COUPLED CLUSTERS AND THE ONE-COMPONENT BOSE PLASMA

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We show that the coupled cluster formalism in its lowest level of approximation provides an excellent description of the one-component Bose plasma at all densities. In particular, using a translationally-invariant description, we derive a unified framework that both exactly describes the high-density plasma and at least qualitatively describes the low-density solid phase.

A general discussion of the coupled cluster formalism of many-fermion theory and its application to the electron gas has recently been given by the present authors [1]. Attention was focussed there on the high-density limit, and in order to make further progress we have now also studied the analytically much simpler, although conceptually very similar, Bose formalism.

In essence, the coupled-cluster formalism employs the linked-cluster theorem for the exact many-body ground-state wavefunction $|\psi\rangle$ (i.e., the usual $\exp(S)$ Ansatz) to decompose the N -body system into a set of mutually interacting n -body subsystems ($n \leq N$) that are described by a set of so-called correlation operators S_n , the matrix elements of which describe the excitation of n "particle-hole pairs" from some suitably defined non-interacting reference (or model) state $|\phi\rangle$. Although it is not necessary to be so restrictive we choose $|\phi\rangle$ here to be a single-state condensate, and we have

$$|\psi\rangle = e^S |\phi\rangle, \quad S = \sum_{n=2}^N S_n, \\ |\phi\rangle = (N!)^{-1/2} (b_0^\dagger)^N |0\rangle, \quad (1) \\ S_n = \frac{1}{n!} \sum_{\rho_1 \dots \rho_n} b_{\rho_1}^\dagger \dots b_{\rho_n}^\dagger S_n(\rho_1 \dots \rho_n) (N^{-1/2} b_0^\dagger)^n,$$

where the operators $b_\alpha^\dagger$ create bosons in a complete orthonormal single-particle (s.p.) set $|\alpha\rangle$ in general, and which henceforth we choose as plane waves. The exact N -body Schrödinger equation for the ground state is thereby exactly decomposed into a coupled set of N (non-linear) microscopic equations for the matrix elements of the correlation operators S_n . In the present case where we are interested only in microscopic two-body (Coulomb) forces, and choosing $|\phi\rangle$ to be the usual (translationally-invariant) zero-momentum condensate; the exact two-body equation (for spin-zero bosons) for $S_2(q) \equiv S_2(\vec{q}, -\vec{q})$ becomes,

$$\frac{\hbar^2 q^2}{m} S_2(q) + T_{\text{RPA}} + T_{\text{CP}} + T_{\text{LAD}} + \sum_{\vec{q}'} V(q') \\ \times [2N^{1/2} S_3(\vec{q}, \vec{q}', -\vec{q}-\vec{q}') + \frac{1}{2} N S_4(\vec{q}, -\vec{q}, \vec{q}', -\vec{q}')] = 0,$$

$$T_{\text{RPA}} = NV(q)[1+S_2(q)]^2, \quad T_{\text{CP}} = -\frac{E}{N} S_2(q), \\ T_{\text{LAD}} = \sum_{\vec{q}'} V(\vec{q}-\vec{q}') S_2(q'), \quad (2)$$

and where the g.s. energy is given by

$$E/N = \frac{1}{2} NV(0) + \frac{1}{2} \sum_{\vec{q}} V(q) S_2(q). \quad (3)$$

The density $\rho \equiv N/\Omega$ is expressed in terms of either the usual dimensionless coupling constant r_s , which is the average interparticle spacing in units of the Bohr radius a , or a fictitious Fermi wavenumber k_F applicable to an analogous unpolarized spin- $\frac{1}{2}$ system, as $\rho = (4\pi r_s^3 a^3/3)^{-1} = k_F^3/3\pi^2$; and the g.s. energy per particle is expressed in Rydberg units as $E/N = \epsilon(e^2/2a)$. The so-called SUB2 approximation is obtained from Eq.(2) by setting S_3 and S_4 to zero. The remaining four terms then represent respectively (i) the kinetic energy (KE) contribution; (ii) the terms that, with KE, generate the random-phase approximation (RPA); (iii) the terms that generate the fully self-consistent (s.c.) energy insertions on the zero-momentum condensate lines, viz., the s.c. condensate potential (CP); and (iv) the terms that repeatedly scatter two particles outside the condensate and hence generate the two-particle ladder (LAD) diagrams. Where all dimensionless momenta are scaled against the fictitious Fermi momentum $\hbar k_F$, the SUB2 equation for Coulomb forces becomes,

$$q^2 S_2(q) + 4\alpha r_s (3\pi q^2)^{-1} [1+S_2(q)]^2 - 2(\alpha r_s)^2 \epsilon S_2(q) \\ + \frac{\alpha r_s}{\pi q} \int_0^\infty dq' q' \ln \left| \frac{q'+q}{q'-q} \right| S_2(q') = 0, \quad (4) \\ \epsilon = 2(\pi \alpha r_s)^{-1} \int_0^\infty dq S_2(q); \quad \alpha^3 = 4/9\pi.$$

Although the nonlinear equation (4) is readily solved numerically, it is more instructive to examine its high- and low-density limits. In the high-density ($r_s \rightarrow 0$) limit it is trivial to show that $\epsilon \rightarrow Qr_s^3/4 + R$; and furthermore that only the KE and RPA terms contribute to leading order to give the well-known exact result $Q \approx -0.8031$ of Foldy [2]. The CP and LAD terms also contribute to next order to give a SUB2 value $R=16/9\pi$. Inspection of Eq.(2) shows that the coupling

terms to S_3 and S_4 also contribute to the constant R^3 (although not to Q). A careful and detailed calculation including these terms leads to the value $R \approx 0.0280$, and an intricate rearrangement shows that our result is identical to the first correct result reported [3], of Brueckner.

In the much more interesting strong-coupling limit, $r_s \rightarrow \infty$, one may not expect the SUB2 approximation to give a reasonable result, since one imagines that n -body clusters with $n \gg 2$ are of importance here. Indeed we expect the system to undergo a phase transition to a Wigner solid, and this crystal phase is an archetype of one where N -body correlations dominate. However, in the SUB2 approximation we find that $\epsilon \rightarrow -Ar^{-1} + Br^{-3/2} + O(r^{-2})$ as $r_s \rightarrow \infty$, and that the S_{KE} term contributes only to the constant B in leading order. Whereas each of the terms RPA, CP and LAD is necessary for a quantitative evaluation of the constant A , they play quite different physical roles. Whereas the RPA terms continue to be vital for the correct analytic behaviour by providing the correct long-range ($q \rightarrow 0$) Coulomb screening, the CP now plays a similarly crucial role in the short-range ($q \rightarrow \infty$) limit. Whereas the inclusion of the LAD term quantitatively changes the constants A and B , it may safely be omitted without changing this analytic form for the low-density energy expansion. Dropping the LAD term leads to the analytic results $A = (32/3\pi^2)^{1/3} \approx 1.03$; $B = 3^2\pi/8 \approx 0.68$. The virial theorem may also be used to show that in this low-density expansion the leading term is purely potential energy, whereas the much more interesting second term is half each kinetic and potential energy — a result strongly indicative of the simple harmonic motion (SHM) expected of a solid. Indeed, Wigner first pointed out that in this limit, where the potential energy dominates, the energy is minimized by the particles crystallizing; and this leads to an electrostatic energy proportional to r_s^{-1} . Whereas in a fluid phase the particles are free to occupy the whole volume and hence by the uncertainty principle have a kinetic energy proportional to r_s^{-2} ; the particles in the Wigner solid are constrained to oscillate about fixed lattice sites and hence to have a greater kinetic energy, which by simple SHM considerations is seen to vary as $r_s^{-3/2}$. Thus our SUB2 g.s. energy has the correct analytic form of a solid, even though the coefficients are not very close to the b.c.c. crystal values of $A \approx 1.792$, $B \approx 2.65$. (We note that inclusion of the LAD term only increases this discrepancy by reducing the value of A by about 20%.) It is important to realize however that even the lowest SUB2 approximation in the coupled cluster scheme gives a low-density energy which cannot possibly represent a fluid phase since the particles are not free to occupy the whole volume.

It is clear therefore that our everywhere translationally-invariant approach well describes both fluid and solid phases. Although one might be

surprised that the fluid-like SUB2 wavefunction is capable of describing an (amorphous) solid state, it is clear that strong many-body correlations are built into the approximate wavefunction. On the other hand it is clear that in the low-density limit the third- and higher-order correlations obtained from the couplings to S_n with $n > 2$ are still very strong, and ought to be incorporated for a better quantitative description. Due to the relative simplicity of the Bose coupled-cluster equations, this remains quite feasible to do (as indeed we have already shown in the high-density limit), and we hope to report later on such further results.

REFERENCES

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