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On the validity of perturbative treatments for the static screening in a charged-boson gas

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Abstract. The static screening of an external charged particle in a three-dimensional charged-boson gas is investigated by employing two different procedures. Both procedures satisfy the Kato–Kimball cusp condition and the proper normalization of induced densities. Self-consistent quadratic response solutions for the induced density and associated screened potential are presented. The solutions, obtained by successive approximations for an integral equation and via perturbative approximations for an integro-differential equation, are compared and analysed. The convergence condition for successive approximations in infinite order is deduced.

1. Introduction

The goal of the research to be described here is to compare perturbative solutions for two well-established procedures for screening calculations, treating the case of a fixed-charge impurity in an ideal, charged-boson gas at $T = 0$. The procedures are based on the Euler equation of density functional theory [1–3] and the density profile relation given by an integral equation [4, 5]. Because of the difference between the two methods, it is useful to compare the results that one obtains.

The perturbative solutions, obtained here up to quadratic order in the external charge Z for the induced densities and screened potentials, allow a valuable investigation to be made via comparison of the results with rigorous, procedure-independent constraints. Furthermore, the solutions provide useful insight into the important question of convergence, and may extend the range of validity of the standard linear screening theory. Clearly, one needs to know the quadratic response at least, in order to see how good the linear response is.

The system of point-like charged bosons embedded in a neutralizing background at $T = 0$ has attracted attention in recent years as an important reference system of quantum statistics with possible application to superconductors, and to systems of astrophysical interest (see references [6, 7] and earlier references cited therein). The charged-boson gas offers a relatively simple many-body model for the above-mentioned problem of screening, and thus parallels the physically more significant system of electrons for the same problem [8–10]. Parallel theoretical efforts on bosons and fermions may be helpful in disentangling the effects of screening due to the Coulomb interaction and those due to the exclusion principle.

The paper is organized as follows. In section 2 we outline the two procedures to be employed. The quadratic approximations are defined there. We summarize rigorous

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constraints for the impurity case. In section 3 our results for the induced densities and potentials are presented and analysed. Section 4 is devoted to a summary and some concluding remarks. The paper ends with a short appendix. We use atomic units ($e^2 = \hbar = m = 1$) throughout this work.

2. Procedures and constraints

The ideal gas of charged boson particles (of mass m and charge e) is characterized by the density parameter r_s which is related to the unperturbed number density n_0 by $r_s = (3/4\pi n_0)^{1/3}$. The ground-state wave-function (ψ_0) of the system is a unique, non-negative symmetric function [11] and, in our case, it is given by $\psi_0 = \sqrt{n_0}$.

Now, suppose we place a charged test particle of mass $M \gg m$ in the many-body system. Then, the total boson density depends on the position $\boldsymbol{r}$ and can be written as

$$n(\boldsymbol{r}) = n_0 + \delta n(\boldsymbol{r}) \tag{2.1}$$

where the induced density ($\delta n(\boldsymbol{r})$) satisfies the screening, i.e. normalization, condition

$$\int \mathrm{d}^3\boldsymbol{r}\, \delta n(\boldsymbol{r}) = Z. \tag{2.2}$$

The spherically symmetric, screened potential ($V(r)$) of the charged impurity is calculated, in our self-consistent treatment, by using the Poisson equation

$$V(r) = -\frac{Z}{r} + \int \mathrm{d}^3\boldsymbol{r}'\, \frac{\delta n(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|}. \tag{2.3}$$

In the first procedure, we consider, according to the Hohenberg–Kohn theorem, the fundamental energy functional for jellium in the presence of a charged test particle. The Euler equation of this variational problem becomes [1–3]

$$-\frac{1}{2}\nabla^2\omega(r) + V(r)[\psi_0 + \omega(r)] = 0 \tag{2.4}$$

in which the convenient notation $\sqrt{n(r)} \equiv \psi(r) = \psi_0 + \omega(r)$ is introduced. Notice that the value of the chemical potential (μ_0), i.e. the Lagrange multiplier, is fixed as $\mu_0 = 0$, for the ideal gas at $T = 0$. This ground-state method gives for equation (2.4), by using equations (2.2) and (2.3) with the appropriate expression $\delta n(r) = 2\psi_0\omega(r) + \omega^2(r)$, a non-linear Schrödinger equation. Generally, the solution of this equation requires an iterative method. Furthermore, an investigation of the short-distance limit of equation (2.4) results in a useful constraint, which is known as the Kato–Kimball nuclear cusp condition [12, 13]:

$$\left.\frac{\delta n'(r)}{n(r)}\right|_{r=0} = -2Z. \tag{2.5}$$

Our quadratic treatment rests on a perturbative expansion, which is defined as follows:

$$\psi(r) = \psi_0 + \psi_1(r, Z) + \psi_2(r, Z^2) + \cdots \tag{2.6}$$

for the ground-state wave-function. Using this notation, the relevant contributions ($n_1(r, Z)$ and $n_2(r, Z^2)$) to the induced density $\delta n(r) = n_1(r, Z) + n_2(r, Z^2) + \cdots$ can be written as

$$n_1(r, Z) = 2\psi_0\psi_1(r, Z) \tag{2.7a}$$

$$n_2(r, Z^2) = 2\psi_0\psi_2(r, Z^2) + \psi_1^2(r, Z). \tag{2.7b}$$

For simplicity, from now on, only the indices (1 and 2) will be used to indicate first- and second-order expansions. The screened potential is defined as $V(r) = V_1(r) + V_2(r)$ in the quadratic approach, and the corresponding expressions are given by

$$V_1(r) = -\frac{Z}{r} + \int \mathrm{d}^3\boldsymbol{r}' \, \frac{n_1(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} \tag{2.8a}$$

$$V_2(r) = \int \mathrm{d}^3\boldsymbol{r}' \, \frac{n_2(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|}. \tag{2.8b}$$

In equations (2.7*a*), (2.7*b*) and (2.8*a*), (2.8*b*) the solutions $\psi_1(r), n_1(r)$ and $\psi_2(r), n_2(r)$ are the results from solving coupled equations, by using equation (2.4) up to the relevant order:

$$-\frac{1}{2}\nabla^2\psi_1(r) + V_1(r)\psi_0(r) = 0 \tag{2.9a}$$

$$-\frac{1}{2}\nabla^2\psi_2(r) + V_2(r)\psi_0 + V_1(r)\psi_1(r) = 0. \tag{2.9b}$$

Notice that equation (2.9*a*) with equations (2.7*a*) and (2.8*a*) gives the self-consistent linear response solution.

In the second procedure to be employed, we consider a density profile relation [5] given in the form of an integral equation, in Fourier-momentum (q-) space. This method is not based on the variational principle for the ground-state energy. It uses an *ansatz* [4, 14] for the effective, screened interaction. The linear integral equation is as follows, for an ideal boson system [4, 5]:

$$\delta n(q) = n_1(q)\left[1 + \frac{1}{\pi\omega_p^2}\int_0^\infty \mathrm{d}k \; k^2 f(k,q)\,\delta n(k)\right] \tag{2.10}$$

where $\omega_p^2 = 4\pi n_0$ is the classical plasma frequency, and the function $f(k,q)$ has the form

$$f(k,q) = 1 + \frac{q^2 - k^2}{2qk}\ln\left|\frac{q+k}{q-k}\right|. \tag{2.11}$$

Notice that in equation (2.10) $n_1(q)$ is the linear response solution, outlined at the end of the preceding paragraph. This linear response solution is unique for our procedures and has the asymptotic form (see section 3, below) $n_1(q) \to Z(16\pi n_0)/q^4$ for high q-values.

Using this together with the well-established relation of Kimball [13]

$$\delta n'(r)\big|_{r=0} = -\frac{1}{8\pi}\lim_{q\to\infty}[q^4\,\delta n(q)] \tag{2.12}$$

we arrive (via equations (2.10)–(2.11) and the trick of inverse Fourier representation with $r \to 0$ in the argument of equation (2.10)) at the standard Kato condition of equation (2.5). Therefore, the nuclear cusp condition is satisfied in the integral-equation procedure. Generally, the solution of equation (2.10) requires an iterative method. Our quadratic treatment, for this case, rests on a successive approximation for equation (2.10), using $n_1(q)$ under the integral sign in order to define the corresponding second-order solution of this procedure.

In the following, we formulate a ground-state energy constraint. According to earlier results, the exact energy change ($\Delta E = E(n, Z) - E(n_0)$) due to the presence of a charged impurity is given by

$$\Delta E = n_0[V_1(q=0) + V_2(q=0)] - \frac{1}{2}\int \frac{\mathrm{d}^3\boldsymbol{q}}{(2\pi)^3}\,|V_1(q)|^2\chi^0(q) \tag{2.13}$$

for our ideal boson system ($E(n_0) = n_0\mu_0 = 0$) up to quadratic order [15]. Here $V_1(q)$ and $V_2(q)$ are the Fourier transforms of $V_1(r)$ and $V_2(r)$, and $\chi^0(q)$ is the static, non-interacting response function (see reference [16] and section 3, below).

3. Results

The present section will be devoted to detailed analytical results, with relevant comparisons and accompanying analysis. For convenience, we introduce new variables (R and Q) via the definitions $R = r\lambda$ and $Q = q/\lambda$, where $\lambda = (4\pi n_0)^{1/4}$. In addition, in order to distinguish quadratic solutions, we shall use (beside the index 2) an asterisk for results obtained from the integral equation (n_2^* and V_2^*).

The linear response solution, which is unique in both procedures, is defined by equations (2.8*a*)–(2.9*a*). The linearized, Schrödinger-like equation (2.9*a*) is solved by standard Fourier transformation and the results obtained are

$$n_1(Q) = 4Z\frac{1}{Q^4+4} \tag{3.1}$$

$$V_1(Q) = -\frac{4\pi Z}{\lambda^2}\frac{Q^2}{Q^4+4} \tag{3.2}$$

in which the above-introduced variables are used. The ratio of $v(q) = -4\pi Z/q^2$ and $V_1(q)$ gives us the usual dielectric function

$$\epsilon(q) = 1 + \frac{4\lambda^4}{q^4} \equiv 1 + \frac{4\pi}{q^2}\chi^0(q) \tag{3.3}$$

of the boson system. The density response function $\chi^0(q)$ is needed in equation (2.13) for energy calculation, at the quadratic order of approximation.

The real-space equivalents of equations (3.1) and (3.2) are calculated by inverse Fourier transformations and have the following forms:

$$n_1(R) = \frac{Z\lambda^3}{2\pi}\frac{\mathrm{e}^{-R}}{R}\sin R \tag{3.4}$$

$$V_1(R) = -Z\lambda\frac{\mathrm{e}^{-R}}{R}\cos R. \tag{3.5}$$

The ratio $n_1(R=0)/n_0 = 2(Z/\lambda)$ shows that the natural expansion (small) parameter in our treatment is, in fact, Z/λ. The ratio suggests, for the case of a negative impurity ($Z < 0$), a physical estimate for the validity range ($|Z/\lambda| < 0.5$) of the solution, due to the obvious $|\delta n(r=0)/n_0| < 1$ constraint. For a positive impurity ($Z > 0$), the appearance of a bound state in a screened potential may signal the validity limit for its perturbative solution. This useful constraint provides [17] the $\lambda/Z > 0.72$ value for the applicability of the form of $V_1(r)$. By using the $\lambda^4 = 3/r_s^3$ representation, one can estimate the corresponding values of the density parameter r_s. According to expectation, the validity of the perturbative solutions is restricted to high densities ($n_0 \sim \lambda^4$) even for the smallest, physical $|Z| = 1$. Finally, from equation (3.5) we can subtract the value of the first-order induced potential ($\phi_1(R) = V_1(R) + (Z\lambda/R)$) at the origin; $\phi_1(r=0) = Z\lambda$ at fixed λ.

Now, we present our quadratic solutions obtained within the frameworks of the procedures applied. Equation (2.9*b*) is solved with the help of Fourier transformation into momentum (q-) space and simultaneous application of equations (2.8*b*), (3.4), (3.5) and (2.7*a*). The result for the induced density ($n_2(q)$) is given, in this case, by

$$n_2(Q) = n_1(Q)\frac{Z}{8\lambda}\left[Q\ln\frac{4+(Q+2)^2}{4+(Q-2)^2} + Q^3\left(\arctan\frac{Q}{2} + \frac{1}{2}\arctan\frac{2-Q}{2} - \frac{1}{2}\arctan\frac{2+Q}{2}\right)\right] \tag{3.6}$$

in which $n_1(Q)$ is given by equation (3.1) and the introduced variable $Q = q/\lambda$ is used. The quadratic, induced potential (see equation (2.8*b*)) has the simple form $V_2(q) = (4\pi/q^2)n_2(q)$.

The corresponding result for the integral-equation procedure is as follows:

$$n_2^*(Q) = n_1(Q)\frac{Z}{\lambda}\left[1 + \frac{Q}{4}\ln\left|\frac{Q^2+2+2Q}{Q^2+2-2Q}\right| + \frac{1}{2Q}\arctan\frac{4Q(Q^2-2)}{(Q^2-2)^2-4Q^2} - \frac{\theta(Q-(\sqrt{3}-1))\pi}{2Q} - \frac{\theta(Q-(\sqrt{3}+1))\pi}{2Q}\right]. \tag{3.7}$$

This equation is obtained by using equation (3.1) in the argument ($q = \lambda Q$) of equation (2.10) and standard application of the residue theorem for integration in the latter. The quadratic, induced potential of this successive approximation is $V_2^*(q) = (4\pi/q^2)n_2^*(q)$.

It is very instructive to discuss the asymptotic limits, on the basis of equations (3.6) and (3.7), for quadratic, induced densities and associated potentials. The high-q limits of these equations are the same: $n_2(q \to \infty) = n_2^*(q \to \infty) \to 8Z^2\lambda^3/q^4$. This is in accordance with the relevant cusp constraint (see equations (2.5) and (2.12)) in a perturbative approximation for the density $n(r) = n_0 + \delta n(r) = n_0 + n_1(r) + n_2(r) + \cdots$. The low-$q$ limits are different, i.e., $n_2(q \to 0) \to q^2(Z^2/8\lambda^3)$ and $n_2^*(q \to 0) \to q^2(Z^2/3\lambda^3)$ respectively; therefore the associated induced potentials become different (see equation (2.13)) in the forward ($q = 0$) direction.

Next, we evaluate equation (2.13) by using equations (3.2), (3.3), (3.6) and (3.7). The integral in equation (2.13) has the value of $-(Z^2\lambda/8)$; therefore one obtains

$$\Delta E = n_0 V_2(q=0) - \frac{Z^2\lambda}{8} = \frac{Z^2\lambda}{8} - \frac{Z^2\lambda}{8} = 0 \tag{3.8a}$$

$$\Delta E^* = n_0 V_2^*(q=0) - \frac{Z^2\lambda}{8} = \frac{Z^2\lambda}{3} - \frac{Z^2\lambda}{8} > 0. \tag{3.8b}$$

Consequently, up to this quadratic order, the procedure based on the Euler equation of ground-state density functional theory, and giving equation (3.8*a*), is superior to the integral-equation procedure which results in equation (3.8*b*).

We performed numerical, inverse Fourier transformations in order to obtain the real-space equivalents of the induced quadratic densities and potentials. This calculation gives, for the important ratios (at $r = 0$) of the densities,

$$n_2(0)/n_1(0) \simeq n_2^*(0)/n_1(0) \simeq Z/\lambda$$

by using equation (3.4), also. We note that $V_2(R=0)$ and $V_2^*(R=0)$ do not depend on the density (remember, $\phi_1(R=0) = Z\lambda$). A similar fact was established for the electron gas model at lower densities (see figure 5 in reference [10]). The density ratios show that (as was stated earlier in this paper) the expansion (small) parameter in the perturbative methods for the charged-boson system is $\sim Z/\lambda$. In the appendix the convergence condition for successive approximations, in infinite order for the integral-equation procedure, is deduced.

4. Summary

The interaction of an external charged particle with a charged-boson gas has been investigated by using two non-linear procedures for static screening. Quadratic response solutions for the induced density and associated screened potential are presented, compared and analysed. The method based on the Euler equation of the variational ground-state theorem is shown to be superior to the one based on the integral equation. We have determined a rigorous mathematical expression for the convergence condition for self-consistent perturbative approximations for

the case of the inhomogeneous, linear integral equation. A condition of similar rigour for the case of the non-linear Schrödinger equation remains an interesting open question.

It is found, by detailed physical considerations, that the perturbative approximations might be useful for small values of the expansion parameter Z/λ of the present problem. The results obtained are applicable, therefore, to high-density systems even for the physically smallest $|Z| = 1$ external charge.

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Appendix

We rewrite equation (2.10) using equation (3.1) via the usual variables $x = q/\lambda$ and $y = k/\lambda$. Next, we multiply the resulting equation by x^2 and introduce the functions $F(x)$, $\Phi(x)$ ($F(x)$ for the free term, $\Phi(x)$ for the unknown function) and the kernel $K(x, y)$ as follows:

$$F(x) = \frac{4Zx^2}{x^4 + 4} \tag{A.1}$$

$$\Phi(x) = x^2\,\delta n(x) \tag{A.2}$$

$$K(x, y) = F(x)\left\{1 + \frac{x^2 - y^2}{2xy}\ln\left|\frac{x + y}{x - y}\right|\right\}. \tag{A.3}$$

Using this notation, we can write the original inhomogeneous, linear integral equation in the transparent and usual form

$$\Phi(x) = F(x) + \Lambda\int_0^\infty \mathrm{d}y\; K(x, y)\Phi(y) \tag{A.4}$$

where the parameter (Λ) of this equation is $\Lambda = (\pi\lambda)^{-1}$.

The Neumann series expansion for equation (A.4) is defined by standard successive approximations. These successive approximations converge uniformly [18] to the limit (unique) solution for all values of $\Lambda < R$, where the radius R is defined by

$$R^{-2} = \int_0^\infty \mathrm{d}x\int_0^\infty \mathrm{d}y\,[K(x, y)]^2. \tag{A.5}$$

By performing the integrations, and taking into account the convergence constraint, we can give for our natural expansion parameter the following final form:

$$\frac{|Z|}{\lambda} < 0.98. \tag{A.6}$$

Therefore, successive approximations, even in infinite order, as discussed in this appendix, are restricted to systems with small charges or high densities ($\lambda \sim n_0^{1/4}$); this is in agreement with our statements based on more physical grounds.

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