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Non-perturbative density expansions for extended Coulomb systems

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Abstract. We present a general non-perturbative argument that combines the Pauli and virial theorems for a multicomponent translationally invariant Coulombic system of fermions at zero temperature, and which by an iteration procedure leads to a series in r_s representing the total energy per particle. It agrees with the form found for the ground state of an electron gas in a uniform positive background by diagrammatic perturbation theory, but is shown to be valid for more general (translationally invariant) multicomponent Coulombic systems as well. Several modifications of the method are also discussed, one of them being applied to a low-density single-component system with inhomogeneous states; it yields the expected result for a harmonic Wigner crystal and a rigorous proof that this state (or any other state with harmonic excitations) must be an insulator.

1. Introduction

Universal scaling properties for thermodynamic and structure functions for neutral multicomponent systems of charged point particles were earlier presented [1] and shown to be useful for obtaining accurate analytical expressions for the ground-state energy of dense hydrogen by scaling from known electron-gas results. Modifications of such scaling properties in the presence of a magnetic vector potential were later studied [2] and proved to be useful for the description of possible metal–insulator transitions. More recently, a procedure based on scaling and an appropriate limiting process involving an infinite division of charge and mass was also given [3] and shown to provide further insight into several aspects of a general many-body system with charged components.

We present here a different non-perturbative process, based on scaling and an appropriate discretization and iteration procedure that leads to a series expansion of the ground-state energy of a multicomponent system with charged components in powers of the density parameter r_s . We demonstrate the generality of the result, and briefly comment on some interesting extensions to shorter-range interactions, to non-vanishing temperature, and to the presence of a magnetic vector potential. A modification to inhomogeneous states is also given that, for the special case of a single component, yields the familiar $r_s^{-3/2}$ -term of a harmonic Wigner crystal as a result of very general principles. A further modification in the presence of a magnetic vector potential provides a rigorous proof that such a harmonic state is an insulator.

2. The system

Let us consider a neutral system of N positive charges (Ze) with mass m_p and ZN negative charges ($-e$) with mass m_e (considered as point particles) in volume V . Examples might be

hydrogen [4] or muonium, or electrons and holes [5]. We work with protons from now on ($Z = 1$), although a generalization to arbitrary Z is rather straightforward. Omitting relativistic corrections, the Hamiltonian of this system is

$$H = \sum_{i=1}^N \frac{p_{i,e}^2}{2m_e} + \sum_{i=1}^N \frac{p_{i,p}^2}{2m_p} + \frac{1}{2} \sum_i \sum_{j \neq i} \frac{e^2}{|\vec{r}_{i,e} - \vec{r}_{j,e}|} + \frac{1}{2} \sum_i \sum_{j \neq i} \frac{e^2}{|\vec{r}_{i,p} - \vec{r}_{j,p}|} - \sum_i \sum_j \frac{e^2}{|\vec{r}_{i,e} - \vec{r}_{j,p}|}. \quad (1)$$

We immediately rescale all variables using

$$V = N \frac{4}{3} \pi r_0^3 \quad r_s = \frac{r_0}{a} \quad a = \frac{\hbar^2}{\bar{m}e^2} = \frac{M}{m_p} a_0 \\ M = m_e + m_p \quad \bar{m} = \frac{m_e m_p}{M}$$

and

$$V = \bar{V} r_0^3 \quad \vec{r}_e = r_0 \vec{r}_e \quad \vec{r}_p = r_0 \vec{r}_p \quad \vec{p}_e = \hbar \vec{p}_e / r_0 \quad \vec{p}_p = \hbar \vec{p}_p / r_0.$$

Equation (1) then reads

$$H = \frac{e^2}{2a} \frac{1}{r_s^2} \left\{ \frac{m_p}{M} \sum_{i=1}^N \bar{p}_{i,e}^2 + \frac{m_e}{M} \sum_{i=1}^N \bar{p}_{i,p}^2 + r_s \sum_i \sum_{j \neq i} \frac{1}{|\vec{r}_{i,e} - \vec{r}_{j,e}|} + r_s \sum_i \sum_{j \neq i} \frac{1}{|\vec{r}_{i,p} - \vec{r}_{j,p}|} - 2r_s \sum_i \sum_j \frac{1}{|\vec{r}_{i,e} - \vec{r}_{j,p}|} \right\} \equiv T_e + T_p + U \quad (2)$$

where T_e and T_p are electron and proton kinetic energies, and U denotes the sum of all interactions.

Applying the Hellmann–Feynman theorem (HFT) with respect to r_s , namely

$$\frac{\partial \langle \Psi | H | \Psi \rangle}{\partial r_s} = \langle \Psi | \partial H / \partial r_s | \Psi \rangle \quad (3)$$

where $H|\Psi\rangle = E|\Psi\rangle$ †, together with the definition of pressure at zero temperature, gives

$$P = - \left(\frac{\partial \langle H \rangle}{\partial V} \right)_N = - \frac{r_s}{3V} \left(\left\langle \frac{\partial H}{\partial r_s} \right\rangle \right)_N = - \frac{r_s}{3V} \left(- \frac{2\langle T \rangle}{r_s} - \frac{\langle U \rangle}{r_s} \right) \quad (4)$$

and hence

$$3PV = 2\langle T \rangle + \langle U \rangle \quad (5)$$

which is the virial theorem (VT) [6]. (T is the total-kinetic-energy operator $T \equiv T_e + T_p$.)

If we also introduce a coupling constant λ in the Hamiltonian

$$H = T + \lambda U \quad (6)$$

(eventually $\lambda = 1$), the HFT with respect to λ gives the Pauli theorem (PT), namely

$$\frac{\partial \langle H \rangle_\lambda}{\partial \lambda} = \left\langle \frac{\partial H}{\partial \lambda} \right\rangle_\lambda = \langle U \rangle_\lambda \equiv U_\lambda. \quad (7)$$

Correspondingly the VT is now modified to read

$$3P_\lambda V = 2T_\lambda + \lambda U_\lambda. \quad (8)$$

† Equation (3) is equivalent to having $|\Psi\rangle$ normalized.

Combination of (7) and (8) with $E_\lambda = T_\lambda + \lambda U_\lambda$ yields

$$\lambda \frac{\partial E_\lambda}{\partial \lambda} = 2E_\lambda - 3P_\lambda V \quad (9)$$

which together with

$$P_\lambda = -\frac{r_s}{3V} \frac{\partial E_\lambda}{\partial r_s} \quad (10)$$

gives

$$r_s \frac{\partial E_\lambda}{\partial r_s} - \lambda \frac{\partial E_\lambda}{\partial \lambda} = -2E_\lambda \quad (11)$$

which is an exact partial differential equation for the internal energy at coupling strength λ . The general solution of this linear first-order partial differential equation is easily found to be in the scaling form

$$E_\lambda(r_s) = f(\lambda r_s) \lambda^2 \quad (12)$$

which agrees with the known solution for non-interacting fermions ($\lambda = 0$):

$$\frac{E_0}{N} = \frac{D}{r_s^2} = \frac{D\lambda^2}{(\lambda r_s)^2}$$

with $D \simeq 2.21(1 + m_e/m_p)$ Ryd, since λ should drop out of the expression in the limit $\lambda \rightarrow 0$.

On the other hand if we differentiate (9) with respect to r_s and assume that the mixed second derivatives of E_λ exist and are continuous[†], we get a corresponding equation for the pressure:

$$\lambda \frac{\partial P_\lambda}{\partial \lambda} - r_s \frac{\partial P_\lambda}{\partial r_s} = 5P_\lambda. \quad (13)$$

Its general solution has the form

$$P_\lambda(r_s) = g(\lambda r_s) \lambda^5 \quad (14)$$

with

$$g(\lambda r_s) = \frac{-f'(\lambda r_s)}{N4\pi a^3(\lambda r_s)^2}$$

which is also in accord with the non-interacting result for the pressure

$$P_0(r_s) = \frac{A}{r_s^5} \quad (15)$$

with $A = D/(2\pi a^3)$, since once again λ has to drop out of the result in the limit $\lambda \rightarrow 0$.

3. Iterative solution

For the purpose of extracting further information from (13), we now propose the following scheme: we partition λ into n infinitesimal pieces of magnitude b each ($\lambda = nb$) with the intention of taking an eventual limit, namely $n \rightarrow \infty$, $b \rightarrow 0$ such that $\lambda \rightarrow 1$. Accordingly we write

$$\lambda \frac{\partial P_\lambda}{\partial \lambda} = \frac{(P_{nb}(r_s) - P_{(n-1)b}(r_s))}{b} nb \quad (16)$$

and inserting this into (13) we must now solve an ordinary differential equation (ODE) for $P_{nb}(r_s)$ assuming that $P_{(n-1)b}(r_s)$ is a known function of r_s . But because we know its form

[†] This is essentially an assumption of no symmetry breaking.

for $n = 1$ (equation (15)), this generates an iteration procedure that gives the form of $P_{nb}(r_s)$ for any n (up to some undetermined integration constants resulting from the solutions of the ODEs). As we will see below, n will be the order of an expansion of the pressure in powers of b . It remains to take the limit $n \rightarrow \infty, b \rightarrow 0$ such that $nb \rightarrow 1$, in order to get the functional form of $P(r_s)$ of our actual physical system.

Applying this procedure, equations (16) and (13) give the ODE

$$r_s \frac{dP_{nb}}{dr_s} + (5 - n)P_{nb} = -nP_{(n-1)b} \quad (17)$$

which when multiplied by the factor r_s^{4-n} can be integrated to yield

$$P_{nb}(r_s) = \frac{-n}{r_s^{5-n}} \int P_{(n-1)b} r_s^{4-n} dr_s + \frac{\bar{C}_n}{r_s^{5-n}} \quad (18)$$

with \bar{C}_n some undetermined function of b . Starting from $n = 1$ and using (15) we get

$$P_b(r_s) = \frac{A}{r_s^5} + \frac{\bar{C}_1}{r_s^4}.$$

But by invoking the general form (14) of the solution, we have $\bar{C}_1 = bC_1$ where C_1 is a further undetermined constant. Similarly, repeating with (18) and invoking (14) at each level, we get

$$P_{2b} = \frac{A}{r_s^5} + \frac{(2b)C_1}{r_s^4} + \frac{(2b)^2 C_2}{r_s^3} \quad P_{3b} = \frac{A}{r_s^5} + \frac{(3b)C_1}{r_s^4} + \frac{\frac{4}{3}(3b)^2 C_2}{r_s^3} + \frac{(3b)^3 C_3}{r_s^2}$$

and so on.

By this means we generate a well-defined iteration procedure that simply renormalizes the constants except those of the first two terms. It is important to carry out this process up to $n \rightarrow \infty$ to ensure that the limiting values of the renormalized constants are actually finite. In fact it is not difficult to see by mathematical induction that the general result for any n can be written as

$$P_{nb}(r_s) = \frac{A}{r_s^5} + \sum_{k=1}^n \frac{B_n^{(k)} (nb)^k}{r_s^{5-k}} \quad (19)$$

with

$$B_n^{(k)} = \frac{k^{k-1}}{(k-1)!} \frac{(n-1)!}{(n-k)! n^{k-1}} C_k$$

where C_k is the undetermined constant that appears in the initial solution of the ODE at level $n = k$.

Now we let $n \rightarrow \infty, b \rightarrow 0$ in such a way that $nb \rightarrow 1$, as indicated above. In this limit,

$$B_n^{(k)} \rightarrow \frac{k^{k-1}}{(k-1)!} C_k$$

which is a finite number provided that C_k is finite. Finally,

$$P(r_s) = \frac{A}{r_s^5} + \frac{C_1}{r_s^4} + \frac{2C_2}{r_s^3} + \frac{\frac{9}{2}C_3}{r_s^2} + \frac{\frac{32}{3}C_4}{r_s} + \frac{625C_5}{24} + \dots = \frac{A}{r_s^5} + \sum_{k=1}^{\infty} \frac{k^{k-1} C_k}{(k-1)! r_s^{5-k}}. \quad (20)$$

For the ground state we can obtain the energy by integrating the pressure: from (10) we have

$$E_\lambda = NC'_\lambda - N4\pi a^3 \int P_\lambda(r_s) r_s^2 dr_s$$

which gives for the energy per particle in the neutral ensemble:

$$\frac{E_{nb}}{N} = 4\pi a^3 \left(\frac{A/2}{r_s^2} + \frac{C_1(nb)}{r_s} - 2C_2 \left(\frac{n-1}{n} \right) (nb)^2 \ln r_s - \sum_{k=3}^n \frac{B_n^{(k)}(nb)^k}{k-2} r_s^{k-2} + \frac{C_b(nb)^2}{4\pi a^3} \right) \quad (21)$$

where C_b must be of the form

$$C - 2C_2 \frac{n-1}{n} 4\pi a^3 \ln(nb)$$

with C a constant in order to comply with (12). Taking the limit $n \rightarrow \infty$, $b \rightarrow 0$ such that $nb \rightarrow 1$ gives the final form for the ground-state energy, namely

$$\frac{E(r_s)}{N} = 2\pi a^3 \left(\frac{A}{r_s^2} + \frac{2C_1}{r_s} - 4C_2 \ln r_s - \sum_{k=3}^{\infty} \frac{2k^{k-1} C_k}{(k-1)!(k-2)} r_s^{k-2} + \frac{C}{2\pi a^3} \right). \quad (22)$$

The value of A is determined from the non-interacting ($\lambda = 0$) result of section 2 and is given by $2\pi a^3 A \simeq 2.21(1 + m_e/m_p)$ Ryd. The constants C_k and C are not determined by this process (some of them are known for the one-component electron gas and are given by $4\pi a^3 C_1 \simeq -0.916$ Ryd from exchange energy, and $C \simeq -0.094$ Ryd and $8\pi a^3 C_2 \simeq -0.0622$ Ryd from correlation energy). Nevertheless, this general argument gives the known functional form for the ground state of the one-component electron gas as determined by perturbation theory [7]. (Note that it also gives a *new reason* behind the appearance of the well-known logarithmic term in the energy, which is the $1/r_s^3$ term in the series expansion of the pressure.) Furthermore, it generalizes the so-called r_s -expansion to higher r_s and to any multicomponent Coulombic system of fermions (provided that translational symmetry is not broken). We should probably emphasize that the expressions (20) or (22) result solely from the form of the Hamiltonian and the assumption that there is no symmetry breaking as we increase λ from 0 to 1.

4. Harmonic Wigner crystal

In order to see how the above method can be used in the case of symmetry-broken states, let us follow an alternative route. If instead of (6) we set $H = \lambda T + U$, then the Pauli theorem now reads

$$\frac{\partial \langle H \rangle_\lambda}{\partial \lambda} = \left\langle \frac{\partial H}{\partial \lambda} \right\rangle_\lambda = \langle T \rangle_\lambda \equiv T_\lambda \quad (23)$$

and the virial theorem now takes the form

$$3P_\lambda V = 2\lambda T_\lambda + U_\lambda \quad (24)$$

as the analogue of (8). Combination then of (23) and (24) with $E_\lambda = \lambda T_\lambda + U_\lambda$ yields

$$2\lambda \frac{\partial E_\lambda}{\partial \lambda} = -2E_\lambda + 6P_\lambda V \quad (25)$$

as the analogue of (9), which if combined with (10) leads to the analogue of (11), namely

$$r_s \frac{\partial E_\lambda}{\partial r_s} + \lambda \frac{\partial E_\lambda}{\partial \lambda} = -E_\lambda \quad (26)$$

which is a new partial differential equation that is exact for symmetry-broken states. Its general solution is easily found to be in a new scaling form, namely

$$E_\lambda(r_s) = \frac{1}{r_s} f(\lambda/r_s) \quad (27)$$

which is seen to agree with the form of a Madelung energy (C/r_s with C a structure-dependent constant) in the limit $\lambda \rightarrow 0$ where interaction energy is the only contribution to the internal energy of the system. This is known to be the case for the single-component problem to which we now turn our attention.

Anticipating small oscillations around some equilibrium positions for small λ , let us now use a different form of the virial theorem that is rigorously valid for harmonic oscillator states: since the energy is equally partitioned into kinetic and potential energies, we must have the following additional virial relation:

$$\lambda T_\lambda = \frac{1}{2}(E_\lambda - E_{\lambda=0}) \quad (28)$$

which must be exact for small λ (or, equivalently due to (27), for large r_s). If this is combined with (23) and (26) it leads to the following ordinary differential equation for E_λ :

$$-E_\lambda - r_s \frac{\partial E_\lambda}{\partial r_s} = \frac{1}{2} \left(E_\lambda + \frac{C}{r_s} \right) \quad (29)$$

which has a general solution of the form

$$E_\lambda = -\frac{C}{r_s} + \frac{D\lambda^{1/2}}{r_s^{3/2}} \quad (30)$$

with C, D constants. Note that it gives the correct functional form of the first two terms in the expansion of the ground-state energy of a Wigner crystal in powers of r_s : the purely electrostatic r_s^{-1} -term (with C close to the spherical-cell approximation value of 1.8 Ryd), and most importantly the crucial $r_s^{-3/2}$ -term (that is equally divided into kinetic and potential contributions, and with $D \simeq 2.67$ Ryd).

We should also draw attention in passing to the importance of the use of a static and homogeneous magnetic vector potential $\vec{A} = A\hat{x}$ in problems where the location of a possible metal-insulator transition is of interest [2] (see also the next section). Let us here briefly give some results for when a vector potential \vec{A} is present. In such a case, the virial theorem (24) is generalized to the following exact relation for the ground state:

$$\frac{\partial}{\partial r_s} \left(\frac{E_\lambda}{N} \right) = -\frac{1}{r_s} \left(\frac{\lambda T_\lambda}{N} + \frac{E_\lambda}{N} \right) + \frac{1}{r_s} \frac{V}{N} \frac{1}{c} \vec{A} \cdot \vec{J}_\lambda \quad (31)$$

with the current density $\vec{J}_\lambda = J_\lambda \hat{x}$ given by [2]

$$J_\lambda = \frac{c}{V} \frac{\partial E_\lambda}{\partial A}. \quad (32)$$

It is then straightforward to see that substitution of (30) and (28) into (31) leads to the exact vanishing of the current density, which rigorously shows that a harmonic Wigner crystal is an insulator. This may have been expected, but it is here shown by means of very general (and non-local) scaling arguments and may actually apply to any inhomogeneous state of the charged system (such as a CDW, for example) that has harmonic excitations; mere scaling suggests that there *cannot* be any current in the system (not even through an overall sliding procedure).

5. Discussion

The procedures described in this work are generalizable to any kind of interactions although they are only useful for sufficiently long-ranged ones. For instance, if we go through the same

argument as in section 3 for interaction potentials of the form $1/r^\alpha$, we obtain a series of the form

$$\frac{E}{N} = C + \frac{A}{r_s^2} + \int \frac{\text{constant } dr_s}{r_s^{\alpha+1}} + \int \frac{\text{constant } dr_s}{r_s^{2\alpha-1}} + \int \frac{\text{constant } dr_s}{r_s^{3\alpha-3}} + \int \frac{\text{constant } dr_s}{r_s^{4\alpha-5}} + \dots$$

which for small r_s is formally convergent only for $\alpha < 2$. Note that for $\alpha = 2$ we obtain the simple result

$$E = \frac{\text{constant}}{r_s^2} + \text{constant}.$$

The ‘transition point’ at $\alpha = 2$ shows that for sufficiently long-ranged potentials ($\alpha < 2$) the high-density limit tends to the ideal gas, while for sufficiently short-ranged systems ($\alpha > 2$) it is the low-density limit that tends to the ideal behaviour (since the series is now convergent only for large r_s).

The method can also be generalized to non-vanishing temperatures. By discretizing λ we now have a two-variable partial differential equation to solve and at the same time an iteration process (using the known $P_0(r_s, T)$ for the ideal system) which will finally give a series for $P_\lambda(r_s, T)$ or $F_\lambda(r_s, T)$ (now the free energy), but with undetermined functions rather than constants. From this we can show that the terms of the series derived in section 3 are the only ones that survive in the limit $T \rightarrow 0$ and hence confirm the results above for the ground state of the translationally invariant system. An interesting scaling property that emerges for the free energy of our two-component system at finite temperature turns out to be

$$F(r_s, T) = \frac{f(m_e r_s, m_p r_s, T r_s)}{r_s} \quad (33)$$

with f an undetermined function of three variables. This generalizes our earlier scaling result [1] and can be useful for extrapolating known results for metallic hydrogen [4] to finite temperatures.

Finally, it should be re-emphasized that scaling procedures through discretization processes like the one we presented here can be useful in several different ways for many-body systems with charged components [3], and if carried out in the presence of an additional magnetic vector potential (and after the so-called minimal substitution in the Hamiltonian) can lead to important conclusions on the location of possible metal–insulator transitions [2]. We saw in section 4 an example of how the use of a vector potential can lead through general arguments to conclusions concerning an inhomogeneous state with harmonic excitations, but the full implementation of the method to the most general case of a multicomponent system is an especially important issue that deserves a separate investigation.

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[6] In the above application of the HFT we assume that the thermodynamic limit exists—see

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and can be taken, and therefore we ignore the question of the possible existence of residual surface terms associated with any non-Hermiticity of H for an enclosed system; see

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The corrections of order $r_s \ln r_s$ or $r_s^2 \ln r_s$ can be included in the above form at least for $0 < r_s \leq 2$ if we write

$$\ln r_s = r_s - 1 - (r_s - 1)^2/2 + (r_s - 1)^3/3 - \dots$$