factor f which can be expressed approximately as

$$f = \exp\left[-\beta V_{\mathrm{s}}(0)\right] , \tag{1}$$

where $\beta = 1/kT$, in which k is Boltzmann's constant, and $V_{\mathrm{s}}(2a)$ is the contribution from screening to the potential of the interaction when the nuclei are separated by a distance $2a$. Under isothermal conditions $V_{\mathrm{s}}(0) = F_{Z_1+Z_2}(0) - F_{Z_1} - F_{Z_2}$ is the free-energy difference between the initial and final configurations, as discussed in Brüggen & Gough [1]. We call V_{s} the screening energy; F_{Z_i} denotes the free energy associated with a single screened ion of charge $Z_i e$, where e is the unit of electron charge, and $F_{Z_1+Z_2}(0)$ denotes the free energy of the two screened charges, $Z_1 e$ and $Z_2 e$, at zero separation, which has the same value as the free energy $F_{Z_1+Z_2}$ of a single ion of charge $Z_1 + Z_2$. We note that the precision required by solar physics in particular renders the JWKB approximation to the nuclear barrier penetration probability inadequate for calculating the nuclear reaction rates; higher-order terms in the Liouville-Green expansion must be included, which requires knowledge of $V_{\mathrm{s}}(2a)$ beyond $2a = 0$.

In main-sequence stars, such as the sun, screening is weak. In such circumstances it is common to adopt Salpeter's analysis [2] of the Poisson-Boltzmann (PB) equation (cf. equation (10) below) to represent screening of an isolated ion. It is assumed that $e\beta\phi \ll 1$ everywhere, ϕ being the electrostatic potential of a screened ion, so that the PB equation can be linearized in $e\beta\phi$. Then, in the vicinity of ion i, ϕ is given approximately by the spherically symmetrical Debye-Hückel potential $\phi \simeq Z_i \exp(-\kappa r_i)/r_i$, were r_i is the distance from the ion and κ is the inverse Debye length given by $\kappa^2 = 4\pi n_{\mathrm{e}} e\beta(1 + Z^*)$, where n_{e} is the mean electron number density; also Z^* is the (number-weighted, relative to all the ions in the plasma) mean charge number of those relatively light ions that also contribute to the screening. In that case $V_{\mathrm{s}}(0) = -Z_1 Z_2 e^2 \kappa$ [2].

Although Debye-Hückel theory provides an adequate approximation for many purposes, it suffers from two obvious deficiencies: (i) it makes the electron density and ϕ diverge as $r_i \to 0$, violating the assumption $e\beta\phi \ll 1$, and (ii) it does not take into account the electrostatic distortion of the screening clouds around each ion as the two ions approach one another. The divergence of the electron density is integrable, and therefore permits at least a finite correction to V_{s}. We remark that that divergence is not itself a consequence of linearization, for the solution to the full nonlinear PB equation, if it exists, is also divergent.

Another aspect of Debye-Hückel theory which is sometimes brought into question is the assumption that the screening electron cloud adjusts to the positions of the (slowly) moving heavy ions so quickly that the charge distribution may be regarded as being instantaneously static; as discussed by Salpeter, the validity of this assumption, which we adopt here too, is a consequence of the thermal velocities of the electrons being much greater than the velocities of the interacting screened ions.

There have been many attempts to obviate the divergence of the screening charge density in the vicinity of the ions. One of the earliest was by Abe [3], via a reordering of cluster expansions of the kind developed in Mayer's [4] classical theory. Furthermore, Graboske *et* *al.* [5] have used many-particle correlation functions to calculate $V_s(0)$ for a range of temperatures and densities. DeWitt [6] used a diagrammatic expansion of the quantum grand canonical ensemble to obtain a general form of the Montroll-Ward [7] ring-sum formula (a quantum-mechanical generalization of the Debye-Hückel free energy), and evaluated it to get the lowest level of the electron-degeneracy correction to the classical Debye-Hückel plasma free energy. The screening contribution to the free energy has also been estimated using a Padé approximation (see e.g. [8], [9]). These methods, however, yield only the leading contribution, $V_s(0)$, to the work done by the particles as they approach each other, which can be calculated under the assumption that the electron screening clouds experience, aside from their own self-interactions, only the (spherically symmetrical) electrostatic potentials of their associated ions. Only Mitler [10] has attempted to take asphericity into account, but that was in quite a crude representation of both the quantum statistics and the electrostatic equilibrium.

When the reaction rate is evaluated within the framework of the JWKB approximation, the greatest contribution to the work integral comes from the outer regions near the classical turning point, where the screening cloud is governed by Maxwell-Boltzmann statistics. However, when corrections from the Liouville-Green expansion about the JWKB approximation to the barrier-penetration problem are considered, regions closer to the ion, where quantum-mechanical effects come into play, become important. We accommodate these effects by using equilibrium Fermi-Dirac statistics to describe the electron cloud. In so doing, we assume the density of states to be given by the many-particle limit, as did Cowan and Kirkwood [11], taking no explicit account of the details of the quantum states of the bound species (cf. [12]). Thus, in the limit of zero temperature, our description would reduce essentially to the Thomas-Fermi model of the atom if interactions with neighbouring charges were ignored. We continue to apply Boltzmann statistics to the more massive ions. Thus our entire system is described by a hybrid equation, which we call the Poisson-Boltzmann-Fermi-Dirac (PBFD) equation.

Although for the linearized form of the PB equation the total screening cloud around an ion pair is – according to the principle of superposition – given by the sum of the screening clouds of the two individual ions, this is not the case when nonlinear higher-order corrections and the effect of degeneracy are taken into account; then the full interaction between the charges that make up the screening cloud must be taken into consideration. As the two ions approach one another the common screening cloud is progressively deformed.

The procedure we adopt for analysing the system, which is valid for weak screening, is facilitated by two properties of the screened two-ion system. Since the screening is weak, electron degeneracy is important only very close to the ions, within a sphere of radius r_d, say. Therefore, provided the ion separation $2a$ exceeds $2r_\mathrm{d}$ by a good margin, the degenerate regions of the electron screening cloud are each close to being spherically symmetric. Consequently, one can conveniently solve the governing equation by expanding about the spherically symmetric states. This yields what we call the inner solutions. The leading-order spherically symmetrical terms must be obtained numerically. An important feature of the higher-order aspherical terms in the expansion is that the differential equations governing them are linear with a common linear differential operator; they differ only by their inhomogeneous terms. Consequently those solutions can be obtained by quadrature. Outside the electron-degenerate regions the PB equation is valid in its weak-potential approximation; we call its solution the outer solution. The PB equation can be expanded about its linearized form, yielding once again a sequence of linear differential equations which also differ only by their inhomogeneous terms. In the calculation of the outer solution we accomodate large deviations from spherical symmetry; there is only axisymmetry, about an axis passing through the two interacting ions. We solve the equations by expanding the solutions in a series involving spheroidal harmonics. As with the expansion of the inner solutions, once the first-order correction to the outer potential has been calculated, further terms in the expansion can be obtained solely by quadrature.

The inner and outer solutions are matched in a region of common validity, in which electron degeneracy is negligible. This requires the ions to be not so close as to cause the regions of electron degeneracy to overlap. Evidently, at very small ion separation, this does not occur, and the procedure breaks down. However, for weak screening the domain of invalidity is small, and the error incurred has only a small influence on the total free energy and the nuclear reaction rates. One could extend the range of validity of the outer solution by regarding the PB equation as the leading term in an expansion of the PBFD equation for weak degeneracy, and including higher-order corrections to the solution before carrying out the matching with the inner solutions.

In section II we briefly review the earlier attempt by Mitler to calculate the higher-order terms of the interaction energy between two screened ions. We then proceed to present our expansion. In section III we expand the PB equation to second order in the potential ϕ. Using perturbation theory about the linear result, we can write down a solution which contains constants that depend on the conditions in the vicinity of the heavy ions. In section IV we derive PBFD equation. We then determine unknown constants of the inner solutions, together with the constants in the perturbative (outer) solution to the PB equation, by matching in the vicinity of each ion separately. Having thus obtained the potential and density distribution, we proceed to calculate the total electrostatic potential energy, U, and finally the Helmholtz free energy, F.

From here on, atomic units, i.e. $\hbar = m_{\mathrm{e}} = e = 1$, will be used.

II. MITLER'S MODEL

A first attempt to calculate higher-order corrections to Salpeter's approximation was made by Mitler [10]. He investigated the screening at all densities with the aim of finding the ignition curve for carbon burning. He constructed the following phenomenological model for the (continuous) charge distribution about a single ion of charge Z: within some sphere of radius r_m the component ρ_in of the electron density associated with the ion is assumed arbitrarily to be constant and equal to the mean value n_e of the total electron density, and outside that sphere the component ρ_out of the electron density associated with the ion has the functional form of the Debye model, i.e., for $r < r_\mathrm{m}$,

$$\rho_\mathrm{in}(r) = Z\delta^{(3)}(r) - n_\mathrm{e}, \tag{2}$$

where $\delta^{(3)}(r)$ represents the Dirac delta function in three dimensions, and, for $r > r_\mathrm{m}$,

$$\rho_\mathrm{out}(r) = -\kappa^2 C\mathrm{e}^{-\kappa r}/4\pi r, \tag{3}$$

where C is a constant and, as usual, $\kappa^2 = 4\pi n_\mathrm{e}\beta(1+Z^*)$. Matching the densities at r_m and demanding that the total charge in the screening cloud is $-Z$ determines both r_m and C, yielding

$$x_\mathrm{m} := \kappa r_\mathrm{m} = \left(\frac{3\kappa^3 Z}{4\pi n_\mathrm{e}} + 1\right)^{1/3} - 1 \tag{4}$$

and

$$C = 4\pi n_\mathrm{e} x_\mathrm{m} \mathrm{e}^{x_\mathrm{m}}/\kappa^3. \tag{5}$$

Thus one can calculate the internal energy as follows:

$$U = \tfrac{1}{2}\int \rho\,\phi\,\mathrm{d}V = -\frac{4\pi^2 n_\mathrm{e}^2 x_\mathrm{m}^2}{\kappa^5}\left(\tfrac{2}{5}x_\mathrm{m}^3 + 2x_\mathrm{m}^2 + 4x_\mathrm{m} + 3\right). \tag{6}$$

On making κ^3 the independent variable, one can integrate this expression for U with respect to β to calculate the Helmholtz free energy for an ion of charge Z_i:

$$F_{Z_i} = \frac{1}{\beta}\int_0^\beta U\,\mathrm{d}\beta = -\frac{8\pi^2 n_\mathrm{e}^2}{5\kappa^5}[(\zeta_i+1)^{5/3} - 1 - \tfrac{5}{3}\zeta_i], \tag{7}$$

where $\zeta_i = 3Z_i\kappa\beta(1+Z^*)$. Thus one finds that the screening energy of ions 1 and 2 (at zero separation) is given by

$$\beta V_{\mathrm{s}}(0) = \frac{1}{10\kappa\beta(1+Z^*)^2}[(\zeta_1+\zeta_2+1)^{5/3} - (\zeta_1+1)^{5/3} - (\zeta_2+1)^{5/3} + 1]. \tag{8}$$

With this result Mitler estimates a first-order correction to the screening energy at nonzero ion separation by assuming there now to be a uniform charge density around the two ions distributed as an ellipsoid of revolution, and thus finds

$$V_{\mathrm{s}}(r) = F_{Z_1+Z_2}(0)(1-0.0104\kappa^2 r^2) - F_{Z_1} - F_{Z_2}, \tag{9}$$

where F_{Z_i} is the free energy associated with a single ion of charge Z_i as given by equation (7).

Mitler's phenomenological model suffers from a few unphysical assumptions, the most significant of which is that the electron density of the screening cloud at the nucleus (ion) is equal to the mean value n_{e} of the total electron density. Evidently the electron density must be higher than average in the vicinity of the nucleus; for instance, Bahcall & Gruzinov [13] have shown that near a beryllium nucleus in the core of the sun the electron density is almost four times its field-free value. Also there is no reason to believe that in general the distorted charge cloud has the form of an ellipsoid of revolution. It is the purpose of this investigation to calculate what the charge distribution actually is.

III. EXPANSION OF THE POISSON-BOLTZMANN EQUATION TO SECOND ORDER: OUTER SOLUTION

As did Salpeter for the linear case, we assume that the screening charges follow a time-averaged potential distribution. The Poisson-Boltzmann equation for an assembly of heavy ions of charge Z_i in a plasma can thus be written

$$\nabla^2\phi = 4\pi n_{\rm e}[{\rm e}^{\beta\phi} - {\rm e}^{-Z^*\phi\beta}] + 4\pi\sum_i Z_i\delta(\mathbf{r}-\mathbf{r}_i), \tag{10}$$

where $\mathbf{r}_i$ is the position of ion i. In the case of *weak screening*, i.e. when $\beta\phi \ll 1$ throughout (almost) all space, this equation can be linearized in $\beta\phi$ far from the ions. For the resulting linear equation the principle of superposition applies, and the solution appropriate to the situation in hand may be written $\phi(\mathbf{r}) = \sum_i \phi_i(r_i)$, where ϕ_i is the screened potential due to the single ion i:

$$\phi_i(r_i;\kappa) = \frac{Z_i}{r_i}{\rm e}^{-\kappa r_i}, \tag{11}$$

where $r_i = |\mathbf{r}-\mathbf{r}_i|$. The associated contribution to the charge distribution is

$$\rho_i = -\frac{Z_i\kappa^2}{4\pi r_i}{\rm e}^{-\kappa r_i} + Z_i\delta(\mathbf{r}-\mathbf{r}_i), \tag{12}$$

the total charge distribution being $\rho = \sum_i \rho_i$. Thus, when linearization is valid, the total screening is simply the superposition of the linearized screening of each ion considered separately.

We now regard two neighbouring ions, 1 and 2, in isolation from the rest of the plasma, and consider their combined screening cloud far from each ion. Expanding the exponential in the Poisson-Boltzmann equation (10) up to second order in $\beta\phi$ yields

$$\nabla^2\phi - \kappa^2\phi = \tfrac{1}{2}\kappa^2(1-Z^*)\beta\phi^2 + 4\pi\sum_{i=1}^{2} Z_i\delta(\mathbf{r}-\mathbf{r}_i). \tag{13}$$

We write

$$\phi = \phi_0 + \phi_1, \tag{14}$$

where ϕ_0 is the appropriate zero-order solution, satisfying

$$\nabla^2\phi_0 - \kappa^2\phi_0 = 4\pi\sum_{i=1}^{2} Z_i\delta(\mathbf{r}-\mathbf{r}_i), \tag{15}$$

namely

$$\phi_0 = \frac{Z_1}{r_1}\mathrm{e}^{-\kappa r_1} + \frac{Z_2}{r_2}\mathrm{e}^{-\kappa r_2}. \tag{16}$$

The function ϕ_1 is the first-order perturbation to the potential, which satisfies

$$(\nabla^2 - \kappa^2)\phi_1 = \tfrac{1}{2}\kappa^2(1 - Z^*)\beta\phi_0^2. \tag{17}$$

We note that

$$\phi_0^2 = \frac{Z_1^2}{r_1^2}\mathrm{e}^{-2\kappa r_1} + \frac{Z_2^2}{r_2^2}\mathrm{e}^{-2\kappa r_2} + \frac{2Z_1Z_2}{r_1r_2}\mathrm{e}^{-\kappa(r_1+r_2)}. \tag{18}$$

The first two terms on the right-hand side (rhs) of equation (18) depend only on r_1 or r_2, so equation (17) can be solved separately in spherical polar coordinates about the appropriate ion for each of the first two terms. The third term, however, requires more analysis. To seek a solution in spheroidal coordinates is the most straightforward approach. Because equation (17) is linear in ϕ_1, the general solution is the sum of the solutions of the homogeneous equation plus the three particular solutions associated with each of the three inhomogeneous terms.

First we calculate the particular solutions, $\phi_1^{(i)}$ ($i = 1$ or 2), corresponding to the first two terms, which depend only on either r_1 or r_2. They satisfy

$$(\nabla^2 - \kappa^2)\phi_1^{(i)} = \tfrac{1}{2}\kappa^2(1 - Z^*)\beta Z_i^2 r_i^{-2}\mathrm{e}^{-2\kappa r_i}. \tag{19}$$

Because the rhs is spherically symmetric, it generates a spherically symmetric particular integral, and one can write $v = r_i\phi_1^{(i)}$, yielding

$$\frac{d^2v}{dr_i^2} - \kappa^2 v = \tfrac{1}{2}\kappa^2(1 - Z^*)\beta Z_i^2 r_i^{-1}\mathrm{e}^{-2\kappa r_i}, \tag{20}$$

whose general solution is

$$v(r_i) = \tfrac{1}{2} Z_i^2 \kappa (1 - Z^*) \beta \int_{r_i}^{r_0} \sinh \kappa (r' - r_i) \frac{\mathrm{e}^{-2\kappa r'}}{r'} \mathrm{d}r' + A_i \mathrm{e}^{-\kappa r_i} + B_i \mathrm{e}^{+\kappa r_i}. \tag{21}$$

Clearly v must vanish as $r \to \infty$, requiring that $r_0 = \infty$ and $B_i = 0$. Therefore

$$v(r_i) = \tfrac{1}{2} Z_i^2 \kappa (1 - Z^*) \beta \int_{r_i}^{\infty} \sinh \kappa (r' - r_i) \mathrm{e}^{-2\kappa r'} r'^{-1} \mathrm{d}r' + A_i \mathrm{e}^{-\kappa r_i}. \tag{22}$$

We note that the first term on the rhs of equation (22) has a logarithmic divergence at the origin, which represents a more severe divergence in $\phi_1^{(i)}$ than the $1/r$ divergence of the zero-order Debye-Hückel term, and which signifies a (positive) change in the total screening charge accumulated in the vicinity of the ion. Indeed, in the complete solution it effectively generates small corrections A_i to the coefficients Z_i in the zero-order solution (16). Any higher-order expansion is expected to suffer a more severe divergence. Nevertheless, we do not extend these particular integrals to the origin. The second term in the expression (22) represents the spherically symmetrical (about ion i) part of the complementary function; we have found it convenient to include the aspherical remainder of the complementary function in the interaction potential $\phi_1^{(3)}$. The unknown constants A_i have to be determined by matching onto solutions that are valid near the heavy ions. This will be discussed later.

For the calculation of the particular integral $\phi_1^{(3)}$ of equation (17) associated with the cross term on the rhs of equation (18) it is convenient to employ dimensionless prolate spheroidal coordinates ξ, η defined as follows:

$$\xi = \frac{r_1 + r_2}{2a}, \tag{23}$$

$$\eta = \frac{r_1 - r_2}{2a}; \tag{24}$$

r_1 and r_2 are the distances to the foci (at which the charges Z_1 and Z_2 are situated) of a family of confocal ellipses and hyperbolae, $2a$ being the distance between the foci. The appropriate solution satisfying $\phi_1^{(3)} \to 0$ as $\xi \to \infty$ is axisymmetric about the line joining the two ions.

One can write the inhomogeneous term on the rhs of (18) as

$$\frac{2Z_1Z_2}{r_1r_2}\mathrm{e}^{-\kappa(r_1+r_2)} = \frac{2Z_1Z_2}{a^2(\xi^2-\eta^2)}\mathrm{e}^{-2\kappa a\xi} \ . \tag{25}$$

The corresponding particular integral of equation (17) satisfies

$$(\nabla^2-\kappa^2)\phi_1^{(3)} = \frac{Z_1Z_2\kappa^2(1-Z^*)\beta}{a^2(\xi^2-\eta^2)}\mathrm{e}^{-2\kappa a\xi}, \tag{26}$$

which is a modified Helmholtz equation with an inhomogeneous term. That inhomogeneous term diverges more slowly at the charges than do the self-interaction terms, and it does not generate a divergence in $\phi_1^{(3)}$. Separating variables in the form

$$\phi_1^{(3)} = \sum_n \Xi_n(\xi)S_n(\eta) \tag{27}$$

yields

$$\sum_n\left\{\frac{\mathrm{d}}{\mathrm{d}\xi}\left[(\xi^2-1)\frac{\mathrm{d}\Xi_n}{\mathrm{d}\xi}\right]-\Lambda_n\Xi_n-\kappa^2a^2\xi^2\Xi_n\right\}S_n(\eta) = Z_1Z_2\kappa^2(1-Z^*)\beta\mathrm{e}^{-2\kappa a\xi} \ , \tag{28}$$

where Λ_n is a separation constant.

The so-called angular functions $S_n(\eta)$ satisfy the equation

$$\frac{\mathrm{d}}{\mathrm{d}\eta}\left[(1-\eta^2)\frac{\mathrm{d}S_n}{\mathrm{d}\eta}\right]+[\Lambda_n+\kappa^2a^2\eta^2]S_n = 0, \tag{29}$$

which, when κa is small, resembles Legendre's equation. Indeed, it is convenient to expand the angular functions in terms of Legendre functions thus:

$$S_n(\eta;\kappa a) = \sum_{m=0,1}^{\infty}{}' \, d_{mn}(\kappa a) P_m(\eta), \tag{30}$$

where $\sum'$ denotes summation over even m if n is even and over odd m if n is odd. It is found that the series expansion (30) converges rapidly for small κa. The coefficients $d_{mn}(\kappa a)$ satisfy three-term recurrence relations and are tabulated, for instance, by Flammer [14]. They are reproduced in the appendix.

To obtain an equation for $\Xi_n(\xi)$ one can multiply equation (28) by $S_m(\eta)$ and integrate over η in the interval [-1,1]. We use the orthogonality relation

$$\int_{-1}^{1} S_m(\eta;\kappa a) S_n(\eta;\kappa a) \mathrm{d}\eta = N_n(\kappa a)\delta_{mn}, \tag{31}$$

where δ_{mn} is the Kronecker symbol; the factor $N_n(\kappa a)$, which is related simply to the expansion coefficients $d_{mn}(\kappa a)$, is tabulated in the appendix. Defining

$$\lambda_n \equiv \int_{-1}^{1} S_n(\eta)\mathrm{d}\eta = \begin{cases} 2d_{0n}(\kappa a) & \text{for } n \text{ even },\\ 0 & \text{for } n \text{ odd },\end{cases} \tag{32}$$

one obtains

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\left[(\xi^2-1)\frac{\mathrm{d}\Xi_n}{\mathrm{d}\xi}\right] - (\Lambda_n - \kappa^2 a^2 \xi^2)\Xi_n = \lambda_n N_n^{-1} Z_1 Z_2 \kappa^2 (1-Z^*)\beta \mathrm{e}^{-2\kappa a \xi}. \tag{33}$$

Equation (33) is an ordinary inhomogeneous second-order equation which one can solve by the method of variation of parameters. If $R_n^{(1)}$ and $R_n^{(3)}$ are two independent solutions of the corresponding homogeneous equation

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\left[(\xi^2-1)\frac{\mathrm{d}R_n}{\mathrm{d}\xi}\right] - [\Lambda_n + \kappa^2 a^2 \xi^2] R_n = 0, \tag{34}$$

one obtains after a few lines of algebra:

$$\Xi_n = \frac{2}{\pi}\lambda_n N_n^{-1} Z_1 Z_2 \kappa^3 (1-Z^*)\beta a \left[\int_{\xi_1}^{\xi} R_n^{(3)}(x;\kappa a)\mathrm{e}^{-2\kappa a x}\mathrm{d}x \; R_n^{(1)}(\xi;\kappa a) \right.$$
$$\left. - \int_{\xi_2}^{\xi} R_n^{(1)}(x;\kappa a)\mathrm{e}^{-2\kappa a x}\mathrm{d}x \; R_n^{(3)}(\xi;\kappa a)\right], \qquad (35)$$

where ξ_1 and ξ_2 are integration constants which are to be determined by boundary conditions. We choose the function $R_n^{(1)}(\xi;\kappa a)$ such that it tends to ∞ as $\xi \to \infty$ and is finite at $\xi = 1$, whereas $R_n^{(3)}(\xi;\kappa a)$ is chosen to tend to 0 as $\xi \to \infty$ and has a logarithmic singularity at $\xi = 1$. At large ξ both behave like modified spherical Bessel functions of the first and third kinds respectively. Imposing the condition that $\Xi_n \to 0$ as $\xi \to \infty$, the solution to equation (33) is given by equation (35) with $\xi_1 = \infty$ and $\xi_2 = 1$.

Now we can write down a representation of the total potential ϕ in terms of some transition value ξ' of ξ of the full first-order solution, which includes a solution to the homogeneous equation:

$$\begin{aligned}\phi = {} & \frac{\tilde{Z}_1}{r_1}\mathrm{e}^{-\kappa r_1} + \frac{\tilde{Z}_2}{r_2}\mathrm{e}^{-\kappa r_2} \\ & + \tfrac{1}{2} Z_1^2 \kappa (1-Z^*)\beta r_1^{-1} \textstyle\int_{r_1}^{\infty} \sinh\kappa(r'-r_1)\mathrm{e}^{-2\kappa r'} r'^{-1}\mathrm{d}r' \\ & + \tfrac{1}{2} Z_2^2 \kappa (1-Z^*)\beta r_2^{-1} \textstyle\int_{r_2}^{\infty} \sinh\kappa(r'-r_2)\mathrm{e}^{-2\kappa r'} r'^{-1}\mathrm{d}r' \\ & + \sum_n S_n(\eta;\kappa a)\left[\Xi_n(\xi;\kappa,a) + C_n \begin{Bmatrix} R_n^{(1)}(\xi;\kappa a) R_n^{(3)}(\xi';\kappa a) & \text{for } \xi < \xi' \\ R_n^{(3)}(\xi;\kappa a) R_n^{(1)}(\xi';\kappa a) & \text{for } \xi > \xi' \end{Bmatrix}\right], \end{aligned} \qquad (36)$$

where $\tilde{Z}_i = Z_i + A_i$ and C_n are constants which will have to be determined by matching onto the solution that is valid near the heavy ions. The constant ξ' is greater than 1 (the lower limit of the possible range of ξ) but can otherwise be chosen arbitrarily. Equation (36) is valid everywhere except very near the ions, where quantum-mechanical exclusion modifies the statistics significantly. The functions S_n are even with respect to η for even n, and odd for odd n. In the special case when the two charges are equal, i.e. $Z_1 = Z_2$, only the even terms contribute, and all C_n with odd n vanish. The constants $\tilde{Z}_i$ differ from Z_i, the differences representing the contribution to the first-order correction to ϕ arising from the complementary function associated with equation (17).

For the purpose of matching the outer Poisson-Boltzmann solutions to the inner solutions valid near the ions, ϕ is expanded in the regions close to each of ions i in terms of local spherical polar coordinates (r_i, θ_i) centered at each ion (see Fig. 1), which are the coordinates with respect to which we shall derive the inner solutions. Close to ion 1, the term $\tilde{Z}_2 \mathrm{e}^{-\kappa r_2}/r_2$ can be approximated:

$$\frac{\tilde{Z}_2 \mathrm{e}^{-\kappa r_2}}{r_2} \approx \frac{\tilde{Z}_2 \mathrm{e}^{-2\kappa a}}{2a}[1 - (\kappa + 1/2a) r_1 \cos\theta_1]. \tag{37}$$

The term $\tilde{Z}_1 \exp(-\kappa r_1)/r_1$ close to ion 2 is approximated similarly. Moreover, in the vicinity of ion i, where $r_i/a \ll 1$, the spheroidal coordinates ξ and η can be written in the form

$$\xi \approx 1 + \frac{r_i}{2a}(1 - \cos\theta_i) \tag{38}$$

and

$$\eta \approx \mp 1 \pm \frac{r_i}{2a}(1 + \cos\theta_i). \tag{39}$$

In equation (39) the upper sign applies to ion 1 and the lower sign to ion 2.

Near $\xi = 1$ the radial function $R_n^{(3)}$ is dominated by the function $R_n^{(2)}$, defined in the appendix, which is singular at that point. Hence one can write (see equations A24, A29 and A21)

$$R_0^{(3)}(\xi; \kappa a) = R_0^{(1)}(\xi; \kappa a) - R_0^{(2)}(\xi; \kappa a) \approx 1 - b_{00}(\kappa a) Q_0(\xi), \tag{40}$$

and for $n > 0$

$$R_n^{(3)}(\xi; \kappa a) = R_n^{(1)}(\xi; \kappa a) - R_n^{(2)}(\xi; \kappa a) \approx -b_{nn}(\kappa a) Q_n(\xi), \tag{41}$$

where Q_n is a Legendre function of the second kind; it is given by (e.g. [15]):

$$Q_n(\xi) = \frac{1}{2} P_n(\xi) \ln\left(\frac{\xi+1}{\xi-1}\right) - W_{n-1}(\xi) \tag{42}$$

with $n = 0, 1, 2, ...$; the function W_{n-1} is given by the sum

$$W_{n-1}(\xi) = \sum_{k=1}^{n} k^{-1} P_{k-1}(\xi) P_{n-k}(\xi). \tag{43}$$

Close to ion i one can expand Ξ_0 in terms of the local polar coordinates using equations (38) and (39). The integrals may thus be approximated by:

$$\int_1^{\xi} R_0^{(1)}(x, \kappa a) \mathrm{e}^{-2\kappa a x} \mathrm{d}x \, R_0^{(3)}(\xi, \kappa a) \simeq \\ \mathrm{e}^{-2\kappa a} \frac{r_i}{2a}(1 - \cos\theta_i) \left[1 - \frac{b_{00}}{2} \ln 2 + \frac{b_{00}}{2} \ln \frac{r_i}{2a} + \frac{b_{00}}{2} \ln(1 - \cos\theta_i)\right] \tag{44}$$

and

$$\int_{\xi}^{\infty} R_0^{(3)}(x, \kappa a) \mathrm{e}^{-2\kappa a x} \mathrm{d}x \, R_0^{(1)}(\xi, \kappa a) \simeq \int_1^{\infty} R_0^{(3)}(x, \kappa a) \mathrm{e}^{-2\kappa a x} \mathrm{d}x \\ - \mathrm{e}^{-2\kappa a} \frac{r_i}{2a}(1 - \cos\theta_i) \left[1 + \frac{b_{00}}{2} + \frac{b_{00}}{2} \ln 2 - \frac{b_{00}}{2} \ln \frac{r_i}{2a} - \frac{b_{00}}{2} \ln(1 - \cos\theta_i)\right]. \tag{45}$$

It is expedient to expand the term $(1 - \cos\theta_i) \ln(1 - \cos\theta_i)$ in orthogonal functions of powers of $\cos\theta_i$, namely in Legendre polynomials $P_n(\cos\theta_i)$:

$$(1 - \cos\theta_i) \ln(1 - \cos\theta_i) = \sum_{n=0}^{\infty} a_n P_n(\cos\theta_i). \tag{46}$$

We do this in anticipation of the natural aspherical expansion of the inner solution to which the outer solution must be matched. Indeed, for compatibility with the expansions (37), in our numerical computations we shall retain only the first two terms. By projecting equation

(46) onto $P_n(\cos\theta_i)$, using the orthogonality of the Legendre polynomials, the expansion coefficients a_n are obtained in the form

$$a_n = (n+1/2)\int_{-1}^{1} P_n(x)(1-x)\ln(1-x)\mathrm{d}x. \tag{47}$$

The integrals can be evaluated from the formulae (e.g. [16])

$$\int x^n \ln(1+x)\mathrm{d}x = (n+1)^{-1}[x^{n+1} - (-1)^{n+1}]\ln(1+x) \\ + (n+1)^{-1}\sum_{k=1}^{n+1}(-1)^k \frac{x^{n-k+2}}{(n-k+2)}, \tag{48}$$

yielding

$$a_0 = 0.19 \quad \text{and} \quad a_1 = -0.86. \tag{49}$$

The angular functions S_n are regular at $\eta = \pm 1$, and can be Taylor expanded in the form

$$S_n(\eta,\kappa a) \approx S_n(\pm 1,\kappa a) \mp S_n'(\pm 1,\kappa a)\frac{r_i}{2a}(1+\cos\theta_i), \tag{50}$$

where the prime denotes differentiation with respect to the first argument. Simple expansions for $S_n(\pm 1,\kappa a)$ and $S_n'(\pm 1,\kappa a)$ exist, and are listed in the appendix. The zeroth-order angular functions take on the special values:

$$S_0(\pm 1;\kappa a) = {\sum_{m=0}^{\infty}}' d_{m0}(\kappa a) \tag{51}$$

and

$$\left.\frac{\mathrm{d}}{\mathrm{d}\eta}S_0(\eta;\kappa a)\right|_{\eta=\pm 1} = \pm{\sum_{m=0}^{\infty}}' d_{m0}(\kappa a)m(m+1)/2. \tag{52}$$

The values at $\xi = 1$ of $R_0^{(1)}(\xi;\kappa a)$ and its derivative with respect to ξ are given by equations (A21) and (A33); these imply that $R_0^{(1)}(1;\kappa a) \simeq 1$, and, for the purpose of estimating the value of expression (A33), $\mathrm{d}R_0^{(1)}(\xi;\kappa a)/\mathrm{d}\xi|_{\xi=1}$ is negligibly small. However, in the computations reported in Sec. VI the precise values were used. Thus in the vicinity of ion 1 or ion 2, ϕ can be written in the form

$$\phi \approx f_0^{(i)}(r_i) + f_1^{(i)}(r_i)\cos\theta_i + \ldots + f_n^{(i)}(r_i)P_n(\cos\theta_i). \tag{53}$$

After incorporating the results derived above into the expansion of $\beta\phi$ about each ion, we find

$$\begin{aligned}\beta f_0 \approx{}& \tilde{Z}\beta\kappa x^{-1}\mathrm{e}^{-x} + \tilde{Z}\beta\kappa(2\kappa a)^{-1}\mathrm{e}^{-2\kappa a}\\ &+ \alpha x\mathrm{e}^{-2\kappa a}b_{00}[\ln(x/2\kappa a) - \ln 2 - 0.62]/2\kappa a + \alpha J + C_0 S_0(\pm 1;\kappa a)\beta R_0^{(3)}(\xi';\kappa a)\\ &+ \tfrac{1}{2}(Z\kappa\beta)^2(1 - Z^*)x^{-1}\textstyle\int_x^\infty x'^{-1}\sinh(x' - x)\mathrm{e}^{-2x'}\mathrm{d}x'\end{aligned} \tag{54}$$

and

$$\beta f_1 \approx -\tilde{Z}\beta\kappa(2\kappa a)^{-1}\mathrm{e}^{-2\kappa a}(1 + 1/2\kappa a)x + \alpha x\mathrm{e}^{-2\kappa a}b_{00}[\ln(x/2\kappa a) - \ln 2 + 0.72]/2\kappa a, \tag{55}$$

where $\alpha = -2S_0(1;\kappa a)(Z\kappa\beta)^2\kappa a(1 - Z^*)\lambda_0(\kappa a)N_0^{-1}(\kappa a)/\pi$ and $x = \kappa r_i$ is the dimensionless radius from ion i. Moreover $J(\kappa a) := \int_1^\infty R_0^{(3)}\mathrm{e}^{-2\kappa a\xi}\mathrm{d}\xi$, whose values are tabulated in the appendix.

The coefficients b_{00} and λ_0/N_0 can be written in the form

$$b_{00}(\kappa a) = -\frac{1}{\kappa a\sum_{m=0}' d_{m0}(\kappa a)} \tag{56}$$

and

$$\frac{\lambda_0}{N_0} = \frac{d_{00}(\kappa a)}{\sum_{m=0}^{\prime}(2m+1)^{-1}[d_{m0}(\kappa a)]^2} \ . \tag{57}$$

Aside from the unknown constants $\tilde{Z}_i$ and C_0, the functions f_n are therefore known for $n = 0$ and $n = 1$. It is straightforward in principle to extend the expansion to higher order.

IV. THE POISSON-BOLTZMANN-FERMI-DIRAC EQUATION

The Debye-Hückel potential describes the effect of electrostatic screening only in the limit of weak screening, far enough from the nuclei where $\beta\phi \ll 1$ [2]. It breaks down in the vicinity of the nuclei where the potential diverges and where the classical Maxwell-Boltzmann distribution is no longer a good approximation to the Fermi-Dirac statistics of the electrons.

In order to find a solution for those regions in which the Debye-Hückel potential is not applicable we shall describe the electrons by nonrelativistic Fermi-Dirac statistics; the much heavier ions are assumed still to obey classical Maxwell-Boltzmann statistics. The resulting model is essentially the finite-temperature Thomas-Fermi model of the atom. This statistical model of the atom, which was first proposed by Thomas and Fermi in 1923, has been used extensively in equation-of-state calculations of high-temperature high-density material (e.g. [17]), and in plasmas (e.g. [12]).

In Fermi-Dirac statistics the mean number of particles in a state of energy ϵ is given by

$$n_\epsilon = \frac{1}{\mathrm{e}^{\beta\epsilon-\delta}+1}, \tag{58}$$

where here δ is the degeneracy parameter, which we trust will not be confused with the delta function. In order to obtain an expression for the number density of electrons, n_{e}, we have to sum up the occupations of all states. Defining $\rho_\epsilon \mathrm{d}\epsilon$ to be the number of translational states lying in the energy range between ϵ and $\epsilon + \mathrm{d}\epsilon$, one obtains the local electron number density:

$$\tilde{n}_{\mathrm{e}} = 2 \int_{-\phi}^{\infty} \frac{\rho_\epsilon \mathrm{d}\epsilon}{\mathrm{e}^{\beta\epsilon - \delta} + 1}. \tag{59}$$

The factor 2 accounts for the fact that the electron can assume either of two spin states in each translational state. An electron that moves inside a potential ϕ has a translational energy $\epsilon = \frac{1}{2}p^2 - \phi$, where p is the magnitude of the momentum, so we can write for the density of states ρ_ϵ in the energy (momentum) subspace of phase space:

$$\rho_\epsilon \mathrm{d}\epsilon = \frac{1}{2\pi^2} p^2 \frac{\mathrm{d}p}{\mathrm{d}\epsilon} \mathrm{d}\epsilon = \frac{p}{2\pi^2} \mathrm{d}\epsilon \ . \tag{60}$$

This approximation, which is strictly correct only in the limit when the characteristic volume in the configuration subspace defined by the cube of the scale height of ϕ is large, is the principal deficiency in our description of the electron-degenerate regions close to the ions from which we obtain the inner solution. Substituting expression (60) in equation (59) and integrating over all ϵ, one obtains the following expression for the electron density in a potential ϕ:

$$\tilde{n}_{\mathrm{e}}(r) = \tilde{n}_{\mathrm{e}}(\infty) \frac{F_{1/2}(\beta\phi + \delta)}{F_{1/2}(\delta)}. \tag{61}$$

Here $\tilde{n}_{\mathrm{e}}(\infty)$ denotes the electron density far from the ion, which we take to be the mean electron density n_{e} of the plasma. The latter is related to the degeneracy parameter δ through

$$n_{\mathrm{e}} = \sqrt{2}\pi^{-2}\beta^{-3/2} F_{1/2}(\delta); \tag{62}$$

$F_{1/2}$ is a Fermi function, defined as

$$F_\alpha(z) = \int_0^\infty \frac{t^\alpha \mathrm{d}t}{\mathrm{e}^{t-z}+1}. \tag{63}$$

Large positive δ corresponds to a strongly degenerate plasma, while large negative δ corresponds to low degeneracy.

The electron density is related to the potential again by Poisson's equation. Substituting expression (62) for n_e and assuming the usual Maxwell-Boltzmann distribution for the density of the light ions, the electrostatic potential around a single ion satisfies

$$\nabla^2\phi = 4\pi n_\mathrm{e}\left[\frac{F_{1/2}(\beta\phi+\delta)}{F_{1/2}(\delta)} - \mathrm{e}^{-Z^*\beta\phi}\right] - 4\pi\sum_i Z_i\delta(\mathbf{r}-\mathbf{r}_i). \tag{64}$$

This is the equation that we call the Poisson-Boltzmann-Fermi-Dirac (PBFD) equation, and is equivalent to that derived by Cowan and Kirkwood [11]. In the limit of zero temperature, it becomes the equation for the Thomas-Fermi atom.

V. EXPANSION OF INNER SOLUTIONS

It is convenient to cast the PBFD equation into dimensionless form by writing $\psi \equiv \beta\phi$ and $\mathbf{x} \equiv \kappa\mathbf{r}$:

$$\nabla^2_\mathbf{x}\psi = \frac{1}{Z^*+1}\left[\frac{F_{1/2}(\psi+\delta)}{F_{1/2}(\delta)} - \mathrm{e}^{-Z^*\psi}\right] + 4\pi\kappa\beta\sum_i Z_i\delta(\mathbf{x}-\mathbf{x}_i), \tag{65}$$

where $\nabla^2_\mathbf{x}$ is the ∇^2 operator referred to the new dimensionless coordinate system. Near ion i the forms of the potential and the associated screening cloud are dominated by the charge of the ion, and therefore they are nearly spherically symmetric. We therefore expand ψ about the spherically symmetric components with respect to spherical polar coordinates (x_i, θ_i, ϕ_i) about each ion, with common axes coincident with the line of centres:

$$\psi^{(i)}(x_i,\theta_i) = \psi_0^{(i)}(x_i) + \psi_1^{(i)}(x_i)\cos\theta_i + ... + \psi_n^{(i)}(x_i)P_n(\cos\theta_i). \tag{66}$$

Substituting into equation (17), expanding the rhs about spherical symmetry, and separating the variables, one obtains

$$\frac{1}{x_i}\frac{\mathrm{d}^2}{\mathrm{d}x_i^2}(x_i\psi_0^{(i)}) = \frac{1}{Z^*+1}\left[\frac{F_{1/2}(\psi_0^{(i)}+\delta)}{F_{1/2}(\delta)} - \mathrm{e}^{-Z^*\psi_0^{(i)}}\right] + 4\pi\kappa\beta Z_i\delta^{(3)}(x_i), \tag{67}$$

and

$$\frac{1}{x_i}\frac{\mathrm{d}^2}{\mathrm{d}x_i^2}(x_i\psi_1^{(i)}) - \frac{2}{x_i^2}\psi_1^{(i)} = \frac{1}{Z^*+1}\left[\frac{F'_{1/2}(\psi_0^{(i)}+\delta)}{F_{1/2}(\delta)} + Z^*\mathrm{e}^{-Z^*\psi_0^{(i)}}\right]\psi_1^{(i)}, \tag{68}$$

where the prime on $F'_{1/2}$ denotes differentiation with respect to the argument. The derivative $F'_{1/2}$ is evaluated by recalling that $F'_{1/2}(z) = 2F_{-1/2}(z)$. The inner boundary conditions to be applied to $\psi_k^{(i)}$ are $x_i\psi_0^{(i)} \to Z_i\kappa\beta$ as $x_i \to 0$ and that $\psi_k^{(i)}$ be regular at $x_i = 0$ for $k \geq 1$. Inspection of the form of the solutions to equations (67) and (68) reveals that the derivative $\mathrm{d}(x_i\psi_0^{(i)})/\mathrm{d}x_i = \Gamma_i$ is undetermined and that the appropriate higher-order solutions satisfy $\psi_k^{(i)} \sim \gamma_i x_i$ as $x_i \to 0$, where γ_i are constants.

VI. MATCHING THE SOLUTIONS

Equations (67) and (68) were integrated numerically outwards from $x_i = 0$. Because we do not know at this stage the values of $\psi_1^{(i)}$ at the origins of their respective coordinates, we constructed normalized solutions $y_1^{(i)}(x_i)$ satisfying $y_1^{(i)} = 0$ and $\mathrm{d}y_1^{(i)}/\mathrm{d}x_i = 1$ at $x_i = 0$. The appropriate solutions can therefore be written $\psi_1^{(i)} = \gamma_1^{(i)}y_1^{(i)}$ for some constants $\gamma_1^{(i)}$. Matching was then achieved by demanding that both terms of the inner solution and their first derivatives be continuous with their outer counterparts in equation (53) at some radius $\tilde{r}$. Thus

$$\psi_0^{(i)}(\tilde{x}) = \beta f_0^{(i)}(\tilde{r}), \tag{69}$$

$$\left.\frac{\mathrm{d}\psi_0^{(i)}}{\mathrm{d}x_i}\right|_{x_i=\tilde{x}} = \kappa^{-1}\beta \left.\frac{\mathrm{d}f_0^{(i)}}{\mathrm{d}r_i}\right|_{r_i=\tilde{r}} \tag{70}$$

and

$$\gamma_1^{(i)} y_1^{(i)}(\tilde{x}) = \beta f_1^{(i)}(\tilde{r}), \tag{71}$$

and

$$\gamma_1^{(i)} \left.\frac{\mathrm{d}y_1^{(i)}}{\mathrm{d}x_i}\right|_{x_i=\tilde{x}} = \kappa^{-1}\beta \left.\frac{\mathrm{d}f_1^{(i)}}{\mathrm{d}r_i}\right|_{r_i=\tilde{r}} \tag{72}$$

for $i = 1, 2$, where $\tilde{x} = \kappa\tilde{r}$. These eight conditions determine the constants Γ_i, $\gamma_1^{(i)}$, $\tilde{Z}_i$ $(i = 1, 2)$ and C_0 and C_1.

Note that by taking the aspherical terms in the expansion (36) up to first order as a first approximation, we have included an odd term (antisymmetric with respect to the midplane perpendicular to the line of centers) to account for the case $Z_1 \neq Z_2$. If the expansion were taken to higher order, at every new order one more term from the expansions (66) of Φ about each ion has to be matched to the sum in equation (36). This yields four more undetermined constants per expansion term: there are two more boundary values, $\gamma_k^{(i)}$, of the inner solution, and two more constants, C_n, of the outer solution for another even and another odd term of $R_n^{(3)}$. These are determined by the four further conditions for the matching of f_k and f_k' to ψ_k and ψ_k' around each ion.

For simplicity let us examine the case when $Z_1 = Z_2 = Z$, and let us take the expansion in (36) up to first order. Again it may be useful to write the potential in dimensionless form: $\psi \equiv \beta\phi$ with $x \equiv \kappa r_{1,2}$. The problem is now dependent only on the parameters $Z\beta\kappa$ and κa, as well as Z^* and δ which appear in the PBFD equation.

The ensuing set of transcendental equations is now solved numerically using a Newton-Raphson method. The parameter κa is varied between 1, which is the value for which the Debye spheres touch, to $\kappa\tilde{r}$, which is the value for which the two 'matching spheres' touch, at and beyond which this method cannot be applied. We have found that to a precision better than 1 part in 10^2 the total charge of the screening cloud is equal and opposite to the charge of the heavy ion pair, which is an independent check on the self-consistency of this solution.

The choice of the matching radius $\tilde{r}$ is constrained by the following two effects. On the one hand, $\tilde{r}$ should be great enough for the nonlinear effects of the PBFD equation not to be significant (i.e. that $\phi \ll \delta$). Thus it is ensured that the asymptotic outer solution in the Poisson-Boltzmann limit which is to be matched onto the inner solution is approximately valid. On the other hand, the matching radius should be small enough for the effect of the second heavy ion on the solution of the PBFD equation to be treated as a small perturbation, i.e. $\psi_1(\tilde{r})/\psi_0(\tilde{r}) \ll 1$, allowing the aspherical perturbation to the PBFD equation to be linearized. It has been confirmed that the dependence of the solutions illustrated below on the exact choice of $\tilde{r}$ within these constraints is weak.

We have terminated the series in equation (53) at the first-order term, although the series is infinite. For improved accuracy the expansion could be taken to higher orders, as we have outlined above, but the computational effort grows substantially, since with every new term the number of transcendental equations that have to be solved at each order increases by eight, for the general case $Z_1 \neq Z_2$, or by four for the special case when $Z_1 = Z_2$.

Finally we estimate the order of magnitude of the neglected second-order term:

$$\frac{\Xi_2(1+\tilde{r}/2a)}{\Xi_0(1+\tilde{r}/2a)} \approx \frac{\lambda_2 N_0 b_{22} \int_1^\infty R_2^{(1)} \mathrm{e}^{-2\kappa a\xi} \mathrm{d}\xi Q_2(1+\tilde{r}/2a)}{\lambda_0 N_2 b_{00} \int_1^\infty R_0^{(1)} \mathrm{e}^{-2\kappa a\xi} \mathrm{d}\xi Q_0(1+\tilde{r}/2a)} \,. \tag{73}$$

We note that

$$\frac{\lambda_2 N_0 b_{22}}{\lambda_0 N_2 b_{00}} \approx \frac{5d_{22}}{4d_{00}} \approx 1, \tag{74}$$

for all values of κa, and that

$$\frac{\int_1^\infty R_2^{(1)} \mathrm{e}^{-2\kappa a\xi} \mathrm{d}\xi Q_2(1+\tilde{r}/2a)}{\int_1^\infty R_0^{(1)} \mathrm{e}^{-2\kappa a\xi} \mathrm{d}\xi Q_0(1+\tilde{r}/2a)} \approx 10^{-2}. \tag{75}$$

The exact value of the last expression depends on κa as well as on $\kappa\tilde{r}$, and the estimated value that we have quoted was obtained for those values within the aforementioned constraints on $\kappa\tilde{r}$. Thus the second-order term is about 1 per cent of the zeroth-order term, which suggests that it is justified to include only the zeroth-order term. Having thus calculated C_0 and $\tilde{Z}$, we can substitute them into equation (53), and the electrostatic potential is then fully determined.

We now proceed to calculate the electrostatic potential energy U, and subsequently the free energy F.

VII. RESULTS AND DISCUSSION

As shown by Mitler [10] and Brüggen & Gough [1], the work done in fusing two heavy ions that are immersed in a plasma is the free-energy difference between the initial and final configurations. In each of these configurations the screening clouds are spherically symmetrical.

In section IV we introduced the (inner) PBFD equation, which can be solved numerically for the density in the vicinity of an isolated ion and matched onto the outer solution (36) to the PB equation according to conditions (69)-(72). The resulting representation of the full solution can be used immediately to calculate the electrostatic energy U, and hence the free energy F associated with the single screening cloud surrounding an ion of charge Z. In Fig. 2 we have plotted the free energy associated with such a single screened ion, as well as the corresponding free energy of Salpeter's Debye-Hückel solution, which is given by:

$$-\beta F_{\mathrm{DH}} = \frac{1}{2} Z^2 \kappa \beta. \tag{76}$$

We show this figure to provide some indication of the influence of electron degeneracy. However, we emphasize that it applies only to the isolated spherically symmetric ion cloud; it does not provide a complete measure of the importance of the phenomena we address in this paper.

Shown are the free energies for a screened ion in conditions similar to those at the center of the sun and in a degenerate plasma. In Fig. 2 b, in which screening is quite strong, the results are compared also with the free energies from the ion-sphere model (see [2]), in which each ion is considered to be surrounded by an electrostatically neutralizing sphere of fully degenerate cold electrons of uniform density:

$$-\beta F_{\mathrm{ion-sphere}} = \frac{9(\kappa\beta)^{2/3} Z^{5/3}}{10\sqrt{3}(1+Z^*)^{1/3}}\ . \tag{77}$$

Whatever the strength of the screening, our estimate of $|F|$ is less than Salpeter's Debye-Hückel value, because our modifications reduce the screening. The reason is twofold: firstly, quantum-mechanical exclusion reduces the electron density in the vicinity of the ion, and secondly, the Debye-Hückel linearization of the exponential Boltzmann factor in the PB equation overestimates the deviation of that factor from unity, thereby overestimating even the nondegenerate screening. The modifications we have computed increase with Z, even when they are measured in units of the total free energy.

For the strongly screened ion (Fig. 2 b), our results lie between Salpeter's two extreme weak- and strong-screening approximations. For low Z, the results are hardly distinguishable from the ion-sphere model; differences, however, become discernible for heavier ions. For high values of Z the ion-sphere model underestimates the screening.

Our principal aim has been to calculate the interaction energy $U_{\rm int}$ by performing the full two-center calculation using the expansions developed in sections III and V. We define

$$U_{\rm int}(a;\kappa) = \frac{\kappa^2}{8\pi}\int_V \phi(\mathbf{r})\rho(\mathbf{r})\mathrm{d}^3\mathbf{r} - U_\infty, \tag{78}$$

where U_∞ represents the internal energy of the two ions at infinite separation, and $U_{\rm int}$ represents the energy arising from the interaction of the two heavy ions. The integration is over the whole of space. U_∞ does not vary with ion separation $2a$, and therefore does not contribute to the force between the ions. In Fig. 3 we plot $\beta U_{\rm int}(a;\kappa)$ against κa for various values of Z and $\kappa\beta$, and we compare it with Salpeter's Debye-Hückel (DH) result, which is

$$\beta U_{\rm int}^{\rm DH}(a;\kappa) = -\frac{Z^2\kappa\beta}{2\kappa a}(1-\kappa a)\mathrm{e}^{-2\kappa a}. \tag{79}$$

Because the DH approximation overestimates the screening, it underestimates $U_{\rm int}$. It is evident that the difference between the DH result and our model increases with decreasing values of κa. This is due to the increasingly strong nonlinear interaction between the screening charges as the two screening clouds merge, which is not taken into account in the linear DH picture. The difference is an increasing function of Z. The interaction energy $U_{\rm int}$ tends to zero as $\kappa a \to \infty$ for both the DH model and our model, but it does so more rapidly for the former because the DH approximation overestimates the screening.

Finally $U_{\rm int}$ is integrated over β, with all other parameters remaining fixed, to yield the interaction free energy:

$$\beta F_{\rm int}(a;\kappa(\beta)) = \int_0^\beta U_{\rm int}(a;\kappa(\beta'))\,\mathrm{d}\beta' \ . \tag{80}$$

The lower limit of the integration is $\beta = 0$; therefore in a lower part of the integration interval κa is small, as κ is proportional to $\beta^{1/2}$, and our model cannot be applied. This is due to the fact that one cannot find a value for the matching radius $\tilde{r}$ at which both the potential is small compared to the thermal energy and the influence of the other nucleus can be treated as a small perturbation to the spherically symmetric solution to the PBFD equation within the sphere of radius $\tilde{r}$. But when $\beta = 0$, i.e. at infinite temperature, there is no screening, and $U_{\rm int}$ is given by the bare Coulomb interaction. This allows us to interpolate $U_{\rm int}$ down to $\beta = 0$ in order to calculate the free energy. The result for $Z = 2$, $\kappa = 2.22$ and $\beta = 0.0215$ (conditions typical of the solar interior) is shown in Fig. 4. We find that $F_{\rm int}$ is bigger than the corresponding free energy obtained using the DH potential. Also shown is the free energy as given by Mitler's formalism.

The screening energy $V_{\rm s}(2a)$ is then found using

$$V_{\rm s}(2a) = F_{\rm int}(a;\kappa) - \frac{Z^2}{2a}. \tag{81}$$

The aim of this work was to present the results of our calculation of the free energy of a screened ion pair. We shall investigate possible astrophysical consequences of these results in a forthcoming paper.

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APPENDIX A: MODIFIED SPHEROIDAL WAVE FUNCTIONS

1. Spheroidal coordinates

Here we define the spheroidal coordinates used in the body of the paper, and we discuss the solutions of the modified Helmholtz equation in these coordinates. The latter are not well studied, and are not easily available in the literature. However, they are analogous to the solutions of the wave equation in spheroidal coordinates, which are described by, for example, Abramowitz & Stegun [15], Morse & Feshbach [18] and in the monograph by Flammer [14]. We derive some properties of these *modified spheroidal functions* in this appendix.

We define spheroidal coordinates appropriate to our problem as follows:

$$\xi = \frac{r_1 + r_2}{2a} \ , \tag{A1}$$

$$\eta = \frac{r_1 - r_2}{2a}, \tag{A2}$$

where r_1 and r_2 are the distances to the foci of a family of confocal ellipses and hyperbolae, $2a$ being the distance between the foci. This system of ellipses and hyperbolae can now be rotated about their major axis, i.e. the line connecting the foci, and the third spatial coordinate, ϕ, denotes the angle about the axis of symmetry. These coordinates are generally called prolate spheroidal coordinates, and they can take the values $1 \leq \xi < \infty$, $-1 \leq \eta \leq 1$, $0 \leq \phi \leq 2\pi$. Their metric coefficients are

$$h_\xi = a\sqrt{\frac{\xi^2 - \eta^2}{\xi^2 - 1}} \ , \tag{A3}$$

$$h_\eta = a\sqrt{\frac{\xi^2 - \eta^2}{1 - \eta^2}} \ , \tag{A4}$$

$$h_\phi = a\sqrt{(\xi^2 - 1)(1 - \eta^2)} \ . \tag{A5}$$

The problem discussed in this paper is symmetric about the major axis (the line connecting the heavy ions) and is thus independent of ϕ. Hence the modified Helmholtz equation

$$\nabla^2\psi - \kappa^2\psi = 0 \tag{A6}$$

reads

$$\frac{\partial}{\partial\xi}\left[(\xi^2-1)\frac{\partial\psi}{\partial\xi}\right]+\frac{\partial}{\partial\eta}\left[(1-\eta^2)\frac{\partial\psi}{\partial\eta}\right]]-\kappa^2a^2(\xi^2-\eta^2)\psi=0. \tag{A7}$$

We can now separate variables by writing

$$\psi(\xi,\eta)=\sum_n R_n(\xi;\kappa a)S_n(\eta;\kappa a), \tag{A8}$$

where the $R_n(\xi;\kappa a)$ are commonly referred to as the 'radial' functions and the $S_n(\eta;\kappa a)$ as the 'angular' functions.

2. The angular functions $S_n(\eta;\kappa a)$

After substituting the ansatz (A8) into equation (A7) and recognizing the orthogonality (equation A14) of S_n, the following differential equation for the angular functions is obtained:

$$\frac{\mathrm{d}}{\mathrm{d}\eta}\left[(1-\eta^2)\frac{\mathrm{d}S_n}{\mathrm{d}\eta}\right]+[\Lambda_n+\kappa^2a^2\eta^2]S_n=0, \tag{A9}$$

where Λ_n is the separation constant. The two regularity conditions at $\eta=\pm1$ require that Λ_n be an eigenvalue.

Equation (A9) has two regular singularities at $\eta=\pm1$, and also an irregular singularity at $\eta=\infty$.

For $\kappa a\ll 1$, equation (A9) is close to Legendre's equation since $|\eta|\leq 1$. It seems natural therefore to expand S_n in terms of Legendre functions, P_n:

$$S_n(\eta;\kappa a)=\sum_{m=0,1}^{\infty}{}' d_{mn}(\kappa a)P_m(\eta); \tag{A10}$$

$\sum'$ denotes summation over even m if n is even and over odd m if n is odd. We find that the series expansion (A10) converges rapidly for small κa. The coefficients $d_{mn}(\kappa a)$ satisfy three-term recurrence relations and are tabulated, for instance, in Ref. [14]. They have also been reproduced at the end of this appendix. There are various normalization schemes in use, and we have used the Flammer scheme, which requires $S_n(0, \kappa a)$ to be equal to the value $P_n(0)$ of the Legendre function at the origin for even n, and $S_n'(0, \kappa a)$ to be equal to $P_n'(0)$ for odd n, i.e.

$$S_n(0; \kappa a) = P_n(0) = \frac{(-1)^{n/2} n!}{2^n (n/2)!^2}, \tag{A11}$$

for even n, and

$$S_n'(0; \kappa a) = P_n'(0) = \frac{(-1)^{(n-1)/2}(n+1)!}{2^n (\frac{n-1}{2})!^2 (\frac{n+1}{2})!^2}, \tag{A12}$$

for odd n. We have plotted S_n as a function of η for two different values of κa in Fig. 5.

For completeness we note that in addition to the solution (A10), which is finite at $\eta = \pm 1$, there is a second solution (called the angular function of the second kind) which diverges at $\eta = \pm 1$, and which can be expanded in the form

$$S_n^{(2)}(\eta; \kappa a) = \sum_{m=-\infty}^{\infty}{}' d_{mn}(\kappa a) Q_m(\eta), \tag{A13}$$

where Q_m denotes a Legendre function of the second kind. Note that the summation now extends from $-\infty$ to $+\infty$. For details of this expansion see [14]. This solution is not relevant to the case at hand, and therefore we discuss it no further.

3. Orthogonality

The angular functions S_n form an orthogonal set over the interval [-1,1]. The orthogonality relation is

$$\int_{-1}^{1} S_m(\eta;\kappa a) S_n(\eta;\kappa a) \mathrm{d}\eta = N_n(\kappa a)\delta_{mn}, \tag{A14}$$

where δ_{mn} is the Kronecker symbol and the factor $N_n(\kappa a)$ is simply related to the expansion coefficients $d_{mn}(\kappa a)$, which follows immediately from the orthogonality relation for Legendre functions:

$$N_n(\kappa a) = 2 \sum_{m=0,1}^{\infty}{}' \frac{1}{2m+1} [d_{mn}(\kappa a)]^2. \tag{A15}$$

Values of N_n are tabulated at the end of this appendix.

4. The radial functions $R_n(\xi;\kappa a)$

The radial functions R_n satisfy the equation

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\left[(\xi^2-1)\frac{\mathrm{d}R_n}{\mathrm{d}\xi}\right] - [\Lambda_n + \kappa^2 a^2 \xi^2] R_n = 0. \tag{A16}$$

Comparing with equation (A9) one finds that R_n and S_n satisfy the same differential equation, namely

$$\mathcal{L}(f) = (1-x^2)f'' - 2xf' + [\Lambda_n + \kappa^2 a^2 x^2] f = 0, \tag{A17}$$

where x is ξ or η. However, the solutions for each coordinate are valid in separate regions. For the angular functions, S_n, defined for $-1 \le x \le 1$, we have expressed the solutions as a sum over Legendre functions $S_n(x) = \sum_m d_{mn} P_m(x)$. We express the radial functions in terms of modified spherical Bessel functions, because equation (A17) is similar to the modified Bessel equation when $x \gg 1$. The radial functions $R_n(x;\kappa a)$, defined for $x \ge 1$, can be obtained from the expansions of S_n using the transformation

$$\hat{f}(x) = \int_{-1}^{1} \mathrm{e}^{-\kappa a x t} f(t)\mathrm{d}t \equiv \mathcal{F}(f) \tag{A18}$$

with $f = S_n$, for if $f(x)$ satisfies $\mathcal{L}(f) = 0$, then so does $\hat{f}$. The corresponding expansion is in terms of modified spherical Bessel functions $i_n(x) = \sqrt{\pi/2x} I_{n+1/2}(x)$, where $I_{n+1/2}(x)$ is the modified Bessel function of the first kind, namely

$$R_n^{(1)}(\xi; \kappa a) = {\sum_{m=0,1}^{\infty}}' a_{mn}(\kappa a) i_m(\kappa a \xi), \tag{A19}$$

because

$$i_n(x) = \tfrac{1}{2}(-1)^n \mathcal{F}(P_n)|_{\kappa a=1}. \tag{A20}$$

Flammer's normalization

$$R_n^{(1)}(1; \kappa a) = 2^n [(n/2)!]^2 d_{0n}(\kappa a)/n! \tag{A21}$$

for even n, and

$$R_n^{(1)}(1; \kappa a) = \frac{2^n \kappa a \left(\frac{n-1}{2}\right)! \left(\frac{n+1}{2}\right)! d_{1n}(\kappa a)}{3(n+1)!} \tag{A22}$$

for odd n, implies the following relation between the coefficients a_{mn} and d_{mn}:

$$a_{mn}(\kappa a) = \left[{\sum_{k=0,1}^{\infty}}' d_{kn}(\kappa a) \right]^{-1} \mathrm{i}^{m-n} d_{mn}(\kappa a)\ . \tag{A23}$$

We have plotted $R_n^{(1)}$ as a function of ξ for two different values of κa in Fig. 6. This solution is regular at $\xi = 1$.

There is a second solution of equation (A16), $R_n^{(2)}$, which has a logarithmic singularity at $\xi = 1$. One could write down a series expansion for $R_n^{(2)}$ by replacing i_n by the modified spherical Bessel functions of the second kind. However it has been shown that this series does not converge well for small values of $\kappa a\xi$. Instead, since R_n and S_n satisfy the same equation, it is possible to find a series expansion in terms of Legendre functions which converges well. If Q_n denotes a Legendre function of the second kind, then

$$R_n^{(2)}(\xi;\kappa a) = \sum_{m=0,1}^{\infty}{}' \, b_{mn}(\kappa a) Q_m(\xi) + \sum_{m=2,1}^{\infty}{}' \, c_{mn}(\kappa a) P_{m-1}(\xi) \tag{A24}$$

[cf. [14], equation 4.2.6]. The coefficients b_{mn} are given by

$$b_{mn}(\kappa a) = -\frac{\mathrm{i}^n n!}{\kappa a 2^n (n/2)!^2 d_{0n}(\kappa a)} \left[\sum_{k=0}^{\infty}{}' \, d_{kn}\right]^{-1} d_{mn}(\kappa a) \tag{A25}$$

for even n, and

$$b_{mn}(\kappa a) = -\frac{\mathrm{i}^{n-1} 3(n+1)!}{(\kappa a)^2 2^n \left(\frac{n-1}{2}\right)! \left(\frac{n+1}{2}\right)! 2 d_{1n}(\kappa a)} \left[\sum_{k=1}^{\infty}{}' \, d_{kn}\right]^{-1} d_{mn}(\kappa a) \tag{A26}$$

for odd n. The coefficients c_{mn} are related to the coefficients $d_{\rho|r}^{mn}$ defined by Flammer. It is straightforward to show that

$$c_{mn}(\kappa a) = -\frac{n!}{\kappa a 2^n (n/2)!^2 d_{0n}(\kappa a)} \left[\sum_{k=0}^{\infty}{}' \, d_{kn}\right]^{-1} d_{\rho|m}^{0n}(\kappa a) \tag{A27}$$

for even n, and

$$c_{mn}(\kappa a) = -\frac{3(n+1)!}{(\kappa a)^2 2^n \left(\frac{n-1}{2}\right)! \left(\frac{n+1}{2}\right)! 2 d_{1n}(\kappa a)} \left[\sum_{k=1}^{\infty}{}' \, d_{kn}\right]^{-1} d_{\rho|m}^{0n}(\kappa a) \tag{A28}$$

for odd n. The coefficients a_{mn}, b_{mn} and c_{mn} are tabulated at the end of this appendix.

Useful to our problem is the radial function of the third kind, which tends to 0 as $\xi \to \infty$, and which is defined by

$$R_n^{(3)}(\xi;\kappa a) \equiv R_n^{(1)}(\xi;\kappa a) - R_n^{(2)}(\xi;\kappa a). \tag{A29}$$

$R_n^{(3)}$ and $R_n^{(1)}$ are linearly independent. The Wronskian $W = R_n^{(1)\prime} R_n^{(3)} - R_n^{(1)} R_n^{(3)\prime}$ is found in the usual manner:

$$W_n = \frac{2}{\pi \kappa a (\xi^2 - 1)}. \tag{A30}$$

5. Asymptotic behaviour and special values

The values of the angular functions and their first derivatives at $\eta = 1$ are given by

$$S_n(1;\kappa a) = \sum_{m=0,1}^{\infty}{}' \, d_{mn}(\kappa a) \ , \tag{A31}$$

$$\frac{\mathrm{d}}{\mathrm{d}\eta} S_n(\eta;\kappa a)\bigg|_{\eta=1} = \frac{1}{2} \sum_{m=0,1}^{\infty}{}' \, m(m+1) d_{mn}(\kappa a) \ . \tag{A32}$$

Derivatives of the radial functions at $\xi = 1$ are given by

$$\frac{\mathrm{d}}{\mathrm{d}\xi} R_n^{(1)}(\xi;\kappa a)\bigg|_{\xi=1} = \frac{2^{n-1}[(n/2)!]^2 d_{0n}(\kappa a) \sum_{m=0}^{\prime\infty} m(m+1) d_{mn}(\kappa a)}{n! \sum_{m=0}^{\prime\infty} d_{mn}(\kappa a)} \tag{A33}$$

for even n, and

$$\frac{\mathrm{d}}{\mathrm{d}\xi} R_n^{(1)}(\xi;\kappa a)\bigg|_{\xi=1} = \frac{2^{n-1}\kappa a \left(\frac{n-1}{2}\right)! \left(\frac{n+1}{2}\right)! d_{1n}(\kappa a) \sum_{m=1}^{\prime\infty} m(m+1) d_{mn}(\kappa a)}{3(n+1)! \sum_{m=1}^{\prime\infty} d_{mn}(\kappa a)} \tag{A34}$$

for odd n.

As $\xi \to \infty$,

$$R_n^{(1)}(\xi;\kappa a) \to \sqrt{\frac{\pi}{2\kappa a \xi}} I_{n+1/2}(\kappa a \xi) \tag{A35}$$

and

$$R_n^{(3)}(\xi;\kappa a) \to \sqrt{\frac{\pi}{2\kappa a \xi}} K_{n+1/2}(\kappa a \xi), \tag{A36}$$

where I and K are modified Bessel functions of the first and third kinds, respectively.

6. Integral J

In section III the following integral occurred:

$$J(\kappa a) \equiv \int_1^\infty R_0^{(3)} \mathrm{e}^{-2\kappa a \xi} \mathrm{d}\xi \ . \tag{A37}$$

This integral could be expressed as a series of Gegenbauer polynomials, but for computational purposes it was just as convenient here to calculate it numerically. Results are displayed in table 1.

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TABLES

$d_{mn}(c)$	m=0	1	2	3	4	5
c=0.0	1.0000	1.0000	0.00000	0.00000	0.00000	0.0
c=0.1	1.0006	1.0006	0.00111	0.00044	0.00019 -3	0.0
c=0.2	1.0021	1.0024	0.00446	0.00160	0.00306 -3	0.0
c=0.4	1.0090	1.0097	0.01803	0.00645	0.04952 -3	0.3
c=0.6	1.0205	1.0219	0.04128	0.01467	0.25555 -3	0.3
c=0.8	1.0373	1.0393	0.07523	0.02645	0.82977 -3	0.3
c=1.0	1.0599	1.0623	0.12138	0.04209	2.0975 -3	0.3

TABLE I. Nonzero coefficients $d_{mn}(c)$ for $n = 0$ or 1 for the expansions of modified spheroidal wave functions from Flammer (1957); $d_{mn}(c) = 0$ if $m+n$ is odd. Note: small numbers are entered in the format A p which denotes $A \times 10^p$.

$a_{mn}(c)$	m=0	1	2	3	4	5
c=0.0	1.0000	1.0000	0.00000	0.00000	0.00000	0.0
c=0.1	1.0006	1.0006	0.00111	0.00044	0.00019 -3	0.0
c=0.2	1.0021	1.0024	0.00446	0.00160	0.00306 -3	0.0
c=0.4	1.0090	1.0097	0.01803	0.00645	0.04952 -3	0.3
c=0.6	1.0205	1.0219	0.04128	0.01467	0.25555 -3	0.3
c=0.8	1.0373	1.0393	0.07523	0.02645	0.82977 -3	0.3
c=1.0	1.0599	1.0623	0.12138	0.04209	2.0975 -3	0.3

TABLE II. Nonzero coefficients $a_{mn}(c)$ for $n = 0$ or 1 for the expansions of modified spheroidal wave functions from Flammer (1957); $a_{mn}(c) = 0$ if $m+n$ is odd. Note: small numbers are entered in the format A p which denotes $A \times 10^p$.

$c_{mn}(c)$	m=1	2	3	4
c=0.0	0.0000	0.0000	0.0000	0.0000
c=0.1	0.2502 0	-1.3338 -2	0.0000	-4.5267 -6
c=0.2	0.1673 0	-1.7824 -2	9.9594 -4	-2.3795 -5
c=0.4	1.0156 -1	-2.1578 -2	2.6948 -3	-1.1534 -4
c=0.6	7.3979 -2	-2.3475 -2	4.4038 -3	-2.8318 -4
c=0.8	5.9163 -2	-2.4883 -2	6.2327 -3	-5.3567 -4
c=1.0	5.0183 -2	-2.6193 -2	8.2012 -3	-8.8525 -4

TABLE III. Nonzero coefficients $c_{mn}(c)$ for $n = 0$ or 1 for the expansions of modified spheroidal wave functions from Flammer (1957); $c_{mn}(c) = 0$ if $m + n$ is odd. Note: small numbers are entered in the format A p which denotes $A \times 10^p$.

$N_n(c)$	n=0	1
c=0.1	0.667467	0.667467
c=0.2	0.669478	0.669872
c=0.4	0.678851	0.679679
c=0.6	0.694962	0.696272
c=0.8	0.719592	0.720376
c=1.0	0.754820	0.753030

TABLE IV. Normalization factors for the angular function S_n as defined by equation (A14).

c	$J(c)$
0.0	0.0
0.1	4.5808
0.2	1.9117
0.3	1.0644
0.4	0.6671
0.5	0.4461
0.6	0.3107
0.7	0.2226
0.8	0.1628
0.9	0.1208
1.0	0.1233

TABLE V. Integrals $J(c)$.

FIGURES

FIG. 1. Coordinates in the expansion of the spheroidal coordinates around their foci.

FIG. 2. Free energy of a single screened ion as a function of ion charge Z in solar core. Results of this work are shown as crosses, the weak screening result as triangles, and (in panel b only) the results from the ion-sphere model (e.g. Salpeter, 1954) as circles. In panel (a) conditions are characteristic of the solar core: $\kappa\beta = 0.047$, $Z^* = 1.45$ and $\delta = 1.4$. In panel (b) conditions are characteristic of a degenerate plasma: $\kappa\beta = 0.2$, $Z^* = 4$ and $\delta = -5$.

FIG. 3. $\beta U_{\rm int}(a;\kappa)$ plotted against the dimensionless semi-separation κa of two screened ions of charge Z. The solid curves represent the results from this paper; the dotted curves denote the Debye-Hückel result. (a) $Z = 2$, $\kappa\beta = 0.1$; (b) $Z = 8$, $\kappa\beta = 0.025$; (c)$Z = 3$, $\kappa\beta = 0.3$.

FIG. 4. $\beta F_{\rm int}(a;\kappa)$ for $Z_1 = Z_2 = 2$, $\kappa = 2.22$ and $\beta = 0.0215$, which represents conditions characteristic of the solar core. The continuous curve is from the model in this paper, the dotted curve is the DH result and the dashed curve represents Mitler's model.

FIG. 5. $S_n(\eta;\kappa a)$: (a) $\kappa a = 0.1$, (b) $\kappa a = 0.8$.

FIG. 6. $R_n^{(1)}(\xi;\kappa a)$: (a) $\kappa a = 0.1$, (b) $\kappa a = 0.8$.