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Pressure and Stress Tensor in a Yukawa Fluid

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Systems of particles interacting through a screened Coulomb potential of the Debye–Yukawa form are considered. The pressure is obtained from the stress tensor of the field corresponding to the Yukawa interaction, by a suitable statistical average. This approach is especially appropriate for systems living in a curved space. In a curved space, a self contribution to the pressure appears, and it is essential to take it into account for retrieving a correct pressure when the Yukawa interaction tends to the Coulomb interaction.

KEY WORDS: Yukawa potential; screened Coulomb interaction; field stress tensor; curved space.

1. INTRODUCTION

In a recent paper[(1)] it has been discussed how the pressure in a Coulomb fluid can be obtained by a suitable statistical average of the Maxwell stress tensor. The present paper is an extension of these calculations to the case of a fluid made of particles with Yukawa interactions. These Yukawa fluids have been recently reviewed.[(2, 3)] They are of interest because they are often used as simplified models for some complex Coulomb fluids (for instance dusty plasmas): one species S of charged particles is given a microscopic description, while the other charged particles are taken into account only through the screening that they cause to the interaction between the S-particles. One is left with one species interacting through a screened Coulomb potential which is assumed to be of the Debye–Yukawa type. In the following, this model will be considered for its own sake. In particular, the case when the fluid is in a curved space (of interest both for numerical simulations and for looking at the curvature effects) will be investigated.

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To start with, the system under consideration is, in $\mathbb{R}^3$, a gas of point-particles of number-density n, each of charge q, with a pair interaction $v(r)=q^2G(r)$ depending on the distance r, where $G(r)$ has the Yukawa form

$$G(r)=\frac{\exp(-\alpha r)}{r} \tag{1.1}$$

which is the Green function of the Helmholz equation. From the thermodynamic expression for the pressure

$$P=-\partial F/\partial V \tag{1.2}$$

where F is the free energy and V the volume, one can derive[4] the standard virial expression for the excess (over ideal) pressure:

$$P_{\text{ex}}=-\frac{1}{6}n^2q^2\int r\,\frac{dG}{dr}\,g(r)\,d\mathbf{r} \tag{1.3}$$

where $g(r)$ is the pair distribution function (in the present paper, integrals without domain specification are meant to be extended to the whole manifold). In Section 2, it will be shown how (1.3) can be alternatively derived from the stress tensor of the field which carries the Yukawa interaction. In Section 3, the above considerations will be extended to the case of a system confined on the surface S^3 of an hypersphere. Section 4 deals with the two-dimensional analogs of these systems. The limiting case of Coulomb systems is considered in Section 5; the case of a pseudosphere (a surface of constant negative curvature) is revisited in Section 6. The results are discussed in Section 7.

2. YUKAWA GAS IN $\mathbb{R}^3$

In terms of the Yukawa field $\phi(\mathbf{r})$ created by some charge distribution, the energy density is $(1/8\pi)[(\nabla\phi)^2+\alpha^2\phi^2]$ and the corresponding stress tensor is[5]

$$T_{\mu\nu}=\frac{1}{4\pi}\left[\partial_\mu\phi\,\partial_\nu\phi-\frac{1}{2}\,\delta_{\mu\nu}((\nabla\phi)^2+\alpha^2\phi^2)\right] \tag{2.1}$$

where the Greek indices label the three Cartesian axes x, y, z. In terms of the particle positions $\mathbf{r}_i$,

$$\phi(\mathbf{r})=q\sum_i G(|\mathbf{r}-\mathbf{r}_i|) \tag{2.2}$$

The excess pressure is the negative of the statistical average of any diagonal element, say $-\langle T_{xx}\rangle$, at some point which can be chosen as the origin. Following the same steps as in ref. 1, one can decompose the excess pressure into nonself and self parts. With the rotational symmetry taken into account, the nonself part can be written as

$$P_{\text{nonself}} = \frac{n^2 q^2}{24\pi} \int d\mathbf{r}_1 \, d\mathbf{r}_2 [\nabla G(r_1) \cdot \nabla G(r_2) + 3\alpha^2 G(r_1) \, G(r_2)] \; g(|\mathbf{r}_2 - \mathbf{r}_1|) \tag{2.3}$$

Writing each G as the Fourier transform of $4\pi/(k^2+\alpha^2)$, using as integration variables $\mathbf{r}_1$ and $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$, and performing first the integration on $\mathbf{r}_1$, one recovers (1.3). As to the self part of $-\langle T_{xx}\rangle$,

$$P_{\text{self}} = -\frac{nq^2}{8\pi} \int d\mathbf{r} [(\partial_x G(r))^2 - (\partial_y G(r))^2 - (\partial_z G(r))^2 - \alpha^2((G(r))^2] \tag{2.4}$$

it is a divergent integral (at small r), which can however be regularized through the use of the same physical argument as in ref. 1: for computing in an unambiguous way the force per unit area across the yOz plane, one must assume that no particle sits on that plane. Thus, one removes from the integration domain in (2.4) a thin slab $-\varepsilon < x < \varepsilon$ and takes the limit $\varepsilon \to 0$ at the end of the calculation. After some algebra with Fourier transforms, this prescription gives $P_{\text{self}} = 0$.

Thus, in $\mathbb{R}^3$,

$$P_{\text{ex}} = P_{\text{nonself}} \tag{2.5}$$

and the stress tensor approach simply reproduces the standard virial formula (1.3).

3. YUKAWA GAS IN S^3

We now consider a Yukawa fluid living on the three-dimensional "surface" S^3 of an hypersphere of radius R. The Yukawa potential (1.1) now must be changed into the Green function of the Helmholtz equation on S^3 which is[3]

$$G(\psi) = \frac{1}{R} \frac{\sinh \omega(\pi - \psi)}{\sin \psi \, \sinh \omega\pi} \qquad \text{for} \quad \alpha R > 1 \tag{3.1a}$$

$$G(\psi) = \frac{1}{R} \frac{\sin \omega(\pi - \psi)}{\sin \psi \, \sin \omega\pi} \qquad \text{for} \quad \alpha R < 1 \tag{3.1b}$$

where ψ is the angular distance seen from the center of the hypersphere ($R\psi$ is the geodesic distance) and $\omega = |\alpha^2 R^2 - 1|^{1/2}$.

3.1. Pressure from the Stress Tensor

The analog of (2.3) is

$$P_{\text{nonself}} = \frac{n^2 q^2}{24\pi} \int dV_1\, dV_2 [\nabla_0 G(\psi_{01}) \cdot \nabla_0 G(\psi_{02}) + 3\alpha^2 G(\psi_{01})\, G(\psi_{02})]\; g(\psi_{12}) \tag{3.2}$$

where 0 is the arbitrary point at which P_{nonself} is evaluated, dV_i is a volume element around point i, and $R\psi_{ij}$ is the geodesic distance between points i and j. After a calculation described in Appendix A, (3.2) becomes

$$P_{\text{nonself}} = -\frac{1}{6} n^2 q^2 \int R \frac{\partial G(\psi)}{\partial R}\, g(\psi)\, dV \tag{3.3}$$

where $G(\psi)$ must actually be regarded as a function of two independent variables: the angular distance ψ and the hypersphere radius R, as seen on (3.1). In (3.3), the volume element is $dV = 4\pi R^3 \sin^2 \psi\, d\psi$. This result (3.3) is the generalization of (1.3) to a curved space (the hypersphere). It should be noted that now the distance r has been replaced by the radius of curvature R. Only in the flat system limit does $G(\psi, R)$ become a function of the sole variable $r = R\psi$ and $R\, \partial G/\partial R = r\, dG/dr$.

Furthermore, now, the stress tensor approach provides another contribution to P_{ex}: the properly regularized part P_{self} does not vanish in the S^3 case. Indeed, the analog of the integral (2.4) can be split into two pieces P_0 and P_1 corresponding to the contributions of geodesic distances to the origin smaller and larger than $R\psi_0$, respectively. Only P_0 is divergent (at the origin) and must be regularized by the same prescription as in the $\mathbb{R}^3$ case. It is convenient to choose an infinitely small ψ_0. Then, the regularized P_0 can be computed by using the small-ψ form of (3.1), which is just the Coulomb potential in $\mathbb{R}^3$. This calculation has been done in ref. 1 with the result

$$P_0 = -\frac{nq^2}{6R\psi_0} + O(\psi_0) \tag{3.4}$$

As to P_1, with the rotational symmetry taken into account, it can be written as

$$P_1 = \frac{nq^2}{24\pi} \int_{\psi > \psi_0} \left[\left(\frac{1}{R} \frac{dG}{d\psi} \right)^2 + 3\alpha^2 G^2 \right] dV \tag{3.5}$$

This integral (3.5) is computed in Appendix A, and the final result is

$$P_{\text{self}} = P_0 + P_1 = \frac{1}{6} n q^2 \left[\frac{\pi \alpha^2 R}{\sin^2 \pi\omega} - \frac{\cot \pi\omega}{R\omega} \right] \qquad \text{for} \quad \alpha R < 1 \tag{3.6}$$

For $\alpha R > 1$, ω must be replaced by $i\omega$ in (3.6).

Thus the stress tensor approach gives a total excess pressure P_{ex} which is the sum of the nonself part (3.3) and the self part (3.6). While the nonself part is the analog of the total excess pressure (1.3) in $\mathbb{R}^3$, there is now in S^3 an additional non-vanishing self term (3.6).

3.2. Pressure from the Free Energy

Another way of defining and computing the pressure in the case of S^3 is to use the standard equation (1.2). If the total potential energy is

$$W = q^2 \sum_{i<j} G(\psi_{ij}) \tag{3.7}$$

the excess free energy is given by

$$\beta F_{\text{ex}} = -\ln \left\{ \frac{1}{V^N} \int dV_1 \cdots dV_N \exp \left[-\beta \sum_{i<j} G(\psi_{ij}) \right] \right\} \tag{3.8}$$

where β is the inverse temperature and N the number of particles. From (1.2), where here $V = 2\pi^2 R^3$, one finds for the excess pressure the value (3.3) which was the nonself part in the stress tensor approach.

The self part (3.6) appears only if one includes in the total potential energy the self-energies of the particles. Up to some (infinite) volume-independent additive constant, the self-energy of a particle is obtained in Appendix A as

$$e_{\text{self}} = -\frac{1}{2} q^2 \frac{\omega}{R} \cot \pi\omega \qquad \text{for} \quad \alpha R < 1 \tag{3.9}$$

If one adds to the free energy the self term $N e_{\text{self}}$, one does obtain from (1.2) the additional self contribution (3.6) to the pressure.

These results will be discussed in Section 7.

4. TWO-DIMENSIONAL YUKAWA FLUIDS

In this section, the above considerations are adapted to the case of two-dimensional systems. These two-dimensional systems are toy models of theoretical interest. It should be remembered that, in many experimental situations of charged particles confined on a surface, the interaction nevertheless is the three-dimensional Coulomb potential rather than the two-dimensional interactions which are considered here.

4.1. Yukawa Gas in $\mathbb{R}^2$

In $\mathbb{R}^2$, the Green function of the Helmholz equation is

$$G(r) = K_0(\alpha r) \tag{4.1}$$

where K_0 is a modified Bessel function and (1.3) is replaced by

$$P_{\text{ex}} = -\frac{1}{4} n^2 q^2 \int r \frac{dG}{dr} g(r) \, d\mathbf{r} \tag{4.2}$$

In the field approach, the energy density is $(1/4\pi)[(\nabla\phi)^2 + \alpha^2\phi^2]$ and the corresponding stress tensor is

$$T_{\mu\nu} = \frac{1}{2\pi}\left[\partial_\mu \phi \, \partial_\nu \phi - \frac{1}{2}\delta_{\mu\nu}((\nabla\phi)^2 + \alpha^2\phi^2)\right] \tag{4.3}$$

where the Greek indices now label two Cartesian axes x, y.

When the rotational symmetry is taken into account, the analog of (2.3) has the simpler form

$$P_{\text{nonself}} = \frac{n^2 q^2}{4\pi} \alpha^2 \int d\mathbf{r}_1 \, d\mathbf{r}_2 \, G(r_1) \, G(r_2) \, g(|\mathbf{r}_2 - \mathbf{r}_1|) \tag{4.4}$$

(in two dimensions, the derivatives of G cancel out). As in the three-dimensional case, the expression (4.4) of P_{nonself} can be brought to the form (4.2) while the properly regularized P_{self} vanishes. Thus, $P_{\text{ex}} = P_{\text{nonself}}$, and the stress tensor approach reproduces (4.2).

4.2. Yukawa Gas in S^2

As shown in Appendix B, the Green function of the Helmholz equation on a sphere S^2 of radius R is

$$G(\theta) = -\frac{\pi}{2 \sin \nu\pi} P_\nu(-\cos\theta) \tag{4.5}$$

where θ is the angular distance, P_ν is a Legendre function, and $\nu = (1/2)[-1+(1-4\alpha^2 R^2)^{1/2}]$ (if $2\alpha R > 1$, ν is complex).

The analog of (4.4) is

$$P_{\text{nonself}} = \frac{n^2 q^2}{4\pi} \alpha^2 \int dS_1 \, dS_2 \, G(\theta_{01}) \, G(\theta_{02}) \, g(\theta_{12}) \tag{4.6}$$

where dS_i is an area element around point i. After a calculation similar to the one for S_3 in Appendix A, (4.6) becomes the analog of (3.3)

$$P_{\text{nonself}} = -\frac{1}{4} n^2 q^2 \int R \frac{\partial G(\theta)}{\partial R} g(\theta) \, dS \tag{4.7}$$

($G(\theta)$ depends also on R through ν). When P_{self} is split into the contributions P_0 (P_1) of geodesic distances smaller (larger) than $R\theta_0$, both parts remain finite as $\theta_0 \to 0$. The regularized P_0 is the same as for a plane two-dimensional Coulomb system[1] ($P_0 = -nq^2/4$) and

$$P_1 = \frac{nq^2}{4\pi} \alpha^2 \int [G(\theta)]^2 \, dS \tag{4.8}$$

The integral in (4.8) involves $\int_{-1}^{1} [P_\nu(x)]^2 \, dx$ which is tabulated in ref. 6, and one obtains

$$P_{\text{self}} = P_0 + P_1 = \frac{nq^2}{4} \left\{ -1 + \frac{\alpha^2 R^2}{2\nu+1} \left[\frac{\pi^2}{\sin^2 \pi\nu} - 2\psi'(\nu+1) \right] \right\} \tag{4.9}$$

where ψ' is the derivative of the psi function (the psi function being the logarithmic derivative of the gamma function).

The pressure can also be derived from the thermodynamic relation (1.2) (with the volume V replaced by the sphere area S). Again, if only the two-body interactions $q^2 G(\theta_{ij})$ are used for defining the free energy F, only P_{nonself} is obtained, and, for P_{self} to appear, it is necessary to add to the free energy the self-energies of the particles. Each particle is found (see Appendix B) to have, up to some (infinite) volume-independent additive constant, the self-energy

$$e_{\text{self}} = \frac{q^2}{2} \left[\ln R - \psi(\nu+1) - \frac{\pi}{2} \cot \pi\nu \right] \tag{4.10}$$

This gives to the pressure the self contribution (4.9).

4.3. Yukawa Gas in a Pseudosphere

The pseudosphere is a surface of constant negative curvature. Since it is infinite, on it it is possible to study systems which are both infinite and curved.

Let a be the "radius" of the pseudosphere, such that the Gaussian curvature is $-1/a^2$ (instead of $1/R^2$ on a sphere) and let $a\tau$ be the geodesic distance (instead of $R\theta$ on a sphere). As shown in Appendix C, the Green function of the Helmholtz equation now is

$$G(\tau) = Q_\nu(\cosh \tau) \tag{4.11}$$

where Q_ν is a Legendre function of the second kind and $\nu = (1/2)[-1 + (1+4\alpha^2 a^2)^{1/2}]$.

The nonself pressure is given by (4.6) where G now is $G(\tau)$ as given in (4.11). After a calculation similar to the one in Appendix A, one finds the analog of (4.7):

$$P_{\text{nonself}} = -\frac{1}{4} n^2 q^2 \int a \frac{\partial G(\tau)}{\partial a} g(\tau)\, dS \tag{4.12}$$

As to the self pressure, its part P_0 is unchanged ($P_0 = -nq^2/4$) while P_1 is given by (4.8) where G is $G(\tau)$. The integral involves $\int_1^\infty [Q_\nu(x)]^2\, dx$ which is tabulated in ref. 6, and one obtains

$$P_{\text{self}} = P_0 + P_1 = \frac{nq^2}{4}\left[-1 + 2\alpha^2 a^2 \frac{\psi'(\nu+1)}{2\nu+1}\right] \tag{4.13}$$

5. COULOMB LIMIT

The results of ref. 1 for a Coulomb fluid, the one-component plasma, can be retrieved in the limit $\alpha \to 0$ of the Yukawa fluid. However, before taking that limit, one must add a neutralizing background to the Yukawa fluid. The presence of a background is taken into account by changing g into $h = g - 1$ in (1.3), (3.3), (4.2), (4.7).

5.1. Coulomb Limit in $\mathbb{R}^3$

As $\alpha \to 0$, $G \to 1/r$ and (1.3) becomes

$$P_{\text{ex}} = P_{\text{nonself}} = \frac{1}{6} n^2 q^2 \int \frac{1}{r} h(r)\, d\mathbf{r} \tag{5.1}$$

i.e., the excess pressure is one third of the potential energy density.

5.2. Coulomb Limit in S^3

As $\alpha \to 0$,

$$R\frac{\partial G}{\partial R} = -\frac{6}{\pi\alpha^2 R^3} - \frac{1}{\pi R}\left[(\pi-\psi)\cot\psi - \frac{1}{2}\right] + o(1) \tag{5.2}$$

Since the system is finite,

$$n\int h(\psi)\, dV = -1 \tag{5.3}$$

and (3.3) becomes

$$P_{\text{nonself}} = \frac{1}{6}n^2q^2\int\frac{1}{\pi R}\left[(\pi-\psi)\cot\psi - \frac{1}{2}\right]h(\psi)\, dV - \frac{nq^2}{\pi\alpha^2R^3} + o(1) \tag{5.4}$$

Furthermore, as $\alpha \to 0$, (3.6) becomes

$$P_{\text{self}} = \frac{nq^2}{\pi\alpha^2R^3} - \frac{nq^2}{4\pi R} + o(1) \tag{5.5}$$

Thus, one retrieves the result of ref. 1 for the total excess pressure in the Coulomb case $\alpha = 0$:

$$\begin{aligned} P_{\text{ex}} &= P_{\text{nonself}} + P_{\text{self}} \\ &= \frac{1}{6}n^2q^2\int\frac{1}{\pi R}\left[(\pi-\psi)\cot\psi - \frac{1}{2}\right]h(\psi)\, dV - \frac{nq^2}{4\pi R} \end{aligned} \tag{5.6}$$

It should be noted that, in the limit $\alpha \to 0$, P_{nonself} and P_{self} have opposite divergent terms $O(\alpha^{-2})$ which cancel each other in their sum P_{ex}. Thus, it is essential to keep the self term for retrieving the finite result (5.6).

5.3. Coulomb Limit in $\mathbb{R}^2$

As $\alpha \to 0$, $K_0(\alpha r) = -\ln(\alpha r/2) - \gamma + o(1)$ (where γ is Euler's constant)[6] and $r\, dG/dr \to -1$. Since the Coulomb fluid exhibits perfect internal screening, i.e.,

$$n\int h(r)\, d\mathbf{r} = -1 \tag{5.7}$$

(4.2) gives the known explicit exact result[7]

$$P_{\mathrm{ex}} = P_{\mathrm{nonself}} = -\frac{nq^2}{4} \tag{5.8}$$

5.3. Coulomb Limit in S^2

As $\alpha \to 0$, $\nu = -\alpha^2 R^2 + o(\alpha^2)$, $P_\nu(-\cos\theta) = 1 + 2\nu \ln \sin(\theta/2) + o(\alpha^2)$,[6] and $R\,\partial G/\partial R = -(1/\alpha^2 R^2) + o(1)$. Since the system is finite,

$$n \int h(\theta)\, dS = -1 \tag{5.9}$$

and (4.7) becomes

$$P_{\mathrm{nonself}} = -\frac{nq^2}{4\alpha^2 R^2} + o(1) \tag{5.10}$$

while (4.9) becomes

$$P_{\mathrm{self}} = \frac{nq^2}{4}\left[-1 + \frac{1}{\alpha^2 R^2} + o(1)\right] \tag{5.11}$$

Thus, one retrieves the result of ref. 1:

$$P_{\mathrm{ex}} = P_{\mathrm{nonself}} + P_{\mathrm{self}} = -\frac{nq^2}{4} \tag{5.12}$$

Here too, P_{nonself} and P_{self} have opposite divergent terms $O(\alpha^{-2})$ which cancel each other.

5.4. Coulomb Limit in a Pseudosphere

As $\alpha \to 0$, $\nu \to 0$, $G(\tau) \to Q_0(\cosh\tau) = -\ln\tanh(\tau/2)$, and $a\,\partial G/\partial a \to 0$. Thus $P_{\mathrm{nonself}} = 0$. On the other hand, (4.13) becomes $P_{\mathrm{self}} = -nq^2/4$. Thus,

$$P_{\mathrm{ex}} = P_{\mathrm{self}} = -\frac{nq^2}{4} \tag{5.13}$$

Here, the excess pressure entirely comes from the self part.

6. VIRIAL EXPANSION IN A PSEUDOSPHERE

In a pseudosphere, Jancovici and Téllez[9] have defined an excess pressure by the virial expansion in powers of the density n

$$\beta p_{\mathrm{ex}} = \sum_{k=2}^{\infty} B_k n^k \tag{6.1}$$

Obviously, (6.1) does not agree with (5.13). The present section is an erratum to ref. 9: (6.1) is *not* a good definition of the pressure. The considerations about the virial expansion in ref. 9 should be replaced by what follows.

Since on a pseudosphere, as the size of a domain is increased, its perimeter grows as fast as its area S, there is no unique thermodynamic limit for the free energy per unit area F/S. A reasonable definition of a bulk quantity is provided by the usual virial expansion of *the free energy*, obtained by manipulations of the partition function: the nonself part of the excess free energy per particle can be defined by

$$\beta f_{\mathrm{nonself}} = \sum_{k=2}^{\infty} \frac{B_k}{k-1} n^{k-1} \tag{6.2}$$

where each virial coefficient B_k is to be computed in the infinite system limit (for eliminating the boundary effects) before the sum is performed.

Fom this free energy (6.2), one can derive the nonself part of the excess pressure by the standard relation $P_{\mathrm{nonself}} = n^2\, \partial f_{\mathrm{nonself}}/\partial n$ provided one takes into account an unusual feature (which has been disregarded in ref. 9): the interaction law G and therefore the excess free energy per particle f_{ex} depends on the radius of curvature a (the virial coefficients B_k do depend on a): it is convenient to consider f_{ex} as a function of the two independent variables n and na^2. The variation of density in the above definition of the excess pressure can be considered as associated to a variation of a while the average number of particles in some domain remains constant as the area of this domain varies proportional to a^2. In other words, for defining the excess pressure, the partial derivative of the excess free energy with respect to n must be taken at constant na^2, and one must write more precisely

$$P_{\mathrm{nonself}} = n^2 \left(\frac{\partial f_{\mathrm{nonself}}}{\partial n} \right)_{na^2} \tag{6.3}$$

In the case of a Coulomb system of point particles, for dimensional reasons, f_{nonself} depends on n and a only through the combination na^2 (B_k is proportional to $a^{2(k-1)}$), and (6.3) gives $P_{\mathrm{nonself}} = 0$.

Furthermore, self effects must be taken into account. For a Coulomb system, with an interaction $G = -\ln \tanh(\tau/2)$, the self-energy of a particle of small radius $r_0 = a\tau_0$

$$e_{\text{self}} = f_{\text{self}} = -\frac{q^2}{2} \ln \frac{r_0}{2a} = -\frac{q^2}{4} \ln \frac{r_0^2 n}{4na^2} \tag{6.4}$$

does give a contribution to the pressure

$$P_{\text{self}} = n^2 \left(\frac{\partial f_{\text{self}}}{\partial n}\right)_{na^2} = -\frac{nq^2}{4} \tag{6.5}$$

in agreement with (5.13).

7. DISCUSSION

In a flat space $\mathbb{R}^3$ or $\mathbb{R}^2$, the stress tensor approach simply reproduces the expected pressure. There is no self contribution.

The situation is more involved in the finite curved spaces S^3 and S^2, and in the infinite pseudosphere. The very definition of the pressure is not obvious. An operational definition would be the force per unit area exerted on a wall bounding the fluid. However, when the system is a finite one, such a pressure would depend on the position and shape of this wall, and also, for a fixed curvature, the mere presence of a boundary would change the size of the system. In the case of a pseudosphere, a system with a boundary makes difficulties because its perimeter grows as fast as its area. The stress tensor approach, which has been used here, has the advantage of defining a bulk pressure which does not refer to any wall. But it raises a question: should the self part be included or not in the definition of the pressure? One might be tempted to follow the usual procedure of discarding self effects. However, as seen in Section 5, it is necessary to keep this self term for retrieving a finite pressure in the Coulomb case. Thus, the nonself and self parts of the pressure are somewhat entangled with each other. For a flat system in $\mathbb{R}^2$ or $\mathbb{R}^2$, the (properly regularized) self pressure vanishes, for a Yukawa system and thus in the Coulomb limit. However, the same pressure for a flat Coulomb system can be obtained by starting with a Yukawa system (plus background) in S^3, S^2, or the pseudosphere, going to the Coulomb limit $\alpha \to 0$, and finally going to the limit $R \to \infty$ or $a \to \infty$ of a flat system; if this route is followed, it is mandatory to keep the self part of the pressure.

The entanglement of the nonself and self parts of the pressure is especially apparent in the two-dimensional case. The result for a flat Coulomb system, $P_{\text{ex}} = -nq^2/4$ can be obtained by starting with a Yukawa system on a sphere S^2, and taking the limits $\alpha \to 0$ and $R \to \infty$. These limits can be taken in one order or in the opposite one, or even for a fixed value of αR, giving the same final result for P_{ex}. However, the separate contributions P_{nonself} and P_{self} do depend on the way the limits are taken.

In a curved space, the pressure from the stress tensor approach can also be retrieved from the usual thermodynamic definition (1.2) (the negative of the derivative of the free energy with respect to the volume, or its two-dimensional analogs). If one deals from the start with a Coulomb fluid in S^3 or S^2, there is some arbitrariness in the definition of the self-energy of a particle,[8] and only a "reasonable" choice allows to retrieve[1] the stress tensor pressure. In the case of a Yukawa fluid, the self-energy (3.9) or (4.10) is sufficiently well-defined for the calculation of the pressure. Starting with a Yukawa fluid and going afterwards to the Coulomb limit avoids the above mentioned arbitrariness.

It should be noted that, in curved spaces, the stress tensor approach defines the pressure as the response to a change of the radius R or a; the thermodynamic approach does the same. However, as R or a changes, the interaction potential changes, and therefore the derivative $-\partial F/\partial V$ is *not* taken at constant interaction potential. This is a bit unusual! It has to be taken into account when using the virial expansion which seems to exist in the pseudosphere.

The conclusion is that there is some arbitrariness in the definition of the pressure in a curved space. However, the stress tensor approach, in which there is some reason for including the self contribution, gives a pressure which seems acceptable.

APPENDIX A. FORMULAS IN S_3

For deriving (3.3) from (3.2), one first note that, since the integrand in (3.2) depends only on the shape of the geodesic triangle formed by points (0, 1, 2), the integration can be performed on another pair of positions (0, 2), rather than (1, 2). By an integration by parts on 0, the term $\nabla_0 G(\psi_{01}) \cdot \nabla_0 G(\psi_{02})$ can be replaced by $-G(\psi_{01}) \triangle_0 G(\psi_{02})$. Using the Helmholtz equation with a point source

$$[-\triangle_0 + \alpha^2]\, G(\psi_{02}) = -4\pi\delta^{(3)}(\psi_{02}) \tag{A.1}$$

gives

$$P_{\text{nonself}} = \frac{n^2 q^2}{24\pi} \Bigg[4\pi \int dV_2\, G(\psi_{12})\, g(\psi_{12}) + 2\alpha^2 \int dV_0\, dV_2\, G(\psi_{01})\, G(\psi_{02})\, g(\psi_{12}) \Bigg] \tag{A.2}$$

Using the Dirac notation

$$G(\psi_{ij}) = \left\langle i \left| \frac{4\pi}{-\Delta+\alpha^2} \right| j \right\rangle \tag{A.3}$$

where i, j are positions, gives for the integral on 0 in (A.2)

$$\begin{aligned}\int dV_0 G(\psi_{10})\, G(\psi_{02}) &= \int dV_0 \left\langle 1 \left| \frac{4\pi}{-\Delta+\alpha^2} \right| 0 \right\rangle \left\langle 0 \left| \frac{4\pi}{-\Delta+\alpha^2} \right| 2 \right\rangle \\ &= \left\langle 1 \left| \frac{(4\pi)^2}{(-\Delta+\alpha^2)^2} \right| 2 \right\rangle = -4\pi \frac{\partial G(\psi_{12})}{\partial(\alpha^2)}\end{aligned} \tag{A.4}$$

Thus, with simpler notations V and ψ instead of V_2 and ψ_{12}, (A.2) becomes

$$P_{\text{nonself}} = \frac{n^2q^2}{6} \int dV \left[G(\psi) - \alpha \frac{\partial G(\psi)}{\partial \alpha} \right] g(\psi) \tag{A.5}$$

Finally, since $RG(\psi)$ as defined in (3.1) depends on α only through αR, $\alpha(\partial G/\partial \alpha) = \partial(RG)/\partial R$ and (A.5) gives (3.3).

For deriving (3.6) from (3.4) and (3.5), first one performs an integration by parts which transforms (3.5) (where $dV = 4\pi R^3 \sin^2 \psi \, d\psi$) into

$$\begin{aligned}P_1 = \frac{nq^2}{24\pi} \Bigg\{ &\int_{\psi > \psi_0} [-G(\psi) \, \Delta \, G(\psi) + 3\alpha^2 [G(\psi)]^2] \, dV \\ &- \left[G(\psi) \frac{dG}{d\psi} 4\pi R \sin^2 \psi \right]_{\psi = \psi_0} \Bigg\}\end{aligned} \tag{A.6}$$

Since G obeys the Helmholz equation and $\psi \neq 0$, in (A.6) the Laplacian Δ can be replaced by α^2. Furthermore, the integral remains convergent as $\psi_0 \to 0$ and can be extended to the whole hypersphere. With G given by (3.1), this is an elementary integral on trigonometric or hyperbolic functions. Adding the small-ψ_0 form of the last term of (A.6), one finds

$$P_1 = \frac{1}{6} nq^2 \left[\frac{\pi \alpha^2 R}{\sin^2 \pi\omega} - \frac{\cot \pi\omega}{R\omega} + \frac{1}{R\psi_0} + O(\psi_0) \right] \qquad \text{for} \quad \alpha R < 1 \tag{A.7}$$

Adding (3.4) and (A.7) gives (3.6). A similar calculation can be done when $\alpha R > 1$.

For computing the self-energy (3.9) of a particle pictured as a spherical surfacic charge of radius $r_0 = R \sin \psi_0$, in the small-ψ_0 limit one can use the point-particle potential (3.1). As $\psi_0 \to 0$

$$e_{\text{self}} = \frac{q^2}{2} G(\psi_0) = \frac{q^2}{2} \left[\frac{1}{r_0} - \frac{\omega \cot \pi\omega}{R} + O(\psi_0) \right] \qquad \text{for} \quad \alpha R < 1 \tag{A.8}$$

Up to the volume independent term $q^2/2r_0$ (which becomes infinite in the $\psi_0 \to 0$ limit), (A.8) does give (3.9). For $\alpha R > 1$, ω must be replaced by $i\omega$.

APPENDIX B. FORMULAS IN S_2

For finding the Green function (4.5), one notes that the Helmholtz equation in S_2 (similar to (A.1) with $2\pi\delta^{(2)}$ instead of $4\pi\delta^{(3)}$) reduces to the Legendre equation,[6] with the variable $\cos\theta$ and the parameters $\nu = (1/2)[-1 + (1 - 4\alpha^2 R^2)^{1/2}]$, $\mu = 0$. The solution singular at $\theta = 0$ and regular at $\theta = \pi$ is the Legendre function

$$P_\nu(-\cos\theta) = F\left(-\nu, \nu + 1; 1; \frac{1 + \cos\theta}{2} \right) \tag{B.1}$$

Indeed, at $\theta = \pi$ the hypergeometric function F is regular, and as $\theta \to 0$ its behavior[10]

$$P_\nu(-\cos\theta) = \frac{2 \sin \nu\pi}{\pi} \left[\ln \sin \frac{\theta}{2} + \gamma + \psi(1 + \nu) + \frac{\pi}{2} \cot \nu\pi \right] + o(1) \tag{B.2}$$

is[2] such that (4.5) does behave like $-\ln\theta$.

For deriving the self-energy (4.10), one looks at the behaviour of $(q^2/2)\, G(\theta_0)$, considering $r_0 = R\theta_0$ as a small fixed particle radius. As $\theta_0 \to 0$, using (B.2) in (B.1) gives (4.10).

APPENDIX C. GREEN FUNCTION IN A PSEUDOSPHERE

The Helmholtz equation in a pseudosphere of "radius" a reduces to the Legendre equation[6] with the variable $\cosh\tau$ and the parameters $\nu = (1/2)[-1 + (1 + 4\alpha^2 a^2)^{1/2}]$, $\mu = 0$. The solution singular at $\tau = 0$ and vanishing at infinity is $Q_\nu(\cosh\tau)$. For small τ, it does behave[10] like $-\ln\tau$.

[2] There is a minor misprint in ref. 10. In Eq. (15) p. 164, γ must be replaced by 2γ for this equation to agree with Eq. (12) p. 110.

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REFERENCES

1. B. Jancovici, *J. Stat. Phys.* **99**:1281 (2000).
2. J. M. Caillol and D. Gilles, *J. Phys. IV France* **10**:Pr5–237 (2000).
3. J. M. Caillol and D. Gilles, *J. Stat. Phys.* **100**:905–932 (2000).
4. J. P. Hansen and I. R. McDonald, *Theory of Simple Liquids* (Academic, London, 1986).
5. C. Itzykson and J. B. Zuber, *Quantum Field Theory* (McGraw–Hill, New York, 1980).
6. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Academic, New York, 1994).
7. E. H. Hauge and P. C. Hemmer, *Phys. Norv.* **5**:209 (1965).
8. J. M. Caillol and D. Levesque, *J. Chem. Phys.* **94**:597 (1991).
9. B. Jancovici and G. Téllez, *J. Stat. Phys.* **91**:953 (1998).
10. A. Erdélyi *et al.*, *Higher Transcendental Functions* (McGraw–Hill, New York, 1953), Vol. I.