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Screening of point charges by an ideal plasma in two and three dimensions

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It is proven, using the Poisson-Boltzmann equation, that a point charge held fixed in an ideal "jellium" plasma attracts a finite amount of opposite charge arbitrarily close to itself. In two dimensions this condensate is insufficient to neutralize the charge completely; in three or more dimensions neutralization is complete. The proof, which extends and simplifies older results, is based on the idea that the concentration $\exp(-q\phi/kT)/\int d\mathbf{r}\exp(-q\phi/kT)$ is a δ function when $\phi(\mathbf{r})$ is such that $\exp(-q\phi/kT)$ has a nonintegrable singularity. It is also proven that the species in the plasma of opposite polarity to the immersed charge condense onto it in strict order of charge, largest first.

I. INTRODUCTION

The self-consistent equation for the potential ϕ in an ideal, "jellium" plasma is given by combining Poisson's equation $\epsilon_0\nabla^2\phi=-\rho$, where ρ is the charge density, with the Boltzmann distribution $\rho\propto\exp(-q\phi/kT)$ for each charged species s. The result is called the Poisson-Boltzmann equation:

$$\epsilon_0\nabla^2\phi(\mathbf{r})=-\rho_t(\mathbf{r})-\nu(\mathbf{r})\sum_s N_s n_s q_s \exp[-q_s\phi(\mathbf{r})/kT] , \tag{1}$$

where ρ_t is a specified, immovable "test" charge distribution, N_s is the total number of particles of the sth species (*not* the concentration), $\nu(\mathbf{r})$ is a Heaviside step function which is only nonzero within the volume V accessible to the plasma:

$$\nu(\mathbf{r})=\begin{cases}0, & \mathbf{r}\notin V\\ 1, & \mathbf{r}\in V\end{cases} \tag{2}$$

and n_s is a normalization factor determined self-consistently:

$$n_s[\phi]^{-1}=\int d\mathbf{r}\,\nu(\mathbf{r})\exp(-q_s\phi/kT) \tag{3}$$

$$=\int_V d\mathbf{r}\exp(-q_s\phi/kT) . \tag{4}$$

The presence of this factor maintains the gauge invariance of (1). Collisions maintain each species of particle at the same temperature T. The assumptions underlying validity of (1) have recently been examined;[1] any unphysical consequences of the present analysis can be traced to their failure.

On the basis of the Poisson-Boltzmann equation, Lampert and Crandall[2] showed that a point test charge immersed in infinite ideal plasma in three dimensions attracts, out of the plasma, a charge of equal magnitude and opposite polarity arbitrarily close to itself. The point charge is therefore perfectly screened; and linearization of (1) far from the charge to give the Debye-Hückel equation, with solutions asymptotically representing exponential decay of the potential, is inappropriate. This phenomenon of charge condensation had already been conjectured to take place, at least in two dimensions.[3] There is an important qualitative difference between the two- and three-dimensional cases: in two dimensions the condensate does not completely neutralize the test charge.[1,4,5] A unified treatment is given by Lampert.[6] In the general case Eq. (1) is intractable; the condensation phenomenon has been confirmed by numerical solution in two and three dimensions.[7]

Lampert and Crandall[2,4] derived their results using a geometrical argument, bounding the solution of (1) for a two- or three-dimensional hyperspherically symmetrical extended test charge by the exact, one-dimensional solution for two species with $q_2=-q_1$. (The Poisson-Boltzmann equation, suitably rescaled, then takes the familiar form $\nabla^2\phi=\sinh\phi$.) The one-dimensional solution is nonsingular. They then shrank the radius of the test charge to zero, and the result emerged. This analysis, while unquestionably a landmark, suffers from several defects: it applies only to two-species plasmas with $q_2=-q_1$; it assumes global spherical symmetry; analogy between one and three dimensions is questionable, since the field of a charge does not diminish with distance in one dimension while any charge at infinity is ignored (correctly) in the three-dimensional case; and it ignores the fact that n_1 and n_2 may differ [though this may be compensated for by a potential shift of $(kT/2q)\ln(n_2/n_1)$ and a rescaling of length by $(n_1n_2)^{1/2}V$]. Moreover, it should be possible to derive the result directly, without introducing an artificial radius into the problem and then shrinking it to zero.

The present paper overcomes these limitations using a new idea based on the nonlinearity of (1)–(3): if the potential $\phi(\mathbf{r})$ is such that $\exp(-q_s\phi/kT)$ has a single nonintegrable nonoscillatory singularity, the concentration of that species depends on ϕ through the factor

$$n_s\exp(-q_s\phi/kT) = \left[\int_V d\mathbf{r}'\exp(-q_s\phi(\mathbf{r}')/kT)\right]^{-1}\exp(-q_s\phi/kT) . \tag{5}$$

But this is zero everywhere except at the singularity, and integrates to unity over V. Consequently it is a δ function, corresponding to condensation of that species onto the singularity. If one makes the initial assumption of no condensation, and then discovers such a singularity, the inconsistency is only resolved by accepting the condensation hypothesis. This line of reasoning can also explain why the test charge is completely neutralized in three (or more) dimensions, but only partly neutralized in two.

The factor n_s plays a crucial role in this argument. It is customarily scaled away to be determined later from (4), or in the limit of infinite plasma ignored completely. This limit is nonsingular and can therefore safely be taken if desired; N_s/V and $n_s V$ are finite, the latter is taken as unity, and $N_s n_s$ as the mean concentration in (1). Such procedures, in fact, constitute an unnecessary handicap; n_s is best taken together with $\exp(-q_s\phi/kT)$, as in (5).

The point test charge can be seen as a limit of the Poisson-Boltzmann equation in which the "test potential" $\phi_t(\mathbf{r})$, given by $\epsilon_0\nabla^2\phi_t=-\rho_t$, becomes singular. Of course, it does not automatically follow because ϕ_t is singular that the overall potential ϕ must be; a close watch must be kept on the interplay between δ functions in ρ_t and in the concentration factors (5) in the Poisson-Boltzmann equation. A different singular limit of (1) which also leads to charge condensation, even onto extended charges with nonsingular charge densities, is the low-temperature limit $kT\rightarrow 0$ (Ref. 1); again this is apparent from (5).

The one-dimensional case is examined briefly in Sec. II; condensation does not occur. In Sec. III the two-dimensional case is studied. For a single-species plasma the exact radial solution of (1) is available, and is used to check the argument based on (5). Section IV examines the three-dimensional case; complete neutralization occurs, and persists in all higher dimensions. In Sec. V it is shown that condensation of each species with opposite polarity to the test charge occurs in reverse order of magnitude of charge of the species, confirming an old conjecture. This idea is central to Rubinstein's demonstration of condensation in two dimensions,[5] based on generalization from the exact single species solution of Sec. III. Section VI examines the immersion of test dipoles and higher-order multipoles in the plasma. By considering the dipole as two arbitrarily large point charges brought arbitrarily close together, it is predicted that all the plasma condenses onto one or the other side of the dipole; higher poles are treated similarly. Conclusions are presented in Sec. VII.

II. THE ONE-DIMENSIONAL CASE

The one-dimensional case is exceptional in that the field of a charge does not alter with distance. It is trivial to write down a first integral of the Poisson-Boltzmann equation, which may in principle be solved by quadrature; details of the quadrature depend on the number and charge of the species present in the plasma. Charge condensation does not occur, since the solution never becomes singular at any point within the plasma. This is true whether the test charge is in contact with plasma on one or on both sides.

[While treating this case, let us quote parenthetically the solution of an interesting one-dimensional problem, namely, the disposition under its own electric field of a single-species plasma confined to $|x|<a$, with no test charge inside or outside the interval.[1] The charge density ρ is proportional to $\sec^2(\Gamma x/a)$, where Γ lies between 0 and $\pi/2$ and satisfies the equation $\Gamma\tan\Gamma=Nq^2a/4\epsilon_0 kT$, N being the number of particles per unit area perpendicular to x (in three dimensions). The constant of proportionality is found by normalization. Since $\rho=Nnq\exp(-q\phi/kT)$, this solution specifies the potential ϕ, satisfying (1), to within a gauge constant.]

III. THE TWO-DIMENSIONAL CASE

The general solution of (1) for a single-species plasma in two dimensions, with dependence only on the radial variable $r=(x^2+y^2)^{1/2}$, can be found by a transformation relating the equation to the one-dimensional form. The solution is[1,8,9]

$$\phi(r)=-\frac{kT}{q}\ln\left[\frac{\epsilon_0 C^2}{2NnkTr^2}\operatorname{cosech}^2\left[\frac{qC}{2kT}\ln\frac{r}{r_0}\right]\right]\;; \tag{6}$$

C and r_0 are the two constants of integration. Embedded in $\mathbb{R}^3$, N is the number of particles per axial length; n, which cannot be determined self-consistently using (4) until the boundary conditions are specified, has dimensions $(\text{length})^{-2}$, so that Nn remains of dimension $(\text{length})^{-3}$. If C is imaginary, the hyperbolic cosecant becomes trigonometric. A one-parameter family of solutions

$$\phi(r)=-\frac{kT}{q}\ln\left[\frac{2\epsilon_0 kT}{Nnq^2r^2\ln^2(r/r_0)}\right] \tag{7}$$

is generated by taking $C\rightarrow 0$.

These results are now applied to a point test charge Q_t' (of dimension charge per unit length, in $\mathbb{R}^3$) residing at $r=0$ in a single-species plasma confined to $r<b$. Only the hyperbolic form of (6) [and its limit (7)] arises in this case, since the trigonometric form undergoes unphysical oscillations as $r\rightarrow 0$. The potential can be worked out in terms of Q_t', b, and the gauge, using (4) together with the requirements

$$-2\pi\epsilon_0 b\,d\phi/dr\,(r=b)=(Q_t'+Nq),\quad \phi(b)=\phi_b$$

to eliminate C, r_0, and n. Should no solution exist for the resulting equations, we are warned that condensation has occurred. The analysis must then be repeated with $Q_t'\rightarrow Q_t'+\lambda Nq,\ n\rightarrow(1-\lambda)n$, where λ is the proportion of plasma which has condensed; this is found by using the auxiliary condition

$$Q_t'+\lambda Nq=\lim_{r\rightarrow 0}\left[-2\pi\epsilon_0 r\frac{d\phi}{dr}\right] \tag{8}$$

$$=-\frac{4\pi\epsilon_0 kT}{q}\left[1-\frac{qC}{2kT}\right]\,. \tag{9}$$

Condensation is clearly only expected to occur when Q_t', q are of opposite polarity.

These results can also be found indirectly, by taking the limit $a \to 0$ of the regular problem in which the plasma is confined to the annulus $a < r < b$.[1,5] Before the limit is taken, both the hyperbolic and the trigonometric version of (6) are needed, and the one-parameter family (7) takes on a special role as the limit of each. The results are

$$-\frac{4\pi\epsilon_0 kT}{Nq^2} < \frac{qQ_t'}{Nq^2}: \text{ no condensation (includes } q, Q_t' \text{ of like polarity)} ,$$

$$-\left[1+\frac{4\pi\epsilon_0 kT}{Nq^2}\right] < \frac{qQ_t'}{Nq^2} < -\frac{4\pi\epsilon_0 kT}{Nq^2}: \text{ partial condensation, leaving net central charge } -4\pi\epsilon_0 kT/q \text{ [described by Eq. (7)]} , \tag{10}$$

$$\frac{qQ_t'}{Nq^2} < -\left[1+\frac{4\pi\epsilon_0 kT}{Nq^2}\right]: \text{ all plasma condenses} .$$

The test charge is never completely neutralized, even when there is sufficient plasma charge to do so ($0 < qQ_t'/Nq^2 < -1$); moreover, the condensate is temperature dependent. Let us now explain these observations on the basis of the δ-function argument.

We begin by supposing that condensation does *not* occur. Then, sufficiently close to the test charge, $\phi \sim -(Q_t'/2\pi\epsilon_0)\ln r$, and the "concentration factor," $\exp(-q\phi/kT)$ behaves as the $-|qQ_t'/2\pi\epsilon_0 kT|$ *th* power of radius. But this has a nonintegrable singularity at $r=0$, corresponding to condensation, when the power index is more negative than -2 [since the concentration is proportional to this factor after normalization by (4)]. In this case we have a contradiction which is resolved only by accepting that condensation occurs. It is expected on variational grounds (see Sec. V) that the condensate will be as small as is consistently possible. Thus for $-|qQ_t'/2\pi\epsilon_0 kT| > -2$ there will be no condensation, while otherwise there will be sufficient condensation to reduce the power index $-|qQ'_{\text{central}}/2\pi\epsilon_0 kT|$ exactly to the critical value -2, unless, of course, there is insufficient plasma charge; then all the charge of requisite polarity will condense. These three cases successfully reproduce the result (10). Obviously, for species of the same polarity as the test charge, the exponent $q\phi/kT$ changes sign, and the concentration factor is always integrable. The concentration of like-charge species near the test charge rises as a positive power of distance.

This argument is entirely independent of the number and charge of species in the plasma and, since it is a local argument, of the global symmetry. It is therefore generally valid in two dimensions; confirmation of (10) stands as a test case.

IV. THE THREE-DIMENSIONAL CASE

In three dimensions there is no exact solution available, and we rely exclusively on the singularity argument. Assuming there is no condensation or insufficient condensation to neutralize the test charge (placed at $r=0$), the potential $\phi \sim O(1/r)$ with the same sign as Q_t, $\exp(-q\phi/kT)$ has a nonintegrable essential singularity at the test charge for species of opposite polarity to Q_t; and the concentration factor $n\exp(-q\phi/kT)$ for all such species is a δ function, corresponding to complete condensation. (The concentration of species of like polarity to Q_t, by contrast, tends to zero more rapidly than any power of r.) Thus the initial assumption of insufficient condensation to neutralize Q_t is contradicted, provided there is at least enough plasma charge of opposite polarity for neutralization; if not, all such charge condenses. It may similarly be shown that starting with the assumption that the test charge is overneutralized leads to contradiction. The only remaining possibility is exact neutralization. This result persists in higher dimensions D, in which $\phi \propto r^{-(D-2)}$ for a bare charge; the effect of geometry is manifest. Perhaps it is no coincidence that the two-species hyperspherically symmetrical Poisson-Boltzmann equation has the Painlevé property for $D=2$, but not for $D \geq 3$.[1,10]

V. PROPORTIONS OF SPECIES IN THE CONDENSATE

We now prove the conjecture[5] that the most highly charged species with polarity opposite to the test charge condenses out first, then the next, and so on until the concentration factor $\exp(-q_s\phi/kT)$ is just integrable for the (remainder of the) last species to condense. The Poisson-Boltzmann equation may be derived from the variational principle

$$\frac{\delta I}{\delta \phi}[\phi; Q_t; N_1, \ldots, N_l] = 0 , \tag{11}$$

where dependence on the first l species, taken to be those of opposite polarity to Q_t, is written explicitly, and

$$I = \int d\mathbf{r}\left(\tfrac{1}{2}\epsilon_0 |\nabla\phi|^2 - \rho_t\phi\right) - kT\sum_s N_s \ln\{n_s[\phi]V\} . \tag{12}$$

Now write the solution of the Poisson-Boltzmann equation with test charge absent as $\phi(\mathbf{r}; N_1, \ldots, N_l)$. Clearly, we must minimize the variand I over all proportions of the l species of opposite polarity:

$$\frac{d}{d\gamma_i} I[\phi(\mathbf{r};N_1-\gamma_1,\ldots,N_l-\gamma_l);0;N_1-\gamma_1,\ldots,N_l-\gamma_l]=0 , \tag{13}$$

where the γ's are constrained by the requirement of test charge neutralization

$$\sum_{s=1}^{l} \gamma_s q_s = -Q_t . \tag{14}$$

(For simplicity we work in three or more dimensions, in which neutralization is complete.) Now

$$\frac{dI}{d\gamma_i} = \frac{\delta I}{\delta\phi}\frac{\partial\phi}{\partial\gamma_i} + \frac{\partial I}{\partial\gamma_i} \tag{15}$$

$$= \frac{\partial I}{\partial\gamma_i} \tag{16}$$

$$= kT \ln\{n_i[\phi]V\} , \tag{17}$$

since the $\delta I/\delta\phi$ term vanishes by construction. We therefore require

$$kT \ln\{n_s[\phi]V\} - q_s\mathcal{L} = 0, \quad s=1,\ldots,l , \tag{18}$$

where $\mathcal{L}$ is the Lagrange multiplier associated with (14). Dependence of (18) on the γ's is implicit through ϕ. Rewrite (18) as

$$V^{-1}\int d\mathbf{r}\, \nu(\mathbf{r}) \exp(-q_s\phi/kT) = \exp(-q_s\mathcal{L}/kT) , \quad s=1,\ldots,l . \tag{19}$$

But this can only be satisfied if everywhere $\phi(\mathbf{r})=\mathcal{L}$, a constant. The proof is elementary: by differentiating with respect to α (>0) it is readily shown that, for a nonnegative function f, the generalized mean $[V^{-1}\int d\mathbf{r}\, f(\mathbf{r})^{\alpha}]^{1/\alpha}$ is a nondecreasing function of α, and is only stationary when f is constant almost everywhere.[11] With $f=\exp(-q_1\phi/kT)$, (19) corresponds to equality of the generalized means for values $\alpha=q_s/q_1$, $s=2,\ldots,l$. Clearly, this is incompatible with the increase of the generalized mean with α unless ϕ is constant, taking the value $\mathcal{L}$.

In general, ϕ is not constant, no solution exists for $\mathcal{L}$, and there is consequently no minimum of I in the space of the γ's on the plane $\sum_{s=1}^{l}\gamma_s q_s = -Q_t$. Since we are restricted to that part of the plane within the hypercube $0 \le \gamma_s \le N_s$, the smallest attainable value of I occurs on the intersection of the plane with the faces of the hypercube, corresponding to complete condensation of certain species. Since the concentration factor $n_s \exp(-q_s\phi/kT)$ is more singular for larger q_s as ϕ becomes singular, it is the more highly charged species which condense out first.

VI. HIGHER-ORDER POLES

So much for the fate of a point test charge in ideal plasma. What of a (point) test dipole, or higher-order multipole? Regard the dipole (of moment $\mathcal{D}$) as consisting of two point charges of magnitude $\pm\mathcal{D}/\sigma$ and separation σ, and let $\sigma\to 0$. The magnitude of the charges increases without bound; they therefore attract all the plasma to condense on to them, negative charge onto positive, and vice versa. This can also be seen from the singularity argument, since the potential of a dipole is more singular in all dimensions than that of a bare charge as $r\to 0$. Complete condensation obviously also occurs on to higher-order multipoles.

VII. CONCLUSIONS

Based on the Poisson-Boltzmann equation, a new and elementary demonstration of plasma charge condensation onto point charges has been made. The method successfully explains why neutralization is incomplete in two dimensions and complete in three or more. The result is important in that linearized theory for an ideal (Poisson-Boltzmann) plasma has a smaller range of applicability than is customarily realized.

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