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van der Waals perturbation theory for fermion and boson ground-state matter

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Using computer algebraic symbolic manipulation techniques, we rearrange the ideal-gas-based low-density expansions for the ground-state energy of a many-fermion and a many-boson system interacting via arbitrary pair central forces, into a repulsive-core-fluid-based perturbation expansion. Applications through second order are reported for liquid ^{4}He and liquid ^{3}He.

I. INTRODUCTION

Few Monte Carlo computer simulations,[1] whether of the Jastrow variational or the more fundamental Green-function variety, have become available as yet for the calculation of even such basic physical quantities as the ground-state energy of the various quantum many-body systems interacting under simple two-body central potential functions. The reason is twofold: (a) the simulations are expensive in terms of required computer time and (b) the Green-function Monte Carlo (GFMC) problem for fermions is still beset with serious practical difficulties.

Simple, inexpensive, and reliable first-principles determinations of the various properties of a strongly interacting many-body system have been the goal of condensed-matter theory for decades. Two approaches have been the well-known *perturbative* and *variational* schemes based at heart, respectively, on the pioneering work of Brueckner and Bethe and of Jastrow. Another approach has been the coupled-cluster (or exponential-S) method. All approaches are at bottom low-density theories in that they eventually either break down or simply become unreliable beyond some density. At vanishing density, they lead to an infinite series for the ground-state energy, the leading term of which is *exact* at very low densities. This leading term is the ladder (or lowest-order Brueckner) energy in the perturbative, or the two-body (or Jastrow) correlation term in the variational, case. Higher-order terms are very difficult to calculate exactly but have been estimated and yield remarkably good agreement, at physical densities, for the various systems studied when compared with experiment or computer simulations. Our approach consists of going back to the original low-density expansions that quantum-field-theory methods applied to the many-body ideal-gas-based-perturbation theory have generated over the past decades for both many-boson[2] and many-fermion[3] ground-state energies. Here, three or four terms are known exactly. These expansions are then rearranged by considering the two-body interaction to be composed of repulsion plus attraction. The motivation for this procedure is based on the fact that, from both classical as well as quantum computer simulations, the pair-distribution function is qualitatively similar for say, a Lennard-Jones fluid as it is for a fluid of purely repulsive cores. The reexpansion leads to a *double* series: one in "density" and one in "attractive strength." This new perturbation scheme now starts from a zero-order reference system which is no longer the ideal gas of interactionless particles but rather a fluid of purely repulsive particles. This fluid state, nontrivial from the many-body standpoint, is then "perturbed" in a systematic fashion by "switching on" the attractions between the particles. Modern series-analyses techniques, like the well-known Padé approximants,[4] can be employed to extrapolate the energy in both variables—density and attractive coupling—towards physically relevant regions in a reliable, accurate manner. The power of such techniques in constructing good descriptions[5] for various *lattice* models of condensed matter in any dimension suggests their possible utility in analyzing now *continuous* many-body systems like those we are considering. Already, Padé analyses[6] of *classical* virial expansions have yielded descriptions of (i) the high-density fluid, (ii) the amorphous solid, as well as indications of, (iii) the crystalline solid known to occur, even in systems of rigid spheres, from classical molecular dynamics and Monte Carlo computer simulations.

One advantage of the approach being proposed for the quantum continuous problem is that in principle it can incorporate twice as much, if not more, hard information about the low-density, weakly interacting system. This is because there are available in the literature[2,3] this many more exact low-density coefficients than would be reproduced correctly by either the Brueckner-Bethe— or Jastrow—based schemes as extended and generalized to date.

For fermions the expansion for the ground-state energy per particle known so far is given by[3]

$$\frac{E}{N}\simeq\frac{3}{5}\frac{\hbar^2k_F^2}{2m}\left[1+K_1k_Fa+K_2(k_Fa)^2+\left[\tfrac{1}{2}K_3\frac{R_0}{a}+K_4\frac{A_1(0)}{a^3}+K_5\right](k_Fa)^3+K_6(k_Fa)^4\ln|k_Fa|\right.$$
$$\left.+\left[\tfrac{1}{2}K_7\frac{R_0}{a}+K_8\frac{A_0''(0)}{a^3}+K_9\right](k_Fa)^4+o((k_Fa)^4)\right]\ . \tag{1}$$

Here m is the particle mass, $\hbar k_F$ is the Fermi momentum of the ideal gas at a particle density $n\equiv N/V=\nu k_F^3/6\pi^2$, where ν is the number of different fermion species (i.e., the spin-, isospin-, etc., degeneracy). The symbols a, R_0, and $A_1(0)$ stand for the well-known scattering parameters of the effective-range theory[7] of low-energy scattering. These three quantities, known respectively as the S-wave scattering length a, the S-wave effective range R_0, and the P-wave scattering length (cubed) $A_1(0)$, characterize the potential assumed to act between pairs of particles in a *shape-independent* way, since they are related within the aforementioned theory to the scattering phase shift $\delta_l(k)$ in the lth partial wave through the low-energy results[7] ($l=0,1,2,\ldots$)

$$k^{2l+1}\cot\delta_l(k)\simeq-\frac{1}{A_l(0)}+\tfrac{1}{2}R_lk^2+O(k^4)\quad\text{as } k\rightarrow 0\ . \tag{2}$$

For S waves, $A_0(0)\equiv a$, defined before, while $\hbar k$ is the relative scattering linear momentum. On the other hand, the S-wave quantity $A_0''(0)$ appearing for the first time in Eq. (1) in the density-squared (i.e., k_F^6) contribution to the energy, is potential-shape-*dependent* and defined via the various many-body selective infinite summations[3] through the integral

$$A_0''(0)\equiv-\frac{m}{3\hbar^2}\int_0^\infty dr\, r^3V(r)u_0(r)\ , \tag{3}$$

where $V(r)$ is the pair potential and $u_0(r)$ the corresponding S wave, zero-energy, radial Schrödinger scattering wave function. The coefficients K_i of Eq. (1) are pure numbers and are listed in Ref. 8 for two- as well as four-species fermion matter, and reflect several corrections on the original coefficients as found in Ref. 3. A misprint still remains in Ref. 8, namely, for $\nu=4$ (complete) K_2 should be 0.556 610 instead of 0.566 610. For two-species fermion matter (neutron, ^{3}He, etc.), $K_6\equiv 0$ so that no log term is present, while for four-species (nuclear matter) K_7, K_8, and K_9 are still unknown, but K_6 is known and is not equal to 0. Thus, in either case one is dealing with a four-term expansion with coefficients known exactly.

The analogous expression for bosons is structurally somewhat simpler, and in fact is given[2] by

$$\frac{E}{N}\simeq\frac{2\pi\hbar^2}{m}na\,[1+K_1(na^3)^{1/2}+K_2na^3\ln(na^3)$$
$$+K_3na^3+O((na^3)^{3/2}\ln(na^3))]\ , \tag{4}$$

where n is the particle density of the many-boson system, the S-wave scattering length is as before, and K_1 and K_2 are pure numbers. The constant (in density) K_3, however, corresponds to genuine three-body cluster diagrams and is thus potential-shape dependent. It will hence very probably depend at least on $A_0''(0)$ as defined in Eq. (3). Both K_1 and K_2 have been evaluated by field theory in the boson case. The coefficient K_1 is in perfect agreement with other techniques.[9] Finally, K_3 is not known so that for bosons one really possesses only a three-term series with exactly known coefficients.

Both expansions, Eqs. (1) and (4), are low-density series but are clearly *not* power series in the density such as the classical virial expansion for an imperfect gas,

$$P/nk_BT\simeq 1+B_2(T)n+B_3(T)n^2+\cdots\ ,$$

where P is the pressure, k_B Boltzmann's constant, T the absolute temperature, and the virial coefficients $B_i(T)$ certain multiple integrals over exponentials of the pair potential. By contrast, in Eqs. (1) and (4) log terms in the particle density n appear, not to speak of fractional powers in n. Because of the latter, consequently, the physically prevailing case for naturally occurring interparticle potentials of *negative a* immediately leads, by inspection of Eq. (4), to imaginary contributions in the ground-state energy. This situation is difficult to interpret. A simple way out of the predicament is to consider the two-body potential $V(r)$ as made up of repulsion plus attraction (the latter times some real perturbation parameter λ, where $0\leq\lambda\leq 1$). In other words, one splits off the intermolecular potential function

$$V(r)=V_{\text{core}}(r)+\lambda V_{\text{att}}(r)\ , \tag{5}$$

in some convenient way. This procedure is reminiscent of well-known classical perturbation treatments[10] which have climaxed in what is presumably the most successful theory of classical liquids.[11] Simultaneously, consider expanding the dynamical parameters a, R_0, $A_1(0)$, and $A_0''(0)$ in powers of λ so that[12]

$$a\equiv\int_0^\infty dr\, rv(r)u_0(r)=a_0(1+a_1\lambda+a_2\lambda^2+\cdots)\ , \tag{6a}$$

$$R_0\equiv\frac{2}{a^2}\int_0^\infty dr[(r-a)^2-u_0^2(r)]$$
$$=r_0(1+r_1\lambda+r_2\lambda^2+\cdots)\ , \tag{6b}$$

$$A_1(0)\equiv\tfrac{1}{3}\int_0^\infty dr\, r^2v(r)u_1(r)$$
$$=t_0(1+t_1\lambda+t_2\lambda^2+\cdots)\ , \tag{6c}$$

$$A_0''(0)\equiv-\tfrac{1}{3}\int_0^\infty dr\, r^3v(r)u_0(r)$$
$$=p_0(1+p_1\lambda+p_2\lambda^2+\cdots)\ . \tag{6d}$$

In these equations $v(r)\equiv mV(r)/\hbar^2$ and $u_l(r)$ is the zero-energy Schrödinger radial wave function satisfying $u_l''(r)-[v(r)-l(l+1)/r^2]u_l(r)=0$, with $u(0)=0$. For large r, on the other hand, $u_0(r)\rightarrow r-a$, $u_1(r)\rightarrow r^2/3-A_1(0)/r$, etc. For simple-enough potentials (5), the different coefficients in (6) can be deduced analytically, as in Ref. 8 for the hard-core—square-well (HCSW) potential, or numerically, as in Ref. 13 for the Lennard-Jones and other intermolecular potentials. Substitution of Eqs. (6) into Eqs. (1) and (4) then ultimately leads [e.g., via algebraic manipulation computer schemes like REDUCE or MACSYMA (Ref. 14)] to expansions of the form

$$\frac{E}{N}\simeq A\frac{\hbar^2}{ma_0^2}x^2\sum_{i=0}^{\infty}e_i(x)\lambda^i\ , \tag{7}$$

where each $e_i(x)$ is a low-density series known to as many terms as are known in the original series, (1) or (4). In (7), x is a dimensionless density variable, defined as $(na_0^3)^{1/2}$ for bosons and k_Fa_0 for fermions, while the constant A is just 2π for the former and $\frac{3}{10}$ for the latter. Equation (7) plainly corresponds to the above-mentioned perturbation scheme *about the fluid of repulsive particles* instead of about the ideal gas. We call this scheme the van der Waals perturbation theory as it was suggested, though never formulated in detail, by him more than a hundred years ago. In contrast to the classical fluids van der Waals perturbation scheme alluded to above,[10,11] the quantum problem [Eq. (7)] permits relatively simple evaluation not only of first- but also of higher-order corrections. Now, whereas Eq. (4) could become *complex* if λ in Eq. (5) were sufficiently large so as to make *a negative*, the rearrangement [Eq. (7)] is clearly *real* for all real λ so that the original predicament of complex energies for a negative has been entirely circumvented.

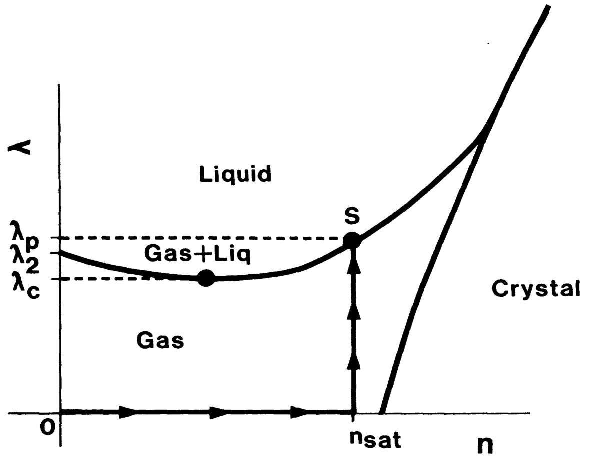

FIG. 1. Schematic attractive coupling λ vs particle density n plane for a typical quantum substance at zero absolute temperature such as ^{4}He or nuclear matter. Three phases, "gas," "liquid," and "crystal" are shown. Thus, a critical attractive two-body coupling strength λ_c is required before any liquid phase can be formed out of the gaseous phase. A maximum value λ_2 exists above which gas *and* liquid cannot coexist in equilibrium, e.g., only liquid can survive. If the density is sufficiently large crystalline order will appear, assuming the repulsive interparticle cores are sufficiently "hard," and for any attraction, no matter how weak. A typical "physical attractive strength" for ^{3}He or ^{4}He, for example, or nuclear matter is labeled λ_p. The zero-pressure equilibrium (or saturation) density state is marked by S. The path marked by arrows corresponds to the procedure of the present paper. Note that no phase boundaries are crossed to reach the ground-state saturation minimum point S.

A second difficulty associated with expansions such as (1) and (4), even if rearranged in the form (7), is, of course, their restriction to low densities, i.e., densities well below those of physically condensed systems such as nuclear matter, the liquid heliums, etc. It is here that extrapolation schemes may play a very useful role, particularly if they can somehow allow us to avoid crossing *phase boundaries* (especially gas-to-liquid ones) and thus obtaining invalid results.

This program is accomplished in the proposed method of attack since it essentially consists of two steps: (i) extrapolation from $n=0$ to finite (physical) n for the ith-order energies $e_i(n)$ in Eq. (7), for $i=0,1,2,\ldots$; and (ii) extrapolation at physical n, from $\lambda=0$ to finite (physical) attractive coupling λ_p. These two procedures are best illustrated in Fig. 1 for the attractive coupling versus density plane[3] of a simple quantum substance. The three common phases (gas, liquid, and crystal), as well as a gas-liquid coexistence region, are displayed. Here λ_c is the minimum attractive strength required to form a liquid (i.e., an N-body self-bound state) at all. On the other hand, λ_2 is the minimum value required for the disappearance of a gas-liquid coexistence region and finally λ_p is the *physical* coupling in a typical quantum liquid (say, ^{3}He or ^{4}He). Consequently, the point S is a typical equilibrium, or saturation (zero pressure), state for the quantum liquid. The two-step series analysis of Eq. (7) sketched above corresponds to (i) the horizontal arrowhead trajectory in Fig. 1 from 0 to the value $n_{\rm sat}$ along the n axis and then (ii) the path vertically up from the point $n_{\rm sat}$ $(\lambda=0)$ to the desired state point S at λ_p. Note that no phase boundaries have been crossed, contrary to what might very easily occur in an ideal-gas-based perturbation scheme.

The first step is then to derive explicitly the $e_0(x)$, $e_1(x),\ldots,$ of Eq. (7), and this is carried out in Sec. II for any central, two-particle potential interaction.

II. van der WAALS PERTURBATION SERIES

We discuss first the many-boson system, given that its low-density expansion (4) is of simpler structure than the corresponding one for fermions (1). Since the coefficient K_3 is not known [though it could conceivably turn out to be similar in structure to the k_F^4 coefficient of (1)] we shall simply put

$$K_3\equiv q_0(1+q_1\lambda+q_2\lambda^2+\cdots)\ . \tag{8}$$

From (5), $\lambda=0$ corresponds to the fluid of purely repulsive cores. For infinitely hard cores the coefficient q_0 has been evaluated[15] by global fit to GFMC data for boson hard spheres. If attractions are then added the coefficients q_1, q_2, etc., could in principle be extracted from the physical constraints $\epsilon_1(x_B)=\text{const}$, $\epsilon_i(x_B)=0$, $i=2,3,\ldots$, etc., respectively, as motivated by Ref. 16. In the two papers quoted under this reference, it is proved that, at least for classical many-particle systems in one and two dimensions, so-called thermodynamic (or van der Waals) first-order perturbation theory is *exact* in the limit of close packing. Hence the constraints just stated. In our case, $x_B=(n_B c^3)^{1/2}$, where $c=a_0$ is the hard-sphere diameter and n_B is the Bernal density, or density of random close packing, as determined, for example, from Ref. 15. Henceforth, the $\epsilon_i(x)$ $(i=0,1,2,3,\ldots)$ stand for the *extrapolants* to nonzero $x\equiv(nc^3)^{1/2}$ for the low-density forms $e_i(x)$ that resulted from the rearrangement (7).

Inserting (8) and (6a) into (4) the form (7) ensues, with the $e_i(x)$ given by

$$e_0(x)=1+K_1x+K_2x^2\ln x^2+q_0x^2+\cdots, \tag{9}$$

$$e_j(x)=a_j[1+(f_{2j}/a_j)x+(f_{3j}/a_j)x^2\ln x^2+(\tilde{q}_j/a_j)x^2+\cdots]. \tag{10}$$

The coefficients f_{ij} $(i=2,3;\ j=1,2,3,\ldots)$ will clearly depend explicitly on the constants K_1 and K_2 as well as on the expansion coefficients a_j of the S-wave scattering length as defined in Eq. (6a). Appendix A lists in MACSYMA format f_{2j} and f_{3j} for $j=1,2,\ldots,6$. (Note that K_i appears as k_i.) The coefficients $\tilde{q}_j$ are linear in the q_j of (8); as neither q_j nor $\tilde{q}_j$ are known, we leave both unspecified. All this will enable one to then carry out van der Waals perturbation theory up to *sixth order*. As mentioned in the Introduction, carrying this out is seen to be not only feasible but relatively simple, in marked contrast with the *classical* van der Waals perturbation scheme[10,11] where even second order has, unfortunately, required estimations. On the other hand, the success of the *quantum* van der Waals scheme to any order will crucially hinge on whether one can construct reliable extrapolants $\epsilon_j(x)$ to the low-density forms (10). A general method for implementing this will be presented and illustrated in Sec. III.

But before that, let us consider the many-fermion problem. We refer to Eq. (1), and substitute the λ expansions of Eqs. (6), which leads to the rearrangement (7). Recalling that $x\equiv k_F a_0$, the sum in Eq. (7) will become

$$e_0(x)+\sum_{i=1}^{5}\sum_{j=1}^{\infty}f_{ij}x^i\lambda^j,\quad f_{1j}\equiv K_1a_j, \tag{11}$$

where

$$e_0(x)\simeq 1+K_1x+K_2x^2+\left[\tfrac{1}{2}K_3\frac{r_0}{a_0}+K_4\frac{t_0}{a_0^3}+K_5\right]x^3+K_6x^4\ln x+\left[\tfrac{1}{2}K_7\frac{r_0}{a_0}+K_8\frac{p_0}{a_0^3}+K_9\right]x^4+\cdots, \tag{12}$$

and where the coefficients f_{ij} $(i=2,3,\ldots,5)$ in (11) are listed in Appendix B for $j=1,2,\ldots,6$, i.e., again through sixth order. In Eq. (11) the x^4 and x^5 terms should be interpreted, respectively, as $x^4\ln x$ and x^4. Note, too, that for two-species fermions there is no $x^4\ln x$ term,[3] or that $f_{4j}\equiv 0$. In the four-species case the f_{5j} are listed for completeness in Appendix B but are in terms of the constants K_7, K_8, and K_9 which are unknown[3] at present.

III. APPLICATIONS

As illustrations of the van der Waals quantum-perturbation scheme, we report the calculation of the ground-state energy through second order for two distinct physical systems. These are (i) liquid ^{4}He under a hard-core-square-well (HCSW) potential parametrized by Burkhardt[17] so as to be phase-shift equivalent (for low-energy and low-partial waves) to the Lennard-Jones pair potential,[18] and (ii) liquid ^{3}He interacting via this latter (soft-cored) pair potential itself.

To extrapolate the low-density series $e_i(x)$ in Eq. (7) we employ a general extrapolation method essentially inspired by, but somewhat more general than, Padé approximation,[4] both standard and generalized, the latter referring to nonpower series. This method is motivated by the very common situation in a physical series (regular, power, or otherwise, with, e.g., log terms) that the earlier terms of the series are numerically known to higher accuracy than the later terms in the "tail" of the expansion.

For the many-boson and many-fermion cases to be dealt with here, the $e_i(x)$ in Eq. (7) have the forms

$$e_i(x)/a_i=1+b_1x+b_2x^2\ln x^2+b_3x^2+\cdots\quad\text{(bosons)}, \tag{13}$$

$$e_i(x)/A_ix=1+f_1x+f_2x^2+f_3x^3+f_4x^4+\cdots\quad(\nu=2\text{ fermions}), \tag{14}$$

with f_4 and b_3 as yet unknown, and A_i being negative constants. Our method begins by expressing the least number of terms in the tails of either (13) or (14) that will allow expression as a ratio of functions, $N(x)$ and $D(x)$, for example, such that expansion about $x=0$ of $N(x)/D(x)$ reproduces the initial tail expression. The next step starts with a tail expression having one more term, etc., until the whole expression—(13) or (14)—has been represented as ratios of such functions. In general then, the series (13) or (14) will be represented by

$$P(x)+\frac{N(x)}{D(x)}\equiv\epsilon(x), \tag{15}$$

where $P(x)$ is always polynomial (or zero or unity) and the single log term in the raw series (13) occurs *either* in $N(x)$ or in $D(x)$.

A. Liquid ^{4}He

The Burkhardt[7] HCSW potential has a hard-sphere diameter $c=1.685$ Å, attractive square well depth $v_0=1.899\,986\,5$ K and range $R=5.5$ Å so that one can define the dimensionless parameters

$$\lambda\equiv mv_0(R-c)^2/\hbar^2=2.281\,416\,5,\qquad \alpha\equiv(R-c)/c=2.264\,095. \tag{16}$$

The S-wave scattering length for this potential is then

$$a = c[1+\alpha(1-\tan\sqrt{\lambda}/\sqrt{\lambda})] = -36.2938\ \text{Å}\ . \tag{17}$$

The λ-power series (6a) is analytical, with

$$a_0 = c,\ \ a_1 = -\tfrac{1}{3}\alpha,\ \ a_2 = -\tfrac{2}{15}\alpha,\ \ldots\ . \tag{18}$$

Equation (7) then becomes, using Appendix A and Eqs. (9) and (10),

$$\frac{E}{N} = \frac{2\pi\hbar^2}{mc^2}x^2 \left\{ \left[1 + \frac{128}{15\sqrt{\pi}}x + 8\left[\frac{4\pi}{3} - \sqrt{3}\right] x^2 \ln x^2 + q_0 x^2 + \cdots \right] \right.$$
$$-0.754\,698\,3(1+12.036\,105x + 78.615\,68x^2\ln x^2 + Q_1x^2 + \cdots)\lambda$$
$$\left. -0.301\,879\,3(1-4.955\,702x - 143.876\,08x^2\ln x^2 + Q_2x^2 + \cdots)\lambda^2 + \cdots \right\}, \tag{19}$$

with q_0, Q_1, and Q_2 unknown. A global fit[15] to the boson hard-sphere GFMC results[19] yields the extrapolant to the first square-bracket series of (19) given by

$$\epsilon_0(x) = \left[1 - \frac{2.407\,209x}{1-8.164\,607x(\ln x + 0.223)} \right]^{-2} . \tag{20}$$

This form possesses a second-order, uncertainty-principle[20] pole at $x = x_B = 0.7082$, which is identified as the Bernal (or random close packing) density for a boson hard-sphere system. This is $n_B = 0.3547n_0$, where n_0 is $\sqrt{2}/c^3$ or the density of primitive hexagonal packing. The classical *empirical*[21] value of n_B is $0.86n_0$. A smaller value is to be expected in the quantum case. Equation (20) gives $q_0 = 26.2$.

The second and third square-bracket expressions of (19), corresponding to second- and third-order perturbation corrections to the hard-sphere fluid due to the pair attractions, were analyzed in the form Eq. (15) with the results summarized in Table I. For each form, Q_1 and Q_2 were determined from the constraints mentioned before, namely,

$$\epsilon_i(x_B) \equiv \epsilon_i(x_B)/a_i = \text{const},\ \ \epsilon_2(x_B) = 0\ . \tag{21}$$

The constant is 2.955 42 for the potential being used, and is obtained by demanding, in accordance with Ref. 16, that the first-order contribution to the energy per particle at close packing be given by the number of sphere centers within the attractive potential range R of a given sphere, namely, $(4\pi/3)R^3n_B$, minus one sphere, times the attractive well depth $-v_0$ (and with the customary factor of $\frac{1}{2}$). Forms for $\epsilon_1(x)/a_1$, and $\epsilon_2(x)/a_2$ listed in Table I are rejected if they possess a pole (marked with a "p") in the physical interval $0 < x < x_B$. In first order, moreover, we expect an acceptable extrapolant to be monotonic increasing; those forms violating this condition are marked "vmi". Furthermore, both first- and second-order corrections must be nonpositive for *all* densities so that because of the two overall negative factors in (19), an acceptable

TABLE I. Possible approximants, with general structure given by Eq. (15), to the second and third parentheses low-density series in Eq. (19). For example, form III to Eq. (13) is explicitly $1+b_1x/(1-b_2x\ln x^2/b_1 - b_3x/b_1)$. The unknown b_3 coefficients, called Q_1 and Q_2 in Eq. (19), are determined as explained in the text and are, respectively, −0.651 64 (form II) and −81.3798 (form III). Note that forms I and V are identical; all others are distinct from each other. The acronyms are as follows: p means pole; vp, violates positivity; ns, no solution; nmi, nonmonotonic increasing; and vma violates monotonicity in order.

Form	No. of terms in $P(x)$	Terms in $N(x)$	Terms in $D(x)$	Order	
				1	2
I	1	$x, x^2\ln x^2$	$1, x$	p	p
II	1	x, x^2	$1, x\ln x^2$		vp
III	1	x	$1, x\ln x^2, x$		
IV	0	$1, x$	$1, x, x^2\ln x^2$	p	p
V	0	$1, x, x^2\ln x^2$	$1, x$	p	p
VI	0	1	$1, x, x^2\ln x^2, x^2$	nmi	ns
VII	0	$1, x, x^2\ln x^2$	$1, x^2$	p	ns
VIII	0	$1, x^2\ln x^2, x^2$	$1, x$	p	vmo
IX	0	$1, x, x^2$	$1, x^2\ln x^2$	nmi	p
X	0	$1, x$	$1, x^2\ln x^2, x^2$	vp	ns
XI	0	$1, x^2\ln x^2$	$1, x, x^2$	p	ns
XII	0	$1, x^2$	$1, x, x^2\ln x^2$	nmi	p

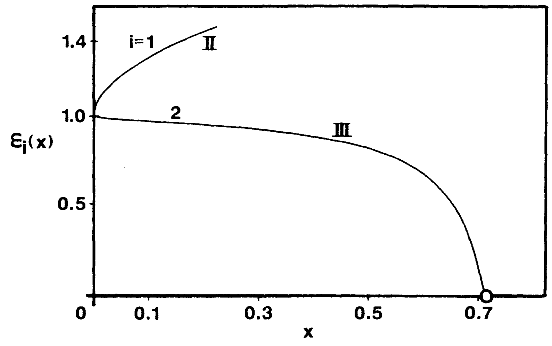

FIG. 2. Density dependence of first- and second-order energy corrections to the hard-sphere Bose fluid described by Eq. (20). The numerals II and III refer to the specific forms in Table I which successfully extrapolate, respectively, the truncated log-bearing series in the second and third parentheses of Eq. (19). The open circle on the $x=(nc^3)^{1/2}$ axis marks the Bernal value $x_B=0.7082$ where Eq. (20) has a second-order pole. The first order $\epsilon_i(x)$ rises smoothly and attains the value of 2.955 42 at x_B as discussed in the text.

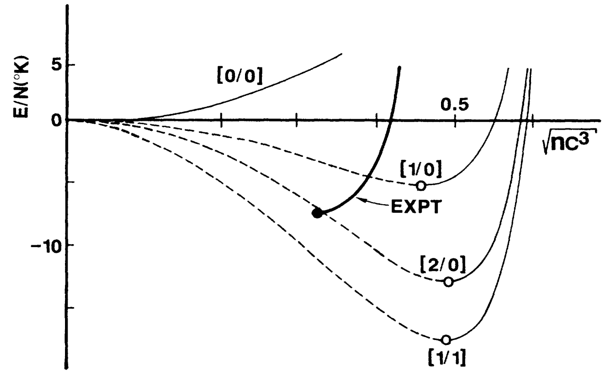

FIG. 3. Zero-order, [0/0], first-order, [1/0], and second-order, [2/0] and [1/1], total ground-state energy of ^{4}He in the van der Waals perturbation scheme with the HCSW model pair potential. The curve marked EXPT refers to the experimental results.

form for either $\epsilon_1(x)/a_1$, or $\epsilon_2(x)/a_2$ must be positive for all x; "vp" in Table I designates violation of positivity. One further restriction imposed on second order is that $\epsilon_2(x)/a_2<\epsilon_1(x)/a_1$, for all x, a property that is observed in *exact* studies[22] through fourth order for fermions interacting with a finite attractive square well pair potential. A single form (VIII) marked "vmo" (violates monotonicity in order) was found to violate this. Finally, entries marked "ns" allow no solution for the constant Q_2 with the equation $\epsilon_2(x_B)=0$ since Q_2 appears in the denominator. In conclusion, only *one* form (III) survives the analysis in second order, and *two* forms (II and III) in first order. These latter two forms, however, are very similar for all $0<x<x_B$; in fact, their difference is at most 0.25% at the maximum value of $\epsilon_1(x)/a_1$, which is $\epsilon_1(x_B)/a_1$, which is equal to 2.955 42. For definiteness, we reject III and keep II. Figure 2 shows a plot of form II for first order and form III for second order. The open circle marks the value of x_B quoted before.

Using these forms as well as Eq. (20) to represent and replace the corresponding square-bracketed series in Eq. (19) we proceed to analyze the resulting power series in λ through second order by constructing standard Padé approximants $[L/M](\lambda)$, with $0\leq L+M\leq 2$ and L,M non-negative integers. The resulting ground-state energy versus $x=(nc^3)^{1/2}$ appears in Fig. 3, where [0/0] refers to the hard-sphere fluid equation of state. First- and second-order total energies are labeled [1/0] and [2/0], respectively. Preliminary higher-order results are found to converge rapidly and lie *above* the $[1/1](\lambda)$ Padé result, but are not reported here. The dashed portions of the curves correspond to metastable and unstable branches, which are eliminated by the appropriate[23] convex-hull construction analogous to the familiar Maxwell equal-area rule. For reference, we give the experimental curve[24] (labeled EXPT) for ^{4}He. We remark that the discrepancy between predicted and empirical results are not necessarily significant at this point since not only have many-body forces been neglected but also a rough schematic model potential is employed. In fact, we found that this discrepancy can be virtually removed by varying the values c, R, and v_0 of the HCSW potential[16] *such that* the empirical bound[25] on the S-wave scattering length

$$|a|>20\ \text{Å}\ , \tag{22}$$

for the ^{4}He-^{4}He system is preserved.

B. Liquid ^{3}He

For the Lennard-Jones[18] (LJ) interaction the expansions (6) must be done numerically, and are published elsewhere[13] for the case in which the splitting implied in Eq. (5) between $V_{\text{core}}(r)$ and $V_{\text{att}}(r)$ is accomplished at the zero of the LJ potential, and $\lambda=1$. Equation (1) and Appendix B together then yield

$$\begin{aligned}\frac{E}{N}=\frac{3}{10}\frac{\hbar^2x^2}{ma_0^2}[&(1+0.353\,678x+0.185\,537x^2+0.384\,632x^3-0.025\,203\,9x^4+\cdots)\\&-0.372\,459x\lambda(1+1.049\,186x+6.280\,439x^2-2.045\,335x^3+f_{41}x^4+\cdots)\\&-0.244\,966\,9x\lambda^2(1+0.209\,218x+0.650\,121x^2+1.290\,48x^3+f_{42}x^4+\cdots)-\cdots]\ ,\end{aligned} \tag{23}$$

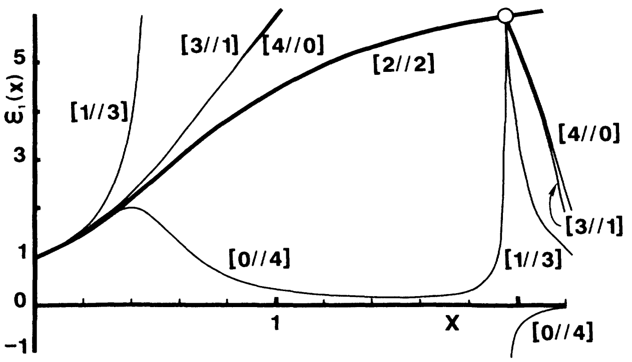

FIG. 4. Density dependence of all two-point, fourth-order Padé approximants to the first-order energy-correction series given by the second parentheses of Eq. (23). The bold curve designates the only acceptable extrapolant, as discussed in text. Open circle marks the corresponding Bernal value $x_B=1.939$ appropriate for two-species fermions.

where f_{41} and f_{42} are to be determined, and where $a_0=2.062\,437\,8$ Å is the S-wave scattering length of the purely repulsive part $V_{\text{core}}(r)$ of the LJ potential. This latter value is understandably somewhat smaller than the value 2.556 Å where the potential changes sign, because of the softness of the LJ repulsive core.

To describe the fluid of repulsive particles, for which we expect energy increasing in density, all Padé approximants in x were constructed to the fourth-order polynomial in the first parentheses of Eq. (23). These are $[4/0](x)$, (the original series), $[3/1](x)$, $[2/2](x)$, $[1/3](x)$ and $[0/4](x)$. The extrapolants [2/2] and [1/3] are immediately discarded since the former has a pole at $x=1.12$ and the latter at $x=1.43$. The form [0/4] rises with x, reaches a maximum at around $x\simeq1.1$ and then decreases to zero as $1/x^4$ as x increases. The two remaining forms [4/0] and [3/1] are very similar in value for $0<x\lesssim2$; while [3/1] continues to rise in x, however, the [4/0] form falls and develops a zero at around $x=20$. We thus retain only the [3/1] form to represent zero order.

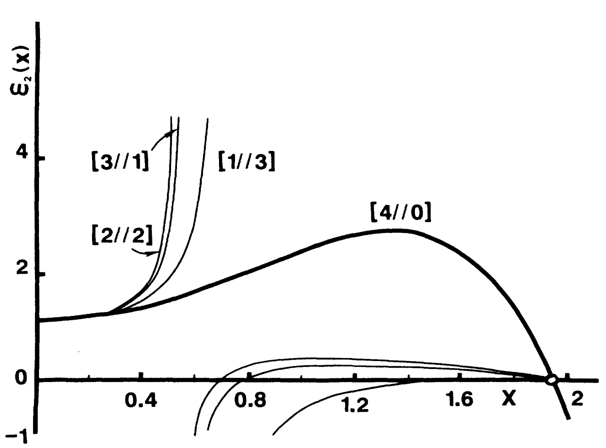

FIG. 5. Same as Fig. 4 but for second-order perturbation energy, referring to the third set of parentheses in Eq. (23).

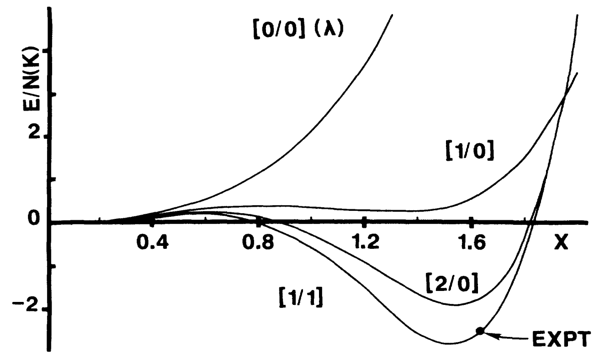

FIG. 6. Same as Fig. 3, but for liquid ^{3}He interacting via the Lennard-Jones pair potential.

All fourth-order Padé approximants $[L/M](x)$, $L+M=4$, were constructed for the second and third parentheses of Eq. (23), fourth-order polynomials corresponding to the first- and second-order perturbation corrections to the soft-sphere fluid energy. To determine the unknown constants f_{41} and f_{42} of Eq. (23) we again impose the conditions (21), where $x_B=1.939$ and $[L//M](x_B)=4.517$. The latter value is the one appropriate for the Burkhardt ^{3}He-^{3}He HCSW, while the former value was the one found[20] for the two-species fermion hard-sphere system. The double slash in the Padé symbol $[L//M](x)$ refers to the fact that it is a *two*-point approximant, about the points $x=0$ *and* $x=x_B$. Figures 4 and 5 display the resulting approximants for the density dependence in first and second order. Open circles mark the value of x_B just quoted. Note that in first order only one approximant, the $[2//2](x)$, satisfies the conditions of being monotonic increasing in x. In second order only one approximant, the $[4//0](x)$, is free of poles. (The [0//4] form is not considered since it has no solution for the constant f_{42}.)

Finally, Fig. 6 shows the Padé approximants through second order for the ground-state energy of the system. For reference, the experimental value of −2.47 K and $n=0.0165$ Å^{-5} for the zero pressure, equilibrium (saturation) binding energy is marked by a dot. Again, the $[1/1](\lambda)$ approximant is below the $[2/0](\lambda)$ curve, as well as below preliminary higher-order results to be reported later in greater detail.

IV. CONCLUSIONS

We start from the well-known low-density k_Fa $[(na^3)^{1/2}]$ expansion for the ground-state energy of a many-fermion (many-boson) system interacting via arbitrary pairwise central interactions. Both expansions are non-power series, and have been obtained over the past fifty years from quantum-field-theoretic techniques applied to a perturbation scheme about the corresponding ideal Fermi or Bose gases. In them, at least twice as many coefficients are presently known as can be reproduced, in the low-density limit, by either the Brueckner-based ladder[26] or Jastrow-based variational theories[27] of these many-particle ground states, although the latter enjoys the advantage of always dealing with explicit ("trial") wave functions. Information originating in the basic, central pair interactions appears in the energy expansions via effective range-theory parameters, except for one potential-shape-dependent S-wave quantity, $A_0''(0)$. Expansion of these dynamical parameters in powers of the two-body attraction coupling constant then leads to a ground-state energy which can be viewed as a perturbation scheme about, not the ideal gas, but rather the nontrivial fluid of repulsive cores.

This rearrangement has been carried out through sixth order utilizing the computer algebraic scheme known as MACSYMA. Extrapolation to nonzero, physical densities of the resulting perturbation energies can now be carried out in principle for any central pairwise interaction.

Finally, the results are applied through second order to ^{4}He and ^{3}He and both calculations already suggest that the perturbation scheme is rapidly convergent.

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APPENDIX A: BOSON EXPANSION COEFFICIENTS

$$f_{2,1}=\frac{5a_1k_1}{2}\ ,$$

$$f_{2,2}=\frac{(20a_2+15a_1^2)k_1}{8}\ ,$$

$$f_{2,3}=\frac{(40a_3+60a_1a_2+5a_1^3)k_1}{16}\ ,$$

$$f_{2,4}=\frac{(320a_4+480a_1a_3+240a_2^2+120a_1^2a_2-5a_1^4)k_1}{128}\ ,$$

$$\begin{aligned}f_{2,5}=[&640a_5+960a_1a_4+(960a_2+240a_1^2)a_3\\&+240a_1a_2^2-40a_1^3a_2+3a_1^5]k_1/256\ ,\end{aligned}$$

$$\begin{aligned}f_{2,6}=[&2560a_6+3840a_1a_5+(3840a_2+960a_1^2)a_4\\&+1920a_3^2+(1920a_1a_2-160a_1^3)a_3+320a_2^3\\&-240a_1^2a_2^2+60a_1^4a_2-5a_1^6]k_1/1024\ ,\end{aligned}$$

$$f_{3,1}=4a_1k_2\ ,$$

$$f_{3,2}=(4a_2+6a_1^2)k_2\ ,$$

$$f_{3,3}=(4a_3+12a_1a_2+4a_1^3)k_2\ ,$$

$$f_{3,4}=(4a_4+12a_1a_3+6a_2^2+12a_1^2a_2+a_1^4)k_2\ ,$$

$$\begin{aligned}f_{3,5}=[&4a_5+12a_1a_4+(12a_2+12a_1^2)a_3\\&+12a_1a_2^2+4a_1^3a_2]k_2\ ,\end{aligned}$$

$$\begin{aligned}f_{3,6}=[&4a_6+12a_1a_5+(12a_2+12a_1^2)a_4+6a_3^2\\&+(24a_1a_2+4a_1^3)a_3+4a_2^3+6a_1^2a_2^2]k_2\ .\end{aligned}$$

APPENDIX B: FERMION EXPANSION COEFFICIENTS

$$f_{2,1}=2a_1k_2\ ,$$

$$f_{2,2}=(2a_2+a_1^2)k_2\ ,$$

$$f_{2,3}=(2a_3+2a_1a_2)k_2\ ,$$

$$f_{2,4}=(2a_4+2a_1a_3+a_2^2)k_2\ ,$$

$$f_{2,5}=(2a_5+2a_1a_4+2a_2a_3)k_2\ ,$$

$$f_{2,6}=(2a_6+2a_1a_5+2a_2a_4+a_3^2)k_2\ ,$$

$$f_{3,1}=\frac{2k_4t_0t_1+a_0^2k_3r_0(r_1+2a_1)+6a_0^3a_1k_5}{2a_0^3}\ ,$$

$$f_{3,2}=\frac{2k_4t_0t_2+a_0^2k_3r_0(r_2+2a_1r_1+2a_2+a_1^2)+a_0^3(6a_2+6a_1^2)k_5}{2a_0^3}\ ,$$

$$f_{3,3}=\{2k_4t_0t_3+a_0^2k_3r_0[r_3+2a_1r_2+(2a_2+a_1^2)r_1+2a_3+2a_1a_2]+a_0^3(6a_3+12a_1a_2+2a_1^3)k_5\}/(2a_0^3)\ ,$$

$$\begin{aligned}f_{3,4}=\{&2k_4t_0t_4+a_0^2k_3r_0[r_4+2a_1r_3+(2a_2+a_1^2)r_2+(2a_3+2a_1a_2)r_1+2a_4+2a_1a_3+a_2^2]\\&+a_0^3(6a_4+12a_1a_3+6a_2^2+6a_1^2a_2)k_5\}/(2a_0^3)\ ,\end{aligned}$$

$$\begin{aligned} f_{3,5}=\{&2k_4t_0t_5+a_0^2k_3r_0[r_5+2a_1r_4+(2a_2+a_1^2)r_3+(2a_3+2a_1a_2)r_2+(2a_4+2a_1a_3+a_2^2)r_1+2a_5+2a_1a_4+2a_2a_3]\\ &+a_0^3[6a_5+12a_1a_4+(12a_2+6a_1^2)a_3+6a_1a_2^2]k_5\}/(2a_0^3)\ ,\end{aligned}$$

$$\begin{aligned} f_{3,6}=\{&2k_4t_0t_6+a_0^2k_3r_0[r_6+2a_1r_5+(2a_2+a_1^2)r_4+(2a_3+2a_1a_2)r_3+(2a_4+2a_1a_3+a_2^2)r_2\\ &+(2a_5+2a_1a_4+2a_2a_3)r_1+2a_6+2a_1a_5+2a_2a_4+a_3^2]\\ &+a_0^3[6a_6+12a_1a_5+(12a_2+6a_1^2)a_4+6a_3^2+12a_1a_2a_3+2a_2^3]k_5\}/(2a_0^3)\ ,\end{aligned}$$

$$f_{4,1}=4a_1k_6\ ,$$

$$f_{4,2}=(4a_2+6a_1^2)k_6\ ,$$

$$f_{4,3}=(4a_3+12a_1a_2+4a_1^3)k_6\ ,$$

$$f_{4,4}=(4a_4+12a_1a_3+6a_2^2+12a_1^2a_2+a_1^4)k_6\ ,$$

$$f_{4,5}=[4a_5+12a_1a_4+(12a_2+12a_1^2)a_3+12a_1a_2^2+4a_1^3a_2]k_6\ ,$$

$$f_{4,6}=[4a_6+12a_1a_5+(12a_2+12a_1^2)a_4+6a_3^2+(24a_1a_2+4a_1^3)a_3+4a_2^3+6a_1^2a_2^2]k_6\ ,$$

$$f_{5,1}=\frac{a_0^2k_7r_0(r_1+3a_1)+k_8p_0(2p_1+2a_1)+8a_0^3a_1k_9}{2a_0^3}\ ,$$

$$f_{5,2}=[a_0^2k_7r_0(r_2+3a_1r_1+3a_2+3a_1^2)+k_8p_0(2p_2+2a_1p_1+2a_2)+a_0^3(8a_2+12a_1^2)k_9]/(2a_0^3)\ ,$$

$$\begin{aligned} f_{5,3}=\{&a_0^2k_7r_0[r_3+3a_1r_2+(3a_2+3a_1^2)r_1+3a_3+6a_1a_2+a_1^3]\\ &+k_8p_0(2p_3+2a_1p_2+2a_2p_1+2a_3)+a_0^3(8a_3+24a_1a_2+8a_1^3)k_9\}/(2a_0^3)\ ,\end{aligned}$$

$$\begin{aligned} f_{5,4}=\{&a_0^2k_7r_0[r_4+3a_1r_3+(3a_2+3a_1^2)r_2+(3a_3+6a_1a_2+a_1^3)r_1+3a_4+6a_1a_3+3a_2^2+3a_1^2a_2]\\ &+k_8p_0(2p_4+2a_1p_3+2a_2p_2+2a_3p_1+2a_4)+a_0^3(8a_4+24a_1a_3+12a_2^2+24a_1^2a_2+2a_1^4)k_9\}/(2a_0^3)\ ,\end{aligned}$$

$$\begin{aligned} f_{5,5}=\{&a_0^2k_7r_0[r_5+3a_1r_4+(3a_2+3a_1^2)r_3+(3a_3+6a_1a_2+a_1^3)r_2+(3a_4+6a_1a_3+3a_2^2+3a_1^2a_2)r_1+3a_5\\ &\quad+6a_1a_4+(6a_2+3a_1^2)a_3+3a_1a_2^2]+k_8p_0(2p_5+2a_1p_4+2a_2p_3+2a_3p_2+2a_4p_1+2a_5)\\ &\quad+a_0^3[8a_5+24a_1a_4+(24a_2+24a_1^2)a_3+24a_1a_2^2+8a_1^3a_2]k_9\}/(2a_0^3)\ ,\end{aligned}$$

$$\begin{aligned} f_{5,6}=(&a_0^2k_7r_0\{r_6+3a_1r_5+(3a_2+3a_1^2)r_4+(3a_3+6a_1a_2+a_1^3)r_3+(3a_4+6a_1a_3+3a_2^2+3a_1^2a_2)r_2\\ &+[3a_5+6a_1a_4+(6a_2+3a_1^2)a_3+3a_1a_2^2]r_1+3a_6+6a_1a_5+(6a_2+3a_1^2)a_4+3a_3^2+6a_1a_2a_3+a_2^3\}\\ &+k_8p_0(2p_6+2a_1p_5+2a_2p_4+2a_3p_3+2a_4p_2+2a_5p_1+2a_6)\\ &+a_0^3[8a_6+24a_1a_5+(24a_2+24a_1^2)a_4+12a_3^2+(48a_1a_2+8a_1^3)a_3+8a_2^3+12a_1^2a_2^2]k_9)/(2a_0^3)\ .\end{aligned}$$

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