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Onsager Molecules for the Yukawa Potentials: Screening Potentials and the Jancovici Coefficient in Strongly Coupled Electron-Screened Plasmas

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Jancovici derived the exact r^2 term in the expansion of the screening potential of the one-component plasma (OCP) around $r=0$, which led to much improved analysis of the simulation data, but the correspondingly important term has never been calculated for electron-screened plasmas. The Onsager molecule approach provides the strong-coupling-limit result for the OCP screening potentials, features the exact Jancovici r^2 term, and gives a comprehensive physical picture of the structure of strongly coupled plasmas. It is used here to derive the Strong-coupling screening potentials of electron-screened plasmas represented by the Yukawa potentials and, in particular, the corresponding Jancovici r^2 term.

KEY WORDS: Strongly coupled plasmas; electron screening; screening potentials; Yukawa potential; Onsager molecules; pair correlation functions; enhancement factors.

I. INTRODUCTION: SCREENING POTENTIALS AND ENHANCEMENT FACTORS

It is our great pleasure to contribute to this issue in honour of Bernard Jancovici, who made important contributions to the subject we address in this paper.

Classical plasmas composed of classical positive ions in a uniform neutralizing background charge density of degenerate electrons, are basic models for dense stellar materials and provide important reference systems

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in condensed matter physics.[1,2] These systems are referred to as "one component plasma" (OCP), "binary ionic mixture" (BIM), or "multi ionic mixture," depending on the number of different ionic species. Electron screening effects change the interionic interactions from pure Coulomb "$1/r$" to "screened-Coulomb," and the standard linear response treatment with the Debye–Huckel or Thomas–Fermi approximations leads to the Yukawa interparticle interaction "$e^{-\alpha r}/r$."[3] Much effort has been invested over the years[4] in increasing the accuracy of the calculations of the short range screening potentials in strongly coupled plasmas, for two main reasons: (1) The enhancement factors for the thermonuclear reaction rates which are important for stellar evolution, particularly for Carbon ignition in degenerate cores, are essentially controlled by the short range part of the screening potential. (2) The screening potentials play a key role in the study of the short range behavior of the bridge functions, notably their universal properties, which proved seminal for developing an accurate theory of liquid structure.[5] They offer consistency checks for the equation of state of the mixture, and for closure approximations in integral equation theories for the fluid pair structure.

The screening potentials $H_{ij}(r)$ of a classical mixture of particles interacting through the pair potentials $\phi_{ij}(r)$ are related to the pair correlation functions $g_{ij}(r)$:

$$H_{ij}(r) = \frac{\phi_{ij}(r)}{k_B T} + \ln[g_{ij}(r)]. \tag{1}$$

The pair correlation function can be expressed through the free energy change upon fixing the positions of the pair of fluid particles in the appropriate configuration to form an interaction-site molecule[6–9]

$$H_{ij}(r) = \frac{1}{k_B T}[-(F_1^{ex}(r) - F_0^{ex}) + \phi_{ij}(r)] \tag{2}$$

Here F_0^{ex} is the configurational (excess over ideal gas) free energy of the N-particle system, and $F_1^{ex}(r)$ is that of the same system but with the pair of particles i and j in question being kept at fixed separation, r, forming a two-site cluster. $F_1^{ex}(r)$ does contain the intramolecular interaction $\phi_{ij}(r)$, so that $H_{ij}(r)$ is finite as $r \to 0$.

In the non screened classical plasma the point ions of charges $Z_i e$ and $Z_j e$ interact through the bare Coulomb potential:

$$\phi_{ij}^{C}(r) = \left(\frac{e^2}{a}\right) Z_i Z_j \frac{1}{r}. \tag{3}$$

It is convenient to measure all distances in units of the Wigner–Seitz radius, $a=(3/4\pi n)^{1/3}$, where $n=N/V$ is the total number density of the ions, and to define the Coulomb coupling parameter $\Gamma=e^2/ak_BT$. After earlier important calculations by DeWitt and collaborators,[10] additional significant contributions were made by Jancovici and collaborators: Using Eq. (2), assuming the validity of the linear mixing rule[11,12] for the free energy of the BIM, and by employing an accurate OCP equation of state,[13] Jancovici[8] obtained a good estimate of $H(0)$ for the OCP. He also derived the exact leading r^2 term in the expansion around $r=0$ (the Jancovici coefficient), which was used by Alastuey and Jancovici[14] to extrapolate the simulation data for $H(r)=\Gamma/r+\ln g(r)$ towards the origin $r=0$.

A convenient starting point for analysing the electron response corrections[15–19] to the interionic screening potentials is to consider classical mixtures of charged particles interacting through the repulsive Yukawa (screened Coulomb) potentials.[19] "Yukawa" mixtures are composed of positively charged, $Z_ie>0$, point particles interacting through the Yukawa pair potentials:

$$\phi_{ij}^{Y}(r)=\left(\frac{e^2}{a}\right)Z_iZ_j\frac{e^{-\alpha r}}{r}. \tag{4}$$

The leading strong coupling terms for the potential energy, direct correlation functions, and screening potentials for the Coulomb and Yukawa fluid mixtures (corresponding to classical plasmas and electron screened classical plasmas), were obtained from the Onsager molecule approach[22,9,17,20,21] with full thermodynamic consistency and in complete agreement with the Alastuey–Jancovici analysis of early simulations[23] in strong coupling, and with recent highly accurate simulations data.[4] This approach follows from Onsager's[24] method for obtaining exact lower bounds for the potential energy of systems of charge distributions. The Onsager molecule theory provides the asymptotic strong coupling properties of classical plasmas analytically and in a simple physically intuitive way. It was used in order to derive explicit expressions[22,9,26] for $H_{ij}(r)$ in Coulomb plasmas, and for $H_{ij}(r=0)$ in Yukawa plasmas.[17,20,21] In this paper we use this method in order to make a semi analytic calculation of (an accurate approximation to) the Onsager molecules for the Yukawa potential. We present the exact Onsager molecule result for the strong coupling limit of the Jancovici coefficient for the Yukawa interaction, and an accurate approximation for the full $H_{ij}(r)$ for strongly coupled Yukawa systems. The classical Coulomb and Yukawa systems are only model systems, and our results can be directly applicable only for weakly screened plasmas ($\alpha\ll 1$). However, many quite

disparate systems with screened Coulomb interactions can be described by Yukawa interparticle potentials which thus make important reference systems in condensed matter physics,[19] and in this broader context our results for the Yukawa potential can be useful also when the screening parameter is large ($\alpha > 1$).

The main thrust of the DeWitt or Jancovici approaches to screening potentials was in relation to enhancement factors for nuclear reaction rates. The leading term in the expression for the enhancement factor is $\exp[H_{ij}(r=0)/k_BT]$ but all the small r expansion of $H_{ij}(r)$ is relevant. The rate of nuclear reactions plays a major role in many astrophysical problems. Not only does it set the time scale for the nuclear energy release in the core of all stars, thus setting the time scale for stellar evolution, but it is crucial in determining the fate of dense stars. In particular, it determines the dynamical evolution of binary systems, accreting white dwarfs and neutron stars. The many body effects reduce the Coulomb barrier, and enhance the probability of a reacting collision, beyond the pair approximation in Gamow's barrier penetration factor. The ratio between the probability of a pair encounter in the medium to that in the low density pair-approximation, is called the enhancement factor. The ions inside dense stars (such as white dwarfs and neutron stars) are strongly coupled, $\Gamma \sim$ (potential energy)/(kinetic energy) ~ 100, the enhancement factor is roughly proportional to $\exp[H(0)]$, and $H(0) \sim \Gamma$, so that an error of 2% in the value of $H(0)$ may yield a reaction rate which is off by an order of magnitude. Relatively small changes in the enhancement factors of nuclear reactions can make a spectacular difference in the outcome of an accreting massive white dwarf: Depending on the exact value of this factor, the star becomes either a type-I supernova or collapses into a neutron star.[27] This demonstrates the importance of accurate calculations for these factors, which have been considered by many authors over several decades,[28–32] but in most cases only the screening of the Coulomb barrier due to the ions has been calculated. In these calculations one usually assumes that the electrons can be treated as a uniform rigid background. In this case, the classical enhancement factor can be calculated by a comprehensive approach for the screening potentials of Coulomb mixtures,[21, 33] which incorporates the concept of "Onsager molecules" entirely within the spirit of the DeWitt or Jancovici approach. The rigid background approximation is valid as long as the electron Thomas–Fermi screening length is larger than the mean distance between the ions. However, in some astrophysical situations, e.g., massive white dwarfs or low-mass stars,[34] this condition is no longer fulfilled, and the electron gas becomes polarized by the field created by the ions. This induces an electronic contribution to the screening of the inter-ionic Coulomb barrier, i.e., an electron-screening contribution to the

reaction rate. Although some calculations including this effect have been conducted in the special case of massive white dwarfs,[35] a comprehensive treatment is yet to be done. Needless to say that the present linear response model, which features a diverging electron density at the nucleus can not provide a serious discussion of the incorporation of electronic effects into the nuclear enhancement factor, which requires a more accurate treatment of the electron density near the nucleus and its effect on the total internuclear potential. Correct treatment of the electron density near the nucleus is outside the scope of any linear response treatment. Nevertheless, there are two features of the present methodology as developed by one of the authors,[21, 9] which make it relevant also to the nuclear enhancement factor problem: (1) The confined-atom and confined-molecule full Kohn-Sham density functional treatment, is a proper way to approach the problem. The Onsager–Thomas–Fermi "atoms" and "molecules" (see below) utilize the same conceptually correct "confined molecule" physical picture. Its deficiency is the use of a very simple, indeed oversimplified electron density functional. This can be improved directly by incorporating the full Thomas–Fermi density functional with further corrections that improve the electron density at the nucleus. (2) Given an effective pair interaction $\phi(r)$ between the nuclei (the result of a proper solution of the electron density problem) then the enhancement factor is closely related to the corresponding screening potential $H(r)$. The Yukawa potential $Ae^{-\alpha r}/r$ is a quite general form for the short range interatomic interaction, and an analytic expression for $H(r)$ in strong coupling for this potential should be useful.

This discussion connects the present "Onsager molecule" approach to screening potentials to the enhancement problem on the basis of the DeWitt–Jancovici approach. This approach relies in general on calculations of the correlation functions in a classical Coulomb gas, followed by construction of an effective two-body potential and a quantum barrier penetration calculation. It should be noted, however, that very recent work (L. S. Brown and R. F. Sawyer, *Rev. Mod. Phys.* **69**, p. 411 (1997)) found that such an approach "will miss physics that is as important as the physics that it includes."

In Sec. II we briefly summarize the Onsager molecule results for Coulomb plasmas. The Onsager-smearing method for obtaining an exact lower bound to the potential energy of Yukawa plasmas is described in Sec. III. In Sec. IV we present a semi-analytic approximation to the Onsager molecule for the one-component Yukawa plasma, which features the exact Onsager-molecule result for $H(r=0)$ and for the Jancovici coefficient. In Sec. V we point out the scalings that relate the one component results to those for the mixture.

II. "ONSAGER MOLECULES" AND SCREENING POTENTIALS FOR COULOMB PLASMA MIXTURES

The leading term in the asymptotic strong coupling expansion of the configurational free energy of the fluid is an exact Onsager-type[24] lower bound,[22, 17] e.g., the ion-sphere result for the classical plasmas.[25] The two free energies in Eq. (2) are bounded from below by the corresponding leading terms. In particular, the excess free energy of the mixture is bounded by the sum of "Onsager-atom" self energies:

$$F_0^{ex} \geqslant \sum_i N_i u_{OA,i} \tag{5}$$

where

$$u_{OA,i} = -0.9 \left(\frac{e^2}{a}\right) \frac{Z_i^2}{R_i} \tag{6}$$

is the self-energy of an "Onsager atom" consisting of a point charge Z_i at the center of a neutralizing sphere of radius R_i having the background charge density, $R_i = (Z_i/\langle Z \rangle)^{1/3}$. Recall that all distances are measured in units of the Wigner–Seits radius. Similarly,[9]

$$F_1^{ex}(x) \geqslant \sum_{k \neq i,\, k \neq j} N_k u_{OA,k} + (N_i - 1)\, u_{OA,i} + (N_j - 1)\, u_{OA,j} + u_{OM,ij}(r) \tag{7}$$

where $u_{OM,ij}$ is the self-energy of an "Onsager molecule" consisting of a pair of ions Z_i, Z_j separated by a distance r in a uniform neutralizing charge cloud of the background charge density. The shape of this molecule is uniquely determined by the surface on which the electrostatic field vanishes. The screening potential is obtained as a difference between two exact lower bounds[9]

$$H_{OM,ij}(r) = \frac{1}{k_B T}\left[\frac{(e^2/a)\, Z_i Z_j}{r} - (u_{OM,ij}(r) + u_{OA,i} + u_{OA,j})\right] \tag{8}$$

For the one component plasma $H_{OM}(r)$, the corresponding function with all $Z_i = 1$ can be expressed through the function $h_2(r)$:

$$\frac{H_{OM}(r \leqslant 2)}{\Gamma} = \frac{9}{10}(2^{5/3} - 2) = \frac{1}{4} r^2 + h_2(r)\, r^4 \tag{9}$$

where the function

$$h_2(r) \cong 0.038 - 0.0026r^2$$

was obtained by fitting the Onsager molecule numerical data.[26] From elementary electrostatics we find that the small-r expansion for general mixtures takes the form

$$\frac{H_{OM,ij}(r)}{\Gamma} = h_{ij,0} - h_{ij,1} r^2 \cdots \tag{10}$$

where

$$h_{ij,0} = \frac{9}{10}\left(\frac{(Z_i+Z_j)^2}{(R_i^3+R_j^3)^{1/3}} - \frac{Z_i^2}{R_i} - \frac{Z_j^2}{R_j}\right) \tag{11}$$

and

$$h_{ij,1} = \frac{1}{2}\frac{Z_i Z_j}{R_i^3+R_j^3} \tag{12}$$

This coefficient of the r^2 term, i.e., the Jancovici coefficient as obtained from the Onsager molecule, is also the exact Jancovici coefficient for the plasma mixture. This can be established[4] by direct generalization of the original derivation by Jancovici.[8] The terminology "Onsager atoms" and "Onsager Molecules" was introduced by one of the authors[9] in view of Onsager's method[24] for obtaining a lower bound for the total energy of a neutral system of charge distributions by immersing the system in a conducting fluid. Onsager's bound turns out[22, 36] to be the relevant method in the present context. We are not aware of a mathematical proof that Onsager's lower bound is the best possible lower bound in strong coupling.

The surface of the molecule is that where the electric field vanishes since the molecule is neutral and since by Onsager's construction it must be an equipotential surface. The finding of the shape of the Onsager molecule, and the calculation of $u_{OM,ij}(r)$ for general separation r, represent a straightforward but rather tedious numerical problem. It is thus helpful to consider limit cases, scaling relations for mixtures, and simple approximations for $u_{OM,ij}(r)$. The function $H_{OM}(r)$ given above is in excellent agreement with an earlier estimate[9] based on (the much simpler to calculate) convolution-smearing approximation to the Onsager molecule self energy. That smearing approximation, which yields the same first two terms in the small-r expansion, $h_{ij,0}$ and $h_{ij,1}$, as the exact Onsager molecule, will be described and employed below for the more general case of the Yukawa potential.

III. "ONSAGER-SMEARING" LOWER BOUNDS FOR THE POTENTIAL ENERGY OF YUKAWA PLASMA MIXTURES

The Yukawa intermolecular potential, $\phi(r) = e^{-\alpha r}/r$, has the special property[18,20] that it gives rise to the same functional form for the potential outside a spherically symmetric distribution of matter: Thus, if a point Yukawa charge Z is smeared out radially with distribution $\rho(r)$ upto a finite radius R, and if at the same time the charge is appropriately renormalized, $Z_{renorm} = q(\alpha, R)Z$,

$$\frac{1}{q(\alpha, R)} = \frac{4\pi}{\alpha} \int \rho(x)\, x \sinh(\alpha x)\, dx \tag{13}$$

then the potential outside the smearing radius R remains the same as for the original point charge. For a uniform distribution inside a sphere of radius R, $\rho(r \leqslant R) = 3/4\pi R^3$, obtain

$$q(\alpha, R)_{uniform} = Q(\alpha R) \tag{14}$$

where

$$Q(t) = \frac{2t^3}{3[e^t(t-1+e^{-t}(t+1)]} = 1 - \frac{t^2}{10} + \frac{9t^4}{1400} + \cdots \leqslant 1 \tag{15}$$

The renormalization property enables[18,20] to follow the Onsager "smearing" procedure as developed for obtaining a lower bound for the potential energy of Coulomb systems[24,25,22] and apply it[18,20] to general Yukawa systems. Consider classical mixtures consisting of $N = \sum_i N_i$ positively charged, $Z_i e > 0$, point particles of types i in a volume V, interacting through the Yukawa pair potentials $\phi_{ij}(r)/k_B T = Z_i Z_j \Gamma e^{-\alpha r}/r$. The interaction potential energy is measured relative to the (infinite) self energy of the point charges making the system. The interaction potential energy of the system is bounded by the Onsager-type best lower bound obtained by uniformly smearing each particle of type i inside a sphere of radius R_i. The bound is given by:[18,20,21]

$$U^{Yukawa} \geqslant U^{Ukawa}_{bound} = -\frac{1}{2} \sum_i N_i \Psi_{ii}(r=0) + \frac{1}{2V} \frac{4\pi}{\alpha^2} \left(\sum_i N_i Z_i Q(\alpha R_i) \right)^2 \tag{16}$$

where $\Psi_{ij}(r)$ is the interaction between two uniform spheres, of radii R_i and R_j, and Yukawa charges $Z_i Q(\alpha R_i)$ and $Z_j Q(\alpha R_j)$, so that $\Psi_{ij}(r \geqslant R_i + R_j) = (e^2/a)\, Z_i Z_j e^{-\alpha r}/r$, and $\Psi_{ii}(r=0)$ is the self energy of the uniformly distributed Yukawa charge in the sphere. The sum $\sum_i N_i Z_i Q(\alpha R_i)$ is the

total smeared Yukawa charge in the system, and the corresponding term in U_{bound}^{Ukawa} is the self energy of a uniform distribution of this charge in the entire volume of the system. Recall that

$$\Psi_{ii}(r) = \left(\frac{e^2}{a}\right)\frac{Z_i^2}{R_i}\psi\left(\frac{r}{R_i}, \alpha R_i\right) \tag{17}$$

where

$$\psi(x, t) = A(t) + B(t)\frac{x}{2} + A(t)\frac{x^3}{16} + \frac{v(t)}{xt}(1 - e^{-xt}) + \frac{v^2(t)}{2xt^2}(1 - \cosh(xt)) \tag{18}$$

and where

$$A(t) = \frac{3Q^2(t)}{t^2};\ B(t) = \frac{3}{2}A(t)\frac{1-t^2}{t^2};\ v(t) = -2u_0(t) = -\frac{3}{t^2}Q(t)(t+1)\,e^{-t} \tag{19}$$

$$u_0(t) = \frac{3}{2t^2}Q(t)(t+1)\,e^{-t} \tag{20}$$

Note that

$$B(t) - tv(t) - \frac{v^2(t)}{2} = 0 \tag{21}$$

so that $\psi(x, t)$ has the following small-x expansion:

$$\psi(x, t) = (A(t) + v(t)) + (\tfrac{1}{6}v(t)\,t^2)\,x^2 + \cdots \tag{22}$$

We also define

$$\psi(x = 0, t) \equiv \varphi(t) = A(t) + v(t) \tag{23}$$

so that

$$u_0(t) = -\tfrac{1}{2}\varphi(t) + \tfrac{1}{2}A(t) \tag{24}$$

It is useful to note the following identity (prime denotes derivative, e.g., $A'(t) = dA(t)/dt$)

$$t\varphi'(t) - \varphi(t) = t(A'(t) + 2A(t) \tag{25}$$

whereby defining $\bar{\varphi}(t) = t^2\varphi(t)$, $\bar{A}(t) = t^2 A(t)$, obtain

$$t\bar{\varphi}'(t) - 3\bar{\varphi}(t) = t\bar{A}(t) \tag{26}$$

Using these identities, the variational equations

$$\frac{\partial U_{bound}^{Ukawa}}{\partial R_i} = 0; \qquad i = 1, 2,... \tag{27}$$

for optimizing the smearing radii, R_i, are easily solved, and the following best Onsager type lower bound was obtained:[18, 20, 21]

$$U_{best-bound}^{Ukawa} = \sum_i N_i u_i \tag{28}$$

expressed as the sum of "self" (dependent only on each type i) terms:

$$u_i = \left(\frac{e^2}{a}\right)\frac{Z_i^2}{R_i} u_0(\alpha R_i) \tag{29}$$

where the smearing radii, R_i, are obtained from the solution of the following set of non-linear coupled algebraic equations:

$$R_i^3 = \frac{Z_i Q(\alpha R_i)}{\sum_i N_i/N\, Z_i Q(\alpha R_i)}, \qquad i = 1, 2,... \tag{30}$$

For a one component system of N charges $Z_i = Z$ we get, $R_i = R = 1$, and

$$U_{best-bound}^{Ukawa}[N \cdot]/Z^2\left(\frac{e^2}{a}\right) = N u_0(\alpha) \tag{31}$$

The interaction potential energy of the mixture (per particle, in temperature units), is given in general by the standard energy integral involving the pair (radial) distribution functions, $g_{ij}(r)$,

$$\frac{U}{Nk_BT} = \frac{n}{2}\sum_{ij} x_i x_j \int g_{ij}(r)\frac{\phi_{ij}(r)}{k_BT}\, d^3r \tag{32}$$

where $x_i = N_i/N$ are the number concentrations, and $n = N/V$. For the Yukawa potential this takes the special form,

$$\frac{U}{Nk_BT} = \frac{3\Gamma}{2}\sum_{ij} x_i x_j \hat{G}_{ij}(\alpha) \tag{33}$$

where $\hat{G}_{ij}(s) = \int_0^\infty r g_{ij}(r)\, e^{-sr}\, dr$ is the Laplace transform of $[r g_{ij}(r)]$. The Onsager bound $U^{Ukawa}_{best-bound}/Nk_BT$ is equal[20] to the expression (33) provided that the $\hat{G}_{ij}(\alpha)$ are taken as the limit $\eta = 1$ of the solution of the Percus–Yevick equation for a mixture of hard spheres with radii R_i given by (30). This $\eta = 1$ limit of the Percus–Yevick equation is also the leading $\Gamma \to \infty$ strong coupling term of the hypernetted-chain approximation for the pair correlation functions. Under the broad assumption of non-singular bridge functions (i.e., those diagrams missing from the hypernetted-chain approximation) it is also the exact Madelung (i.e., asymptotic strong coupling) energy term for the fluid. The $\Gamma \to \infty$ limit of the hypernetted-chain Ornstein–Zernike direct-correlation functions, $c_{ij}(r)$, is given by the interaction between the optimal distributions in the Onsager smearing process, $c_{ij}(r)/\Gamma = -\Psi_{ij}(r)$. Indeed, by Eq. (16) we verify the Mean-Spherical-Model form of the Ewald identity:[22, 36]

$$\frac{U^{Yukawa}_{best-bound}}{\Gamma N k_B T} = \frac{n}{2} \sum_{ij} x_i x_j \tilde{\Psi}_{ij}(k=0) - \frac{1}{2} \sum_i x_i \Psi_{ii}(r=0) \tag{34}$$

IV. "ONSAGER MOLECULES" AND SCREENING POTENTIALS FOR THE ONE-COMPONENT YUKAWA PLASMA

The optimal Onsager atoms and molecules for obtaining the exact energy lower bound for the Yukawa potential, require the solution of the confined-atom or confined-molecule linearized Thomas–Fermi equations.[17, 18, 20, 21] These equations can be solved analytically for the atom but become tedious numerically for the molecule. Thus, we shall use here the convolution-smearing approximation,[9] and will check its small-r results by comparison with the exact Onsager molecules for the Yukawa plasma. The convolution-smearing approximation provides a quantity which is still a tight lower bound, but not as good as the Onsager molecules.

Consider the one component system composed of $(N-2)$ point Yukawa charges of charge Z, and of one pair of charges Z at fixed distance r. Denote the smearing radius of each the $(N-2)$ free charges by R_a, and that for each of the constrained pair by R_m. The total smeared charge of the system is

$$\sum_i N_i Z_i Q(\alpha R_i) = (N-2)\, ZQ(\alpha R_a) + 2ZQ(\alpha R_m) \tag{35}$$

The self energy of each of the free smeared charges is $(e^2/a)\, Z^2/R_a \varphi(\alpha R_a)$, while that of the pair of constrained charges (viewed as a single two-site "molecule") is $[2(e^2/a)\, z^2/R_m \varphi(\alpha R_m) + (e^2/a)\, Z^2/R_m \psi(r/R_m, \alpha R_m)]$. Recall

that we measure distances in units of a and that $V=4\pi/3Na^3$, so that an exact Onsager-smearing lower bound to the energy is given by

$$\frac{U_{bound}^{Ukawa}[(N-2)\cdot, \cdot - \cdot]}{(e^2/a)}$$

$$= -(N-2)\frac{Z^2}{R_a}\varphi(\alpha R_a) - \left[2\frac{Z^2}{R_m}\varphi(\alpha R_m) + \frac{Z^2}{R_m}\psi\left(\frac{r}{R_m}, \alpha R_m\right)\right]$$

$$+ N\frac{3}{2\alpha^2}\left(\frac{N-2}{N}ZQ(\alpha R_a) + \frac{2}{N}ZQ(\alpha R_m)\right)^2 + Z^2\frac{e^{-\alpha r}}{r} \tag{36}$$

The term $Z^2e^{-\alpha r}/r$ takes into account the "intramolecular" interaction as required for $F_1^{ex}(r)$ in Eq. (2). The optimization equations for the bound, Eqs. (27), take the form

$$R_a^3 = \frac{Q(\alpha R_a)}{((N-2)/N)\,Q(\alpha R_a) + (2/N)\,Q(\alpha R_m)} \tag{37}$$

$$R_m^3 = \frac{Q(\alpha R_m)}{((N-2)/N)\,Q(\alpha R_a) + (2/N)\,Q(\alpha R_m)}$$

$$\times\left[1 + \frac{\alpha R_m^3}{6Q(\alpha R_m)\,Q'(\alpha R_m)}\frac{\partial}{\partial R_m}\left(\frac{1}{R_m}\psi\left(\frac{r}{R_m}, \alpha R_m\right)\right)\right] \tag{38}$$

In the limit $N\to\infty$ the first equation above gives

$$R_a = 1$$

and $R_m(r)$ is obtained from the following form of the second equation above:

$$R_m^3 = \frac{Q(\alpha R_m)}{Q(\alpha)}\left[1 + \frac{\alpha R_m^3}{6Q(\alpha R_m)\,Q'(\alpha R_m)}\frac{\partial}{\partial R_m}\left(\frac{1}{R_m}\psi\left(\frac{r}{R_m}, \alpha R_m\right)\right)\right] \tag{39}$$

where $Q'(t) = dQ(t)/dt$. For $r=0$ we have $R_m^3 = 2Q(\alpha R_m)/Q(\alpha)$ as expected from Eqs. (30), and the result $R_m(\alpha)$ is displayed in Fig. 1. For $r\geqslant 2$ we have $R_m^3(r\geqslant 2) = Q(\alpha R_m)/Q(\alpha)$ so that $R_m^3(r\geqslant 2) = 1$, as expected by the dissociation property of the "molecules" in this convolution smearing construction. The energy bound takes the form:

$$\frac{U_{bound}^{Ukawa}[(N-2)\cdot, \cdot - \cdot]}{(e^2/a)}$$

$$= -(N-2)\,u_0(\alpha) + \frac{2}{R_m}u_0(\alpha R_m) - \frac{1}{R_m}\psi\left(\frac{r}{R_m}\alpha R_m\right)$$

$$+ \frac{1}{R_m}A(\alpha R_m)\left(\frac{R_m^3 Q(\alpha)}{Q(\alpha R_m)} - 1\right) + \frac{e^{-\alpha r}}{r} \tag{40}$$

The "Onsager-molecule" result, in the convolution smearing approximation (CSA), for the screening potential takes the form (recall that $\Gamma = (e^2/a)\,1/k_B T$)

$$\frac{H_{OM,\,CSA}^{Yukawa}(r)}{Z^2\Gamma} = 2u_0(\alpha) - \frac{2}{R_m}u_0(\alpha R_m)$$

$$+ \frac{1}{R_m}\psi\left(\frac{r}{R_m}, \alpha R_m\right) - \frac{1}{R_m}A(\alpha R_m)\left(\frac{R_m^3 Q(\alpha)}{Q(\alpha R_m)} - 1\right) \tag{41}$$

For $r \geqslant 2$ we have $R_m^3(r \geqslant 2) = 1$ so that

$$\frac{H_{OM,\,CSA}^{Yukawa}(r \geqslant 2)}{Z^2(e^2/a)\,1/k_B T} = \psi(r \geqslant 2, \alpha) = \frac{e^{-\alpha r}}{r} \tag{42}$$

For $r = 0$ we have $R_m^3 Q(\alpha)/Q(\alpha R_m) = 2$ and we get

$$\frac{H_{OM}^{Yukawa}(r=0)}{Z^2\Gamma} = 2u_0(\alpha) - \frac{4}{R_m}u_0(\alpha R_m) \tag{43}$$

i.e., it is the exact OM result as expected from Eqs. (28). The leading small-r term is found analytically to be of order r^2, and is given by the corresponding term in Eq. (22)

$$\frac{h_{OM,\,1}^{Yukawa}}{Z^2\Gamma}r^2 = \frac{-1}{R_m}\left(\frac{1}{6}v(\alpha R_m)(\alpha R_m)^2\right)\left(\frac{r}{R_m}\right)^2 = \frac{\alpha^2}{3R_m}u_0(\alpha R_m)\,r^2 \tag{44}$$

where, as above, $R_m(\alpha)$ is obtained from the solution of $R_m^3 = 2Q(\alpha R_m)/Q(\alpha)$. In the limit $\alpha = 0$ it recovers the Jancovici result, $h_{OM,\,1}^{Coulomb}/Z^2\Gamma = 1/4$, for the Coulomb potential. Analytic calculation, in the $r \to 0$ limit, of the confined-molecule linearized Thomas–Fermi equation, shows that our CSA result, Eq. (44), is the exact OM result (as we expected on the basis of the corresponding results for the Coulomb potential). Thus, the small-r expansion of the screening potential of the Yukawa system in the

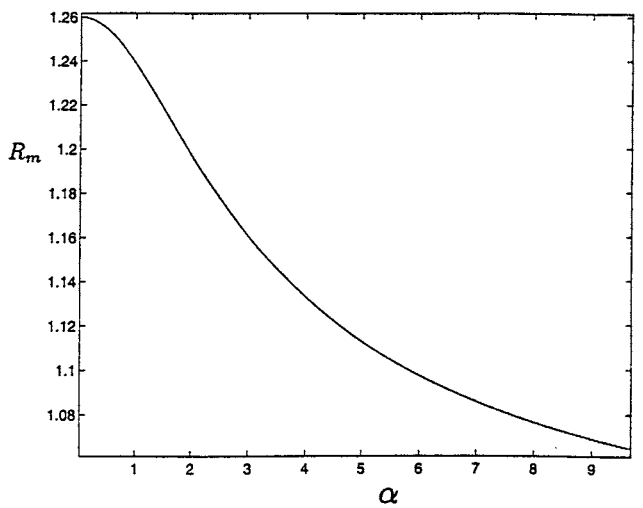

Fig. 1. The smearing radius, R_m at $r=0$ as function of α (i.e., $R_m(r=0)$ as obtained from the solution to Eq. (39)). The value at $\alpha=0$, namely $2^{1/3}$, is the ion-sphere result for the Coulomb potential. See the text.

strong coupling limit takes the form (where R_m is again the $r=0$ result, given in Fig. 1):

$$H_{OM}^{Yukawa}(r)=Z^2\Gamma\left[\left(2u_0(\alpha)-\frac{4}{R_m}u_0(\alpha R_m)\right)-\left(\frac{\alpha^2}{3R_m}u_0(\alpha R_m)\right)r^2+\cdots\right] \tag{45}$$

The Jancovici coefficient for the Yukawa potential is given by

$$h_1^{Yukawa}(\alpha)=\frac{\alpha^2}{3R_m}u_0(\alpha R_m). \tag{46}$$

Recall that

$$u_0(t)=u_0(t)=\frac{3}{2t^2}-\frac{9}{10}+\frac{t}{2}-\frac{18}{175}t^2+\cdots \tag{47}$$

so that, by using

$$R_m=2^{1/3}\left(1-\frac{2^{1/3}-1}{30}\alpha^2+\cdots\right) \tag{48}$$

we obtain

$$h_1^{Yukawa}(\alpha) = \frac{(\alpha R_m)^2}{3R_m^3} u_0(\alpha R_m) = \frac{1}{4} - \left(\frac{5 \cdot 2^{2/3} + 1}{40}\right)\alpha^2 + \cdots \tag{49}$$

It is displayed in Fig. 2, along with a simple fit, given by

$$(h_1^{Yukawa}(\alpha))_{fit} = \left(\frac{1}{4}\right)\frac{1 - 0.18991\alpha}{1 - 0.18991\alpha + 0.56948\alpha^2} \tag{50}$$

The Yukawa screening potentials for $H^{Yukawa}_{OM,\,CSA}(r)/Z^2/\Gamma$ are displayed in Fig. 3 for different values of α. The CSA cannot be expected to be very accurate for relatively large values of α. Our numerical calculations indicate that the CSA is accurate for $\alpha < \sim 0.5$, essentially for all values of α for which the linear-response treatment leading to the Yukawa potential is valid. If it is needed in the general context of the Yukawa potential for $\alpha > 0.5$ then the screening potential can be approximated by a polynomial interpolation between $r = 0$ and $r = 2$, using the OM Jancovici coefficient as we derived, and the smoothness of the function at these end points.

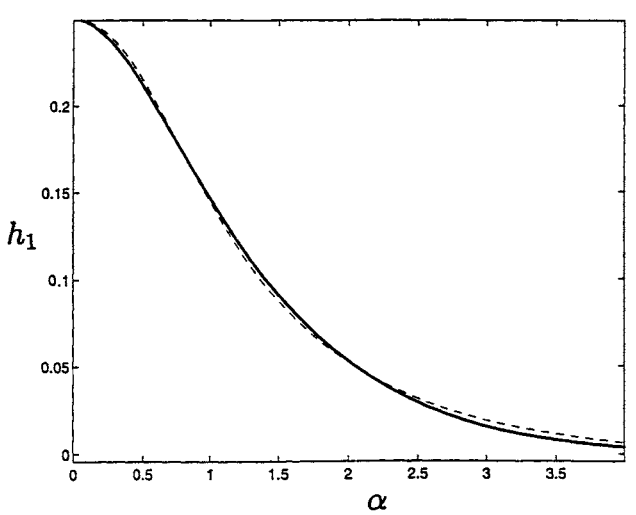

Fig. 2. The Jancovici coefficient, h_1, for the Yukawa potential as function of α: the full line represents $h_1^{Yukawa}(\alpha)$, Eq. 46), and the broken line represents the fit $(h_1^{Yukawa}(\alpha))_{fit}$, Eq. (50). The value at $\alpha = 0$, namely 1/4 is equal to the original Jancovici result[8] for the Coulomb potential. See the text.

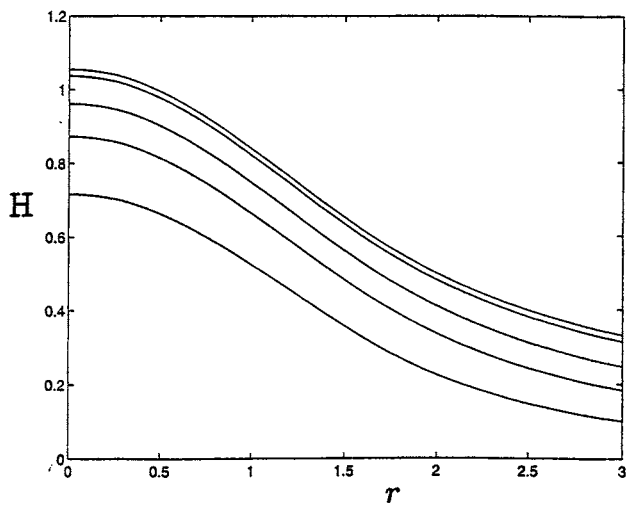

Fig. 3. The Yukawa screening potentials $H = H^{Yukawa}_{Om.\,CSA}(r)/Z^2/\Gamma$ as function of r for different values of α (from top to bottom $\alpha = 0.002, 0.02, 0.1, 0.2, 0.4$). For $\alpha = 0$, the function is equal to the original CSA result[9] for the Coulomb potential. Recall from Eq. (42) that $H = e^{-\alpha r}/r$ for $r \geqslant 2$. See the text.

It is instructive to make connection with Jancovici's original exact method. Using (33) and (31) we can rewrite (46) in the form

$$h_1^{Yukawa}(\alpha) = \left(\frac{\alpha^2}{3R_m} u_0(\alpha R_m)\right) = \frac{\alpha^2}{4} \int_0^\infty r g_{PY}(r)\, e^{-\alpha r}\, dr$$

$$= \frac{1}{4} + \frac{\alpha^2}{4} \int_0^\infty r[g_{PY}(r) - 1]\, e^{-\alpha r}\, dr \tag{51}$$

where $g_{PY}(r)$ is the limit $\eta = 1$ of the solution of the Percus–Yevick equation for the pair correlation function between an impurity of radius R_m, given by $R_m^3 = 2Q(\alpha R_m)/Q(\alpha)$, at the origin and a fluid particle of a hard sphere fluid with spheres of radius $R_a = 1$. According to the general asymptotic strong coupling relation between the Onsager Molecule result and fluid energy integrals, this indicates the following exact result, which can be obtained by following Jancovici's method:

$$h_1^{Yukawa}(\alpha) = \frac{1}{4} + \frac{\alpha^2}{4} \int_0^\infty r[g_\alpha(r) - 1]\, e^{-\alpha r}\, dr \tag{52}$$

Here $g_\alpha(r)$ is the pair correlation between an impurity with charge $2Ze$ at the origin and a charge Ze at r in a Yukawa OCP of charge Ze. Indeed,

this exact result can be obtained by following Jancovici's method. In the limit, the above integral goes to its Coulomb counterpart obtained by replacing $g_\alpha(r)$ by $g_0(r)$ computed with pure Coulomb interactions, for which the asymptotic fluid Madelung term is given by,[36, 20]

$$\lim_{\Gamma\to\infty}\int_0^\infty r[\,g_0(r)-1\,]\,e^{-\alpha r}\,dr=-\left(\frac{5\cdot 2^{2/3}+1}{10}\right) \tag{53}$$

so that we recover the expansion (49).

V. SCALING PROPERTIES FOR THE SCREENING POTENTIALS OF YUKAWA MIXTURES

The screening potential between two identical ions, each of charge Z_i, in the general mixture is obtained by a simple generalization of Eq. (41):

$$\frac{H^{Yukawa}_{OM,\,CSA,\,ii}(r)}{\Gamma}=2\frac{Z_i^2}{R_i}u_0(\alpha R_i)-\frac{2Z_i^2}{R_m}u_0(\alpha R_m)$$
$$+\frac{Z_i^2}{R_m}\psi\left(\frac{r}{R_m},\alpha R_m\right)-\frac{Z_i^2}{R_m}A(\alpha R_m)\left(\frac{R_m^3\,Q(\alpha R_i)}{R_i^3\,Q(\alpha R_m)}-1\right) \tag{54}$$

where the R_i are obtained from Eqs. (30), and where R_m is obtained from

$$R_m^3=R_i^3\frac{Q(\alpha R_m)}{Q(\alpha R_i)}\left[\,1+\frac{\alpha R_m^3}{6Q(\alpha R_m)\,Q'(\alpha R_m)}\frac{\partial}{\partial R_m}\left(\frac{1}{R_m}\psi\left(\frac{r}{R_m},\alpha R_m\right)\right)\right] \tag{55}$$

From either the convolution smearing approximation or from the exact small-r solution of the confined molecule linearized Thomas–Fermi equations (corresponding to the exact Onsager molecules), we obtain the following small-r expansion for the general Yukawa plasma mixture:

$$\frac{H^{Yukawa}_{OM,\,ij}(r)}{\Gamma}=\left(\frac{Z_i^2}{R_i}u_0(\alpha R_i)+\frac{Z_j^2}{R_j}u_0(\alpha R_j)-\frac{(Z_i+Z_j)^2}{R_{i+j}}u_0(\alpha R_{i+j})\right)$$
$$-\frac{Z_iZ_j}{R_{i+j}^3}\left(\frac{(\alpha R_{i+j})^2}{3}u_0(\alpha R_{i+j})\right)r^2+\cdots \tag{56}$$

where

$$R_{i+j}^3=R_i^3\frac{(Z_i+Z_j)\,Q(\alpha R_{i+j})}{Z_iQ(\alpha R_i)} \tag{57}$$

Like their Coulomb counterparts, the Yukawa Onsager molecules as defined have the property to "dissociate" when the distance between the two point charges is larger than $R_i + R_j$, i.e.,

$$u_{OM,ij}^{Yukawa}(r) = u_{OA,i}^{Yukawa} + u_{OA,j}^{Yukawa} \quad \text{for} \quad r \geqslant R_i + R_j \tag{58}$$

$$\frac{H_{OM,ij}^{Yukawa}(r)}{\Gamma} = Z_i Z_j \frac{e^{-\alpha r}}{r} \quad \text{for} \quad r \geqslant R_i + R_j \tag{59}$$

The continuity of the function $H_{OM,ij}^{Yukawa}(r)$ and its first derivatives implies that near "dissociation" a few-term Taylor series expansion of $H_{OM,ij}^{Yukawa}(r)$ around $r = R_i + R_j$ (using the above Yukawa functional form for $H_{OM,ij}^{Yukawa}$ $(r \geqslant R_i + R_j)$) will provide a good estimate of the function. The Onsager Molecule results show the relevance of two different lengths: $d_{ij} = R_i + R_j/2$ which is the "dissociation" radius, and R_{i+j} which is the radius of the molecule at small values of r (for the Coulomb potential $R_{i+j} = (R_i^3 + R_j^3)^{1/3}$). We need to consider separately the cases of "like" $(i = j)$ and "unlike" $(i \neq j)$ ions. For "like" $(i = j)$ ions, $d_{ii} = R_i$ by definition, and the Onsager-molecule screening potentials for the Coulomb plasma obey $H_{OM,ii}(r) = Z_i^2/R_i H_{OM}(r/R_i)$. For "unlike" $(i \neq j)$ ions there is a cross-over of the relevant scaling length, as r changes from "dissociation" to "zero separation," between d_{ij} and R_{i+j}.

At zero separation the expansion in powers of α takes the form[20]

$$\frac{H_{OM,ij}^{Yukawa}(0)}{\Gamma} = -\frac{9}{10}\left(\frac{Z_i^2}{R_i} + \frac{Z_j^2}{R_j} - \frac{Z_{i+j}^2}{R_{i+j}}\right) - Z_i Z_j \alpha$$
$$- \frac{18}{175}\alpha^2 (Z_i^2 R_i + Z_j^2 R_j - (Z_i + Z_j)^2 R_{i+j}) + \cdots \tag{60}$$

which for the one-component system is:

$$\frac{H_{OM}^{Yukawa}(0)}{\Gamma} = -\frac{9}{10}(2 - 2^{5/3}) - \alpha$$
$$+ \left(\frac{18}{175}(2^{7/3} - 2) + \frac{3}{100}(2^{7/3} - 2^{5/3})\right)\alpha^2 + \cdots$$
$$= 1.05732 - \alpha + 0.36860\alpha^2 + \cdots \tag{61}$$

Note however that in the physics context of the linear response for electron screening, the bare interaction between the ions is Coulomb, and the Yukawa potential is just a "device" in order to get the correct pair

correlation function between the ions in the system. Thus,[17, 20, 21] the interionic screening potential for a pair of ions in the electron screened plasma, is an even function of α:

$$H_{ij}^{interionic}(r) = H_{ij}^{Yukawa}(r) + \frac{1}{k_B T}(\phi_{ij}^{C}(r) - \phi_{ij}^{Y}(r))$$
$$= H_{ij}^{Yukawa}(0) + Z_i Z_j \Gamma \alpha + \cdots \tag{62}$$

For the one component system in the strong coupling limit it takes the form (recall the expansion (47)):

$$\frac{H_{OM}^{interionic}(r)}{\Gamma} = (1.05732 + 0.36860\alpha^2 + \cdots) - \frac{1}{2}\alpha^2 r$$
$$-\left(\frac{1}{2R^3} - \frac{9}{10R}\alpha^2 - \frac{18}{175}\alpha^4 R^2 + \cdots\right) r^2 + \cdots \tag{63}$$

where R is obtained from the solution of

$$R^3 = \frac{2Q(\alpha R}{Q(\alpha)} \tag{64}$$

and thus

$$\frac{H_{OM}^{interionic}(r)}{\Gamma} = (1.05732 + 0.36860\alpha^2 + \cdots)$$
$$-\frac{1}{2}\alpha^2 r - (0.25 - 0.22343\alpha^2 + \cdots) r^2 + \cdots \tag{65}$$

$H_{OM}^{interionic}(r)$ is obtained automatically[17, 20, 21] when the confined-atom and confined-molecule linearized Thomas–Fermi treatment is employed in order to obtain the Onsager energy bounds, because that approach already includes the linear-response approximation which is the physical way to define a Yukawa effective potential between the ions in the electron-screened plasma. We note from Eq. (63) that the first effect of electron screening on $H(r)$ is to introduce a linear term in its short distance form. In the limit $\alpha \to 0$ we get $R^3 = 2$ so that we recover the Coulomb result, $H_{OM}(r) = \frac{9}{10}(2^{5/3} - 2) - \frac{1}{2}r^2 + \cdots$, featuring the ion-sphere value for $r = 0$ and the exact Jancovici coefficient.

In summary, we have estimated the function $H(r)$ by a difference of the form $F_2 - F_1$ by using lower bounds for F_2 and F_1, $F_2 > A_2$ and $F_1 > A_1$. The replacement of $F_2 - F_1$ by $A_2 - A_1$ is not justified in general.

Here, however, each lower bound represents the leading term (a fluid Madelung constant) in an asymptotic strong coupling $\Gamma \to \infty$ expansion[36] for the excess (over ideal gas) free energy of a classical Coulomb or Yukawa fluid. In the region of validity of the linear response treatment, namely $\alpha < \sim 0.5$, these lower bounds are expected to be close to the quantities of interest in strong coupling (in particular, the fluid Madelung constant is close to the lattice Madelung constant; e.g., for the Coulomb OCP the ion-sphere result of -0.9 is close to the bcc value of -0.895929). Thus, for weak screening the present estimates for $H(r)$ in strong coupling should be accurate. As the value of α increases, the fluid Madelung constants as given by the Onsager bounds deviate more from the lattice Madelung constants of close packed structures, and the present estimates in strong coupling become less accurate. In general, the Onsager molecule approximation entirely mises the oscilating structure of $H(r)$ at large distances, which has to be incorporated by terms beyond the leading Madelung terms.[36] $H(r)$ for arbitrary r, Γ, and α can be obtained numerically very accurately from a recently introduced density-functional approximation for pair correlations in uniform classical fluids.[37] The availability of the analytic Onsager molecule results greatly facilitates the solution of the density-functional integral equation.[38]

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