Highly Charged Ions in a Weakly Coupled Plasma:
An Exact Solution

Lowell S. Brown, David C. Dooling, and Dean L. Preston
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

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The ion sphere model introduced long ago by Salpeter is placed in a rigorous theoretical setting. The leading corrections to this model for very highly charged but dilute ions in thermal equilibrium with a weakly coupled, one-component background plasma are explicitly computed, and the sub-leading corrections shown to be negligibly small. Such analytic results for very strong coupling are rarely available, and they can serve as benchmarks for testing computer models in this limit.

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Here we shall describe a plasma configuration that is of considerable interest: very dilute “impurity” ions of very high charge $Z_p e$, $Z_p \gg 1$, in thermal equilibrium with a classical, one-component “background” plasma of charge $ze$ and number density $n$, at temperature $T = 1/\beta$. The background plasma is neutralized in the usual way, and it is weakly coupled. We use rationalized electrostatic units and measure temperature in energy units so that the background plasma Debye wave number appears as $\kappa_D^2 = \beta (ze)^2 n$. The weak coupling of the background plasma is conveyed by $g \ll 1$, where $g = (ze)^2 \kappa_D^2/(4\pi T)$. Although the background plasma coupling to itself is assumed to be very weak and the impurity ions are assumed to be so very dilute that their internal interactions are also very small, we shall require that the ionic charge $Z_p$ is so great that the coupling between the impurity ions and the background plasma is large, $gZ_p \gg 1$. This strongly coupled system is interesting from a theoretical point of view and our results can be used to check numerical methods.

This limit can be solved exactly. The solution is given by the ion sphere result presented by Salpeter [1] plus a simple smaller correction. This is accomplished by using the effective plasma field theory methods advocated by Brown and Yaffe [2]. In this field-theory language, the old Salpeter result corresponds to the tree approximation and our new correction is the one-loop term.

In usual perturbative expansions, the tree approximation provides the first, lowest-order term. Here, on the contrary, we express the impurity ion number in terms of an effective field theory realized by a functional integral. This corresponds to a mixed thermal ensemble in which the very dilute impurity ions are represented by a canonical ensemble, with the remaining background plasma described by a grand canonical ensemble. The saddle point of this form of the functional integral involves a classical field solution driven by a strong point charge.

The result for the impurity ion number reads

$$N_p = N_p^{(0)} \exp \left\{ \frac{3}{10} \frac{(3g)^{2/3}}{\beta} Z_p^{5/3} \right\} + \left( \frac{9}{g} \right)^{1/3} C Z_p^{2/3} + \cdots - \frac{1}{3} g Z_p \right\} . \quad (1)$$

Here $N_p^{(0)} \sim \exp\{\beta\mu_p\}$ is the the number of impurity ions defined by the chemical potential $\mu_p$ in the absence of the background plasma; keeping this chemical potential fixed, the background plasma alters this number to be $N_p$. The final $-gZ_p/3$ term in the exponent is the relatively small one-loop correction. The added $\cdots$ represent corrections to the evaluation of the classical action that may or may not be significant — if needed, they may be obtained numerically. The constant $C = 0.8498 \cdots$.

The number correction $[1]$ can be used to construct the grand canonical partition function $\mathcal{Z}$ for the combined system by integrating the generic relation $\mathcal{Z} = \frac{\beta}{\beta\mu_p} \ln \mathcal{Z}$. The equation of state is then determined from $pV = \ln \mathcal{Z}$. To simply bring out the main point, we include here only the leading terms,

$$pV \simeq \left\{ N - Z_p \frac{(3gZ_p)^{2/3}}{10} N_p \right\} T . \quad (2)$$

Although the fraction of impurity ions in the plasma $N_p/N$ may be quite small, there may be a significant pressure modification if $Z_p$ is very large.
The number result also directly yields the plasma correction to a nuclear fusion rate, since

\[ \Gamma = \Gamma_C \frac{N_1^{(0)}}{N_1} \frac{N_2^{(0)}}{N_2} \frac{N_{1+2}}{N_{1+2}}, \]

where \( \Gamma_C \) is the nuclear reaction rate for a thermal, Maxwell-Boltzmann distribution of the initial \((1,2)\) particles in the absence of the background plasma. We use the notation \(1 + 2\) to denote an effective particle that carries the charge \((Z_1 + Z_2)e\). Thus

\[
\Gamma = \Gamma_C \exp \left\{ \frac{3}{10} g^2 \left[ (Z_1 + Z_2)^{5/3} - Z_1^{5/3} - Z_2^{5/3} \right] \right\} \exp \left\{ \left( \frac{g}{g} \right)^{1/3} C \left[ (Z_1 + Z_2)^{2/3} - Z_1^{2/3} - Z_2^{2/3} \right] \right\}. \tag{4}
\]

The first line agrees with the calculation of Salpeter, the second is new. Again the correction can be large.

We turn now to sketch the basis for these results. The effective field theory expresses

\[ N_p = N_p^{(0)} \int d|x| e^{-S[x]} , \tag{5} \]

where the effective action is given by

\[ S[x] = \int (d^3r) \left\{ \frac{\beta}{2} (\nabla \chi(r))^2 - n \left[ e^{i\beta Z e \chi(r)} - 1 - i\beta Z e \chi(r) + i\beta Z_p e \delta(r) \chi(r) \right] \right\}. \tag{6} \]

The normalizing partition function \(Z\) is the same functional integral except that the point source \(\delta\) function term is removed from the effective action. The terms subtracted from the exponential in the action remove an overall number contribution and account for the effect of the rigid neutralizing background. As described in Brown and Yaffe, one can establish this result by expanding the exponential in powers of the number density \(n\) and performing the resulting Gaussian functional integrals to get the usual statistical mechanical form.

The loop expansion is an expansion about the saddle point of the functional integral. At this point, the action \(S[x]\) is stationary, and the field \(\chi\) obeys the classical field equation. The tree approximation is given by evaluating \(S[i\phi_{cl}(r)]\), where \(\phi_{cl}(r)\) obeys the classical field equation

\[ -\nabla^2 \phi_{cl}(r) = Z e n \left[ e^{-\beta Z e \phi_{cl}(r)} - 1 \right] + Z e \delta(r). \tag{7} \]

This equation is of the familiar Debye-Huckle form. We have placed it in the context of a systematic perturbative expansion in which the error of omitted terms can be ascertained. We shall describe the one-loop correction automatically produced by our formalism and prove that higher-order corrections may be neglected.

The one-loop correction to this first tree approximation is obtained by writing the functional integration variable as \(\chi(r) = i\phi_{cl}(r) + \chi'(r)\), and expanding the total action in Eq. \(\phi_{cl}\) to quadratic order in the fluctuating field \(\chi'\). Since \(i\phi_{cl}\) obeys the classical field equation, there are no linear terms in \(\chi'\). The leading quadratic terms define a Gaussian functional integral that produces a Fredholm determinant. Hence, to tree plus one-loop order,

\[ N_p = N_p^{(0)} \frac{\text{Det}^{1/2} \left[ -\nabla^2 + \kappa^2 \right]}{\text{Det}^{1/2} \left[ -\nabla^2 + \kappa^2 e^{-\beta Z e \phi_{cl}} \right]} \exp \left\{ -S[i\phi_{cl}] \right\}. \tag{8} \]

To solve the classical field equation in the large \(Z_p\) limit, we note that \(\phi_{cl}\) must vanish asymptotically, hence Eq. \(\phi_{cl}\) reduces at large distances to the Debye form and thus, for \(|r|\) large,

\[ \phi_{cl}(r) \simeq (\text{const}) e^{-\kappa |r| \left| \left| \frac{\kappa r}{|r|} \right| \right|}. \tag{9} \]

The coordinate integral of \(\nabla^2 \phi_{cl}\) vanishes by Gauss’ theorem, and from Eq. \(\phi_{cl}\) we obtain the integral constraint

\[ zn \int (d^3r) \left[ 1 - e^{-\beta Z e \phi_{cl}(r)} \right] = Z_p. \tag{10} \]

For small \(|r|\), the point source driving term in the classical field equation dominates, giving the Coulomb potential solution. Thus we write

\[ \phi_{cl}(r) = \frac{Z_p e}{4\pi r} u(\xi), \tag{11} \]

where \(\xi = \kappa r\), and the point driving charge \(Z_p e\) is now conveyed in the boundary condition \(u(0) = 1\). The large \(r\) limit requires that \(u(\xi) \sim e^{-\xi}\) for large \(\xi\).

To compute the action corresponding to the classical solution, we must first regularize it and remove the vacuum self-energy of the impurity ion. It is not difficult to show that this gives, on changing variables to \(\xi = \kappa r\),

\[
S_{reg}[i\phi_{cl}] = -\int_0^\infty d\xi \left\{ \frac{g Z_p^2}{2} \left( \frac{d u(\xi)}{d\xi} \right)^2 + \frac{\kappa^2}{g} \left[ \exp \left\{ -\frac{g Z_p}{\kappa} u(\xi) \right\} - 1 + \frac{g Z_p}{\kappa} u(\xi) \right] \right\}. \tag{12} \]

The classical field equation now appears as

\[ -g Z_p \frac{d^2 u(\xi)}{d\xi^2} = \xi \exp \left\{ -\frac{g Z_p}{\kappa} u(\xi) \right\} - 1, \tag{13} \]

according to the variation of Eq. \(\phi_{cl}\).

In our large \(Z_p\) limit, the short distance form of Eq. \(\phi_{cl}\) (multiplied by \(\beta Z e\)) is large over a wide range of \(|r|\), and \(\exp\{\beta Z e \phi_{cl}(r)\}\) is quite small there, leading to
the “ion sphere model” introduced long ago by Salpeter \[1\]. This model makes the step-function approximation obeying the boundary conditions is

\[ 1 - \exp \left\{ -\frac{gZ_p}{\xi} u(\xi) \right\} \simeq \theta (\xi_0 - \xi) . \quad (14) \]

Placing this in the integral constraint \[10\] determines the ion sphere radius \( \xi_0 = \kappa r_0 \) to be given by \( \xi_0^2 = 3gZ_p \). Approximating Eq. \[13\] with the replacement Eq. \[14\] produces a simple differential equation whose solution obeying the boundary conditions is

\[ u_0(\xi) = \begin{cases} 1 - (\xi/2gZ_p)^2 \left[ \xi_0^2 - \frac{1}{4} \xi^2 \right] , & \xi < \xi_0 , \\ 0 , & \xi > \xi_0 , \end{cases} \quad (15) \]

The nature of this “ion-sphere” solution \( u_0(\xi) \) together with the exact solution \( u(\xi) \) obtained by the numerical integration of Eq. \[13\], as well as the first correction described below, are displayed in Fig. \[1\].

We have appended the subscript \( 0 \) to indicate that this is the solution for the ion sphere model. Placing this solution in the new version \[12\] of the action gives

\[ -S_0 [i\phi_{cl}] = \frac{3Z_p}{10} (3gZ_p)^{2/3} - Z_p . \quad (16) \]

To find the leading correction, we first write the full solution \( u(\xi) \) as \( u(\xi) = u_0(\xi) + (\xi_0/Z_p g) v(\xi) \), where \( u_0(\xi) \) is the solution \[15\] to the ion sphere model. The exact differential equation \[13\] now reads

\[ \frac{d^2 v(\xi)}{d\xi^2} = \frac{\xi}{\xi_0} \left[ \theta (\xi - \xi_0) - e^{\frac{-gZ_p u_0(\xi)}{\xi}} \exp \left\{ -\frac{\xi_0}{\xi} v(\xi) \right\} \right] . \quad (17) \]

Since \( u_0(0) = 1 \) and since the solution must vanish at infinity, the proper solution to Eq. \[17\] obeys \( v(0) = 0 \), and \( v(\xi) \to 0 \) for \( \xi \to \infty \). Some algebra yields

\[ S_{\text{reg}} [i\phi_{cl}] = S_0 [i\phi_{cl}] - \frac{\xi_0}{g} \int_{\xi_0}^{\infty} d\xi \ v(\xi) - \frac{\xi_0^2}{2g} \int_{0}^{\infty} d\xi \left( \frac{d v(\xi)}{d\xi} \right)^2 . \quad (18) \]

Thus far we have made no approximations. To obtain the leading correction to the ion sphere result, we note that the factor \( \exp \left\{ -gZ_p / \xi u_0(\xi) \right\} \) is very small for \( \xi < \xi_0 \), and so it may be evaluated by expanding \( u_0(\xi) \) about \( \xi = \xi_0 \). Using Eq. \[15\], the leading terms yield

\[ \exp \left\{ -\frac{gZ_p}{\xi} u_0(\xi) \right\} \simeq \exp \left\{ -\frac{1}{2} (\xi_0 - \xi)^2 \theta (\xi_0 - \xi) \right\} . \]

This approximation is valid for all \( \xi \) because when \( \xi \) is smaller than \( \xi_0 \) and our expansion breaks down, the argument in the exponent is so large that the exponential function essentially vanishes. Since we consider the limit in which \( \xi_0 \) is taken to be very large and the Gaussian contribution is very narrow on the scale set by \( \xi_0 \), we may approximate

\[ \exp \left\{ -\frac{gZ_p}{\xi} u_0(\xi) \right\} \simeq \sqrt{\frac{\pi}{2}} \frac{\delta (\xi - \xi_0) + \theta (\xi - \xi_0)}{\xi} . \quad (19) \]

Here the delta function accounts for the little piece of area that the Gaussian provides near the ion sphere radius. One may verify that, with this approximation inserted into Eq. \[17\], the leading solution is given for \( \xi < \xi_0 \) and \( \xi \to \infty \) by

\[ v_1(\xi) = c_1 \xi \]

where \( c_1 \) is a constant that is yet to be determined, while

\[ \xi > \xi_0 : \]

\[ \frac{d^2 v_1(\xi)}{d\xi^2} = 1 - e^{-v_1(\xi)} . \quad (20) \]

This differential equation is akin to a one-dimensional equation of motion of a particle with \( \xi \) playing the role of time, and \( v_1(\xi) \) playing the role of position. Thus there is the usual “energy constant of motion”. The integration constant is fixed by requiring that \( v_1(\xi) \) vanishes at infinity. Then choosing the proper root to ensure that asymptotically \( v_1(\xi) \) decreases when \( \xi \) increases gives

\[ \frac{dv_1(\xi)}{d\xi} = -\sqrt{2} \left( e^{-v_1(\xi)} + v_1(\xi) - 1 \right) . \quad (21) \]

The different functional forms for \( v_1(\xi) \) in the two regions \( \xi < \xi_0 \) and \( \xi > \xi_0 \) are joined by the continuity constraint \( c_1 \xi_0 = v_1(\xi_0) \), and a slope jump to produce the \( \delta \) function introduced by Eq. \[15\]. This requires

\[ \sqrt{2} \left( e^{-v_1(\xi_0)} + v_1(\xi_0) - 1 \right) = \frac{\pi}{\sqrt{2}} \frac{e^{-v_1(\xi_0)} - v_1(\xi_0)}{\xi_0} . \quad (22) \]

For \( \xi_0 \gg 1 \), the second term on the right-hand may be neglected, giving \( v_1(\xi_0) = 0.6967 \cdots \).

We now evaluate the leading correction in the action \[15\]. In computing the leading term we can set \( \xi = \xi_0 \) in the integral that is linear in \( v_1(\xi) \). The leading correction is given by \( S_{\text{reg}} [i\phi_{cl}] = S_0 [i\phi_{cl}] + S_1 \), in which

\[ S_1 = -\frac{\xi_0^2}{g} C \]

where

\[ C = \int_{\xi_0}^{\infty} d\xi \left\{ v_1(\xi) + \frac{1}{2} \left( \frac{dv_1(\xi)}{d\xi} \right)^2 \right\} . \quad (23) \]
Here we have omitted a part that is of the negligible relative order $1/\kappa_0$. We change variables from $\xi$ to $v_1$ and use the result \[21\] for the derivative to get simple numerical integrals yielding $C = 0.8498 \cdots$.

In summary, we now find that

$$- [S_0 + S_1] + Z_p = \frac{3Z_p}{10} (3gZ_p)^{2/3} \left\{ 1 + \frac{10C}{(3gZ_p)} \right\}. \quad (24)$$

The leading correction to the ion sphere model is of relative order $1/(gZ_p)$. Fig. [2] displays the exact numerical evaluation of the action compared with the ion sphere approximation and the corrected ion sphere model.

The one-loop correction for the background plasma with no “impurity” ions present is given by \[2\]

$$\text{Det}^{-1/2} \left[ -\nabla^2 + \kappa^2 \right] = \exp \left\{ \int (d^3r) \frac{\kappa^3}{12\pi} \right\}. \quad (25)$$

We assume that the charge $Z_p$ of the “impurity” ions is so large that not only $Z_p \gg 1$, but also $gZ_p \gg 1$ as well, even though we require that $g \ll 1$. Then $\kappa_0 \gg 1$, and the ion sphere radius $r_0$ is large in comparison to the characteristic distance scale for spatial variation in the background plasma, the Debye length $\kappa^{-1}$. In this case, the term $\kappa^2 \exp \left\{ -\beta z e \phi_1(r) \right\}$ in the one-loop determinant $\text{Det}^{-1/2} \left[ -\nabla^2 + \kappa^2 e^{-\beta z e \phi_1} \right]$ in Eq. \[2\] can be treated as being very slowly varying — essentially a constant — except when it appears in a final volume integral akin to that in Eq. \[2\]. Therefore, for very strong coupling,

$$\frac{\text{Det}^{1/2} \left[ -\nabla^2 + \kappa^2 \right]}{\text{Det}^{1/2} \left[ -\nabla^2 + \kappa^2 e^{-\beta z e \phi_1} \right]} = \exp \left\{ -\frac{\kappa^3}{12\pi} \int (d^3r) \left[ 1 - \exp \left\{ -\beta z e \phi(r) \right\} \right] \right\} = \exp \left\{ -\frac{\kappa^3}{12\pi} \frac{4\pi}{3} r_0^3 \right\} = \exp \left\{ -\frac{1}{3} gZ_p \right\}, \quad (26)$$

where in the second equality we have used the ion sphere model that gives the leading term for large $Z_p$.

This result is physically obvious. The impurity ion carves out a hole of radius $r_0$ in the original, background plasma. The original, background plasma is unchanged outside this hole. The corrections that smooth out the sharp boundaries in this picture only produce higher-order terms. The original, background plasma had a vanishing electrostatic potential everywhere, and the potential in the ion sphere picture vanishes outside the sphere of radius $r_0$. The grand potential of the background plasma is now reduced by the amount originally contained within the sphere of radius $r_0$, and this is exactly what is stated to one-loop order in Eq. \[2\].

This argument carries on to the higher loop terms as well. As shown in detail in the paper of Brown and Yaffe \[2\], $n$-loop terms in the expansion of the background plasma partition function with no impurities present involve a factor of $\kappa^2 \kappa^n$ which combines with other factors to give dimensionless terms of the form $g^{n-1} \int (d^3r) \kappa^3$. With the very high $Z_p$ impurity ions present, each factor of $\kappa$ is accompanied by $\exp \left\{ -\left( 1/2 \right) \beta z e \phi_1(r) \right\}$ whose spatial variation can be neglected except in the final volume integral. Thus, an $n$-loop term is of order

$$g^{n-1} \kappa^3 \int (d^3r) \left[ 1 - \exp \left\{ -\frac{n+2}{2} \beta z e \phi_1(r) \right\} \right] \sim g^{n-1} \kappa^3 r_0^3 \sim g^n Z_p. \quad (27)$$

Since we assume that $g$ is sufficiently small that $g^2 Z_p \ll 1$ (even though $gZ_p \gg 1$), all the higher loop terms may be neglected \[3\].

We have now established the results quoted above.

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[1] E. E. Salpeter, Aust. J. Phys. 7, 373 (1954).
[2] L. S. Brown and L. G. Yaffe, Phys. Rep. 340, 1 (2001).
[3] This formula holds when the Coulomb barrier classical turning point of the nuclear reaction is small in comparison with the plasma Debye length. It was obtained in a different guise by H. E. DeWitt, H. C. Graboske, and M. S. Cooper, Astrophys. J. 181, 439 (1973). A more general derivation is given by L. S. Brown, D. C. Dooling, and D. L. Preston, Rigorous Formulation of Nuclear Reaction Rates in a Plasma, in preparation. It limits of validity have been previously spelled out by L. S. Brown and R. F. Sawyer, Rev. Mod. Phys. 69, 411 (1997).
[4] See Eq. (2.79) of Brown and Yaffe \[2\] and the discussion leading to that result.
[5] We have glossed over powers of $\ln g$ and quantum corrections that appear in higher orders. They vanish in our strong coupling limit.