Improved quantum hard-sphere ground-state equations of state

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The London ground-state energy formula as a function of number density for a system of identical boson hard spheres, corrected for the reduced mass of a pair of particles in a "sphere-of-influence" picture, and generalized to fermion hard-sphere systems with two and four intrinsic degrees of freedom, has a double-pole at the ultimate *regular* (or periodic, e.g., face-centered-cubic) close-packing density usually associated with a crystalline branch. Improved fluid branches are constructed based upon exact, field-theoretic perturbation-theory low-density expansions for many-boson and many-fermion systems, extrapolated to intermediate densities via Padé and other approximants, but whose ultimate density is irregular or *random* closest close-packing as suggested in studies of a classical system of hard spheres. Results show substantially improved agreement with the best available Green-function Monte Carlo and diffusion Monte Carlo simulations for bosons, as well as with ladder, variational Fermi hypernetted chain, and so-called *L*-expansion data for two-component fermions.

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I. INTRODUCTION

An analytical formula for the ground-state energy E of an N-hard-sphere-boson system of volume Ω for all particle-number densities $\rho \equiv N/\Omega$ was proposed by London [1] as

$$E/N = \frac{2\pi\hbar^2 c}{m} \frac{1}{(\rho^{-1/3} - \rho_0^{-1/3})^2} \frac{1}{(\rho^{-1/3} + b\rho_0^{-1/3})}, \tag{1}$$

where m is the particle mass, c is the hard-sphere diameter and the constant b equals $2^{5/2}/\pi - 1$. Here, $\rho_0 \equiv \sqrt{2}/c^3$ is the assumed ultimate regular (or periodic) close-packing density at which a system of identical classical hard spheres close-pack in a primitive-hexagonal arrangement, e.g., face-centered-cubic or hexagonal. As remarked by Rogers [2], this is what "many mathematicians believe and all physicists know" to be the case. However, the Kepler 1611 conjecture [3] that $\rho_0 \equiv \sqrt{2}/c^3$ is the ultimate packing density for identical hard spheres seems to be approaching theorem status [4] after many attempts of proof.

The justification given for Eq. (1) is that it reduces smoothly to limiting expressions at both low and high densities, namely

$$E/N \underset{\rho \to 0}{\to} (2\pi\hbar^2/m)\rho c, \tag{2}$$

$$E/N \underset{\rho \to \rho_0}{\to} A(\hbar^2/2m)(\rho^{-1/3} - \rho_0^{-1/3})^{-2}, \tag{3}$$

but gives no indication of a "freezing" or Kirkwood [5] phase transition at some number density ρ between 0 and ρ_0. Here $A = \pi^2/2^{1/3} \simeq 7.8335$ is a constant called the *residue* of the second-order (or double) pole at close packing. Using the polyhedron cell method suggested in Ref. [6], the value of A has been predicted [7] theoretically to lie within the rigorous range

$$1.63 \leq A \leq 27.0. \tag{4}$$

The low-density leading term (2) is the celebrated Lenz [8] term, calculated by him as the leading correction to the energy arising from an "excluded volume" effect. The Lenz term has finally been rigorously established [9]. The limit (3) comes from the lowest Schrödinger equation eigenvalue of a particle in a spherical cavity, and is just the kinetic energy of a point particle of mass m inside the cavity of radius $r-c$, where r is the average separation between two neighboring hard spheres and $r = (\sqrt{2}/\rho)^{1/3}$ by assuming a primitive-hexagonal packing arrangement for the cavities.

More recently it was found [10], however, that the arguments leading to the high-density limit of the original [1] (boson) London Eq. (1) are flawed by a fundamental error: the spherical cavity of radius $r-c$ alluded to above in reality refers to the "sphere of influence" of *two* particles. Thus the particle mass used in obtaining Eq. (3) should refer to the *reduced mass* $m/2$ of the pair. This yields the constant

$$b \equiv 2^{3/2}/\pi - 1 \tag{5}$$

instead of the constant $2^{5/2}/\pi - 1$ given by London for Eq. (1). The result (1) with Eq. (5) is designated the *modified London (ML) equation*. It continues to satisfy Eq. (2) as this is independent of the constant b but the residue A in Eq. (3) now becomes $2^{2/3}\pi^2 \simeq 15.667$ instead of the previous $\pi^2/2^{1/3} \simeq 7.8335$ associated with the original London equation, and fully agrees with the empirical residue of 15.7 ± 0.6, extracted by Cole [11] from high-pressure crystalline-branch data in ^{3}He, ^{4}He, H_2, and D_2 systems. Moreover, this ML

equation exhibits dramatically better agreement than the original London (L) equation with Green-function Monte Carlo (GFMC) [12] computer-simulation data points for both fluid and crystalline branches of the boson hard-sphere system.

A generalized London equation has also been proposed [13] for *N-fermion* hard-sphere systems with ν intrinsic degrees of freedom for each fermion. Here $\nu=2$ for, say, liquid ^{3}He or neutron matter, both constituent fermions of which have spin 1/2, and $\nu=4$ for nuclear matter consisting of both neutrons *and* protons of spin 1/2. As ν is essentially the maximum occupation in a given single-particle quantum state, it can be taken as infinite in the case of bosons. For fermions, two differences appear with respect to the boson London formula: (i) unlike the boson case, the ground-state kinetic energy for fermions is nonzero and is added as a well-known [14] ν-dependent leading term; and (ii) the constant b is allowed to be ν dependent, being replaced by

$$b_\nu(\nu) = [(\nu-1)/\nu](b+1) - 1, \tag{6}$$

which clearly approaches b as $\nu\to\infty$. The latter form also ensures a *ν-independent* energy at close-packing where, since the spheres can be labeled so that indistinguishability as well as particle statistics disappears, as expected in this classical limit. Substitution of b_ν for the constant b in Eq. (1) gives a generalized form of the modified London equation (ML_ν),

$$E/N = C_\nu \rho^{2/3} + \left(\frac{\nu-1}{\nu}\right)\frac{2\pi\hbar^2 c}{m}\frac{1}{(\rho^{-1/3}-\rho_0^{-1/3})^2}\frac{1}{[\rho^{-1/3}+b_\nu(\nu)\rho_0^{-1/3}]} \tag{7}$$

with

$$C_\nu \equiv \frac{3\hbar^2}{10m}\left(\frac{6\pi^2}{\nu}\right)^{2/3} \underset{\nu\to\infty}{\to} 0. \tag{8}$$

For $\nu\to\infty$, $b(\nu)\to b$ according to Eq. (6), and Eq. (7) goes over into the boson case (1) because C_ν vanishes in this limit. The low-density limit of Eq. (7) is

$$E/N \underset{\rho\to 0}{\to} C_\nu \rho^{2/3} + \left(\frac{\nu-1}{\nu}\right)\frac{2\pi\hbar^2}{m}\rho c, \tag{9}$$

where the second term on the right-hand side is the Lenz term for ν-component fermions in three dimensions. On the other hand, for $\rho\to\rho_0\equiv\sqrt{2}/c^3$ one sees that Eq. (7) reduces to Eq. (3) as it should. In other words, hard-sphere fermions, bosons, or "boltzons" must all close-pack regularly *at the same density*. From this it follows that the residue for bosons or fermions is the same and equal to $2^{2/3}\pi^2 \simeq 15.667$, in excellent agreement with the empirical Ref. [11] value of 15.7 ± 0.6.

For bosons, in addition to the Lenz term (2) for the low-density fluid branch, several higher-order corrections to the ground-state energy per particle have been derived using quantum field-theoretic many-boson perturbation theory [15,16]. They give

$$E/N = \frac{2\pi\hbar^2\rho c}{m}\{1 + C_1(\rho c^3)^{1/2} + C_2\rho c^3 \ln(\rho c^3) + C_3\rho c^3 + o(\rho c^3)\} \tag{10}$$

for $\rho c^3 \ll 1$, where $C_1 = 128/15\sqrt{\pi}$ and $C_2 = 8(4\pi/3-\sqrt{3})$, but C_3 is an as yet unknown constant. Here, c denotes the S-wave scattering length for a general potential; for a hard-core potential it is just the hard-sphere diameter. The series is clearly not a *pure* power series expansion, and is at best an asymptotic series.

Similarly, for an N-fermion hard-sphere system the corresponding series is [17]

$$E/N = \frac{3}{5}\frac{\hbar^2 k_F^2}{2m}\{1 + C_1(k_F c) + C_2(k_F c)^2 + [C_3 r_0/2c + C_4 A_1(0)/c^3 + C_5](k_F c)^3 + C_6(k_F c)^4 \ln(k_F c) + [C_7 r_0/2c + C_8 A_0''(0)/c^3 + C_9](k_F c)^4 + o(k_F c)^4\} \tag{11}$$

for $k_F c \ll 1$ and where the C_j $(j=1,2,\ldots,9)$ are dimensionless coefficients depending on ν; they are given in Ref. [18] for $\nu=2$ and $\nu=4$. The Fermi momentum $\hbar k_F$ is defined through the fermion-number density

$$\rho \equiv N/\Omega = \nu k_F^3/6\pi^2 \tag{12}$$

with Ω the system volume, so that the Lenz term expressed in terms of ρ is identical to the boson Lenz term apart from a factor of $(\nu-1)/\nu$ which is the average number of fermions the Pauli principle allows a given fermion to interact with at the shortest possible range.

Unfortunately, both low-density expansions (10) and (11) lack accuracy at moderate to high densities, including the saturation (or equilibrium, zero-pressure) densities of liquid ^{4}He ($\nu=\infty$) [19] and liquid ^{3}He ($\nu=2$) or nuclear matter ($\nu=4$). However, one can extrapolate the series for hard-sphere systems to physical and even to close-packing densities through the use of Padé [20] and/or a modest extension of these called the "tailing" [21] approximants. The so-called quantum thermodynamic (or van der Waals) perturbation theory (QTPT) [22,23] has provided fairly accurate representations of the *fluid* branch of the equation of state of quantum hard-sphere systems [24], even beyond freezing (or Kirkwood) phase transition densities, but without sufficient credibility as one approaches close packing. This is clear since one does not possess a *single* ground-state energy function with implicit information of *both* fluid and crystalline branches, with presumably different close-packing ultimate densities.

In Sec. II we discuss the double (or second-order) pole behavior for the equation-of-state fluid branch conceivably ending at *random* closest close-packing, instead of the *regular* close-packing at which the crystalline branch terminates; in Secs. III and IV we construct analytical expressions for the fluid branches for hard-sphere bosons and fermions, respectively. Section V gives our conclusions.

II. DOUBLE-POLE CONDITIONS AT CLOSE PACKING

We shall assume that the fluid branch of the hard-sphere equation of state will terminate not at the regular close-

packing density ρ_0 but rather at the random closest close packing (rccp), sometimes called the Bernal, density ρ_{rccp} (or "maximally random jammed" packing [25]). Its value was originally determined empirically [26] with actual ball-bearing packings. Near the density ρ_{rccp} we expect, based on Eq. (3), that the energy for a hard-sphere boson or fermion gas has the following behavior:

$$E/N \underset{\rho\to\rho_{rccp}}{\to} A(\hbar^2/2m)(\rho^{-1/3}-\rho_{rccp}^{-1/3})^{-2}, \tag{13}$$

with A the *residue* which could be different for each system. Random close-packing densities range [27] from about $0.06\rho_0$ to $0.86\rho_0 \equiv \rho_{rccp}$.

The derivative of Eq. (13) with respect to ρ then tends asymptotically to

$$\frac{d(E/N)}{d\rho} \underset{\rho\to\rho_{rccp}}{\to} \frac{A(2/3)(\hbar^2/2m)}{(\rho^{-1/3}-\rho_{rccp}^{-1/3})^3\rho^{4/3}} \tag{14}$$

while

$$\frac{d\ln(E/N)}{d\rho} \underset{\rho\to\rho_{rccp}}{\to} \frac{2/3}{(\rho^{-1/3}-\rho_{rccp}^{-1/3})\rho^{4/3}} \tag{15}$$

is residue independent. We shall assume that A is the same for boson as for fermion hard spheres and that their rccp density is likewise identical since at closest close-packing the particles become localized by definition, enabling one to formally label each particle; this makes them distinguishable thus rendering (quantum) statistics irrelevant. Note that the pressure $P=\rho^2[d(E/N)/d\rho]$ from Eq. (14) also diverges as $\rho\to\rho_{rccp}$, as expected.

III. BOSON HARD-SPHERE FLUID

In order to extrapolate the low-density series (10) to higher densities we start by writing it as

$$E/N = \frac{2\pi\hbar^2}{m}\rho c e_0(x), \tag{16}$$

where $x \equiv (\rho c^3)^{1/2}$ and

$$e_0(x) \equiv 1 + C_1 x + C_2 x^2 \ln x^2 + C_3 x^2 + O(x^3 \ln x^2) \tag{17}$$

for $x \ll 1$. Alternatively, one can rewrite this series as

$$e_0^{-1/2}(x) = 1 + K_1 x + K_2 x^2 \ln x^2 + K_3 x^2 + O(x^3 \ln x^2), \tag{18}$$

where the K_i's are expressible in terms of the C_i's. As C_3 is to date unknown, consequently K_3 is also unknown. Values of the C_i's and K_i's are given in Table I. We analyze the series $e_0^{-1/2}(x)$ instead of the series $e_0(x)$ to ensure that any zeros in its extrapolants, say $\epsilon_0^{-1/2}(x)$, are double (or second-order) poles in the energy as one expects at any kind of close packing. The extrapolants are generated as a quotient of two polynomials such that on expansion one recovers the first terms of the original series. Series (18) with three terms beyond unity has 12 extrapolants correctly generated in Ref. [28] but fitted there to erroneous values (i.e., to one-half the correct values) GFMC data points [12]. Adjusting various extrapolants [24] to best fit the four known GFMC data points ensures a good value for the unknown coefficient K_3 in Eq. (18). The extrapolant designated "XI (bosons)" in Fig. 2 of Ref. [24] had the least mean-square deviation with respect to the four GFMC fluid-branch data points. Therefore we adopt it as our best initial extrapolant. The ground-state energy per particle for boson hard spheres was thus represented (symbol $\doteq$) by

TABLE I. Coefficients C_i and K_i for bosons appearing in Eqs. (17) and (18), respectively. Numbers in quotation marks are determined as indicated in text.

Bosons ($\nu=\infty$)	$i=1$	2	3
C_i	4.81441778	19.65391518	"73.296"
K_i	−2.40720889	−9.826957589	"−27.956"

$$E/N \doteq \frac{2\pi\hbar^2}{m}\rho c \epsilon_0(\rho) \tag{19}$$

with $K_3 \simeq -27.956$. However, as diffusion Monte Carlo (DMC) calculations became available [29] spanning a wider range of densities in the fluid region than GFMC data, we realized that although our expression XI (x) in Eq. (17) of Ref. [24] agrees well with DMC and GFMC data around the freezing transition, its disagreement with the DMC data at low to intermediate densities suggested the possibility of improving the extrapolant. As will be seen, the new extrapolant $\epsilon_0^{-1/2}$ predicts a random closet close-packing (rccp) density $\rho_{rccp}/\rho_0 \simeq 0.776$ which is only about 10% below the classical hard-spheres empirical [26] rccp value $\simeq 0.86$ mentioned before and also assumed to be the ultimate rccp density for quantum hard-sphere fluids.

In order to improve the fluid-branch expression of Ref. [24] for *low to intermediate* densities we use the two double-pole conditions (13) and (14) which lead to the following conditions on the extrapolant $\epsilon_0(x)$ to be used in Eq. (19) namely

$$\epsilon_0 = \frac{mE}{N2\pi\hbar^2\rho c} \underset{\rho\to\rho_{rccp}}{\to} \frac{A}{4\pi\rho c}(\rho^{-1/3}-\rho_{rccp}^{-1/3})^{-2}.$$

This is equivalent to

$$\epsilon_0^{-1/2}(\rho) \underset{\rho\to\rho_{rccp}}{\to} [A/4\pi\rho c]^{-1/2}(\rho^{-1/3}-\rho_{rccp}^{-1/3}) \underset{\rho\to\rho_{rccp}}{\to} 0. \tag{20}$$

The condition (14) gives

$$\frac{d(\epsilon_0^{-1/2})}{d\rho} \underset{\rho\to\rho_{rccp}}{\to} -\frac{1}{3}[A/4\pi c]^{-1/2}\rho_{rccp}^{-5/6}. \tag{21}$$

Strictly, any log term should be accompanied by a constant, if known, because the scaling of ρ by c^3 is arbitrary. We thus propose the representation of $e_0(x)$ in Eq. (17) as given by

$$e_0^{-1/2}(x) \doteq \frac{1+K_1 x+\beta x^2+\gamma x^3}{1-K_2 x^2 \ln x^2+\alpha x^2} \equiv \epsilon_{0B}^{-1/2}(x), \tag{22}$$

where α, β, and γ are to be determined from Eqs. (20) and (21) and by fitting both DMC [29] and GFMC ([12], Table I)

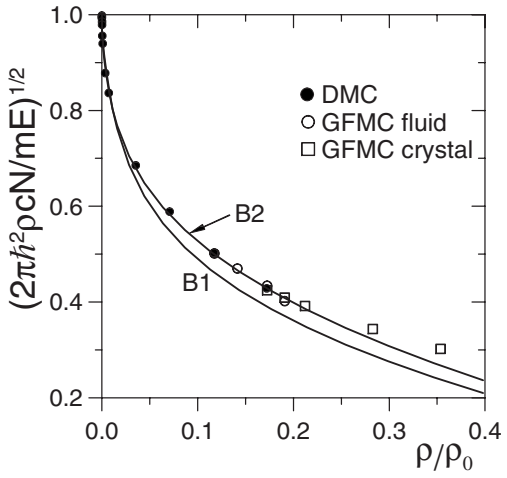

FIG. 1. The quantity $\epsilon_0^{-1/2}=\sqrt{2\pi\hbar^2\rho cN/mE}=[1-(\rho/\rho_0)^{1/3}]\sqrt{1+b(\rho/\rho_0)^{1/3}}$ as a function of x/x_0 for boson hard sphere systems: B1 and B2 refer to Eqs. (22) and (24) with $A\simeq 15.7$ and $A\simeq 11.9$, respectively. Larger dots are GFMC fluid data and smaller dots refer to DMC (fluid) calculations.

data. In this approximant the terms in $x^2\ln x$ and x^2 are kept together. Condition (20) applied to Eq. (22) gives

$$1+K_1x_{rccp}+\beta x_{rccp}^2+\gamma x_{rccp}^3=0. \tag{23}$$

The second condition (21) can be rewritten as

$$\left.\frac{d(\epsilon_{0B}^{-1/2})}{dx}\frac{dx}{d\rho}\right|_{x=x_{rccp}}=\frac{K_1+2\beta x_{rccp}+3\gamma x_{rccp}^2}{1-K_2x_{rccp}^2\ln x_{rccp}^2+\alpha x_{rccp}^2}\frac{c^3}{2x_{rccp}}$$
$$=-\frac{1}{3}[A/4\pi c]^{-1/2}\rho_{rccp}^{-5/6}. \tag{24}$$

Substituting Eq. (23) in the last equation we obtain β in terms of α, namely,

$$-\beta x_{rccp}^2=3+2K_1x_{rccp}-[A/4\pi]^{-1/2}\frac{2}{3}$$
$$\times x_{rccp}^{1/3}(1-K_2x_{rccp}^2\ln x_{rccp}^2+\alpha x_{rccp}^2). \tag{25}$$

Now substituting Eq. (25) in Eq. (23) we arrive at

$$\gamma x_{rccp}^3=2+K_1x_{rccp}-[A/4\pi]^{-1/2}\frac{2}{3}$$
$$\times x_{rccp}^{1/3}(1-K_2x_{rccp}^2\ln x_{rccp}^2+\alpha x_{rccp}^2). \tag{26}$$

Introducing Eqs. (25) and (26) in Eq. (22), we get

$$\epsilon_{0B}^{-1/2}(x)=\Big[1+K_1x+(x/x_{rccp})^2\{-3-2K_1x_{rccp}\}+(x/x_{rccp})^3$$
$$\times\{2+K_1x_{rccp}\}+[A/4\pi]^{-1/2}\frac{2}{3}x_{rccp}^{1/3}(1-K_2x_{rccp}^2$$
$$\times\ln x_{rccp}^2+\alpha x_{rccp}^2)\{(x/x_{rccp})^2-(x/x_{rccp})^3\}\Big]$$
$$\times[1-K_2x^2\ln x^2+\alpha x^2]^{-1} \tag{27}$$

from which after some algebra one obtains a single equation for α, namely,

$$[\epsilon_{0B}^{-1/2}(\alpha,A,x)](1-K_2x^2\ln x^2)-1-K_1x+(x/x_{rccp})^2$$
$$\times\{3+2K_1x_{rccp}\}-[A/4\pi]^{-1/2}\frac{2}{3}x_{rccp}^{1/3}(1-K_2x_{rccp}^2\ln x_{rccp}^2)$$
$$\times\{(x/x_{rccp})^2-(x/x_{rccp})^3\}-(x/x_{rccp})^3\{2+K_1x_{rccp}\}$$
$$=\alpha\Big\{x_{rccp}^2[A/4\pi]^{-1/2}\frac{2}{3}x_{rccp}^{1/3}[(x/x_{rccp})^2-(x/x_{rccp})^3]$$
$$-x^2[\epsilon_{0B}^{-1/2}(\alpha,A,x)]\Big\}, \tag{28}$$

where we have explicitly written the dependence of $\epsilon_{0B}^{-1/2}(x)$ on α and A. To determine α from the DMC [29] and/or GFMC data we must calculate the values α_i^{DMC} [from Eq. (28) after replacing $\epsilon_{0B}^{-1/2}(\alpha,A,x)$ by the $\epsilon_{0-DMC}^{-1/2}(x_i^{DMC})$ obtained from Eq. (19) as $(2\pi\hbar^2\rho cN/Em)^{1/2}$ with E/N the energy from DMC calculations] for each x_i^{DMC} for $i=1,2,\ldots N$ values, and then minimizes $\Sigma_{i=1}^N(\alpha_i^{DMC}-\alpha)^2$ by imposing

$$\frac{d}{d\alpha}\sum_{i=1}^{N}(\alpha_i^{DMC}-\alpha)^2=0,$$

which gives

$$\alpha=\sum_{i=1}^{N}\alpha_i^{DMC}/N.$$

Since the fluid branch GFMC data are a subset of DMC data, we have used these to calculate α here, determining A in the next step. For residue A fixed at $2^{2/3}\pi^2\simeq 15.667$ as described below Eq. (5), we obtain an optimal $\alpha\simeq 114.282$ which from Eqs. (25) and (26) leads to $\beta\simeq 74.0891$ and $\gamma\simeq -65.9475$. The curve then corresponding to Eq. (22) is labeled B1 in Fig. 1.

Alternatively, if we allow the residue A to be free one may ask for a solution minimizing $\Sigma_{i=1}^N[\epsilon_{0-DMC}^{-1/2}(x_i^{DMC})-\epsilon_{0B}^{-1/2}(\alpha,A,x_i^{DMC})]^2$ with respect α and A, i.e.,

$$\frac{d}{d\alpha}\sum_{i=1}^{N}[\epsilon_{0-DMC}^{-1/2}(x_i^{DMC})-\epsilon_{0B}^{-1/2}(\alpha,A,x_i^{DMC})]^2$$
$$=-\sum_{i=1}^{N}2[\epsilon_{0-DMC}^{-1/2}(x_i^{DMC})-\epsilon_{0B}^{-1/2}(\alpha,A,x_i^{DMC})]$$
$$\times\frac{d}{d\alpha}\epsilon_{0B}^{-1/2}(\alpha,A,x_i^{DMC})=0$$

or

$$\sum_{i=1}^{N} 2[\epsilon_{0-DMC}^{-1/2}(x_i^{DMC}) - \epsilon_{0B}^{-1/2}(\alpha,A,x_i^{DMC})]\frac{-Y(\alpha,A,x_i)x^2 + (A/4\pi)^{-1/2}\frac{2}{3}x_{rccp}^{1/3}x_{rccp}^2[(x/x_{rccp})^2 - (x/x_{rccp})^3]}{1 - K_2x^2\ln x^2 + \alpha x^2} = 0 \tag{29}$$

as well as of

$$\frac{d}{dA}\sum_{i=1}^{N}[\epsilon_{0-DMC}^{-1/2}(x_i^{DMC}) - \epsilon_{0B}^{-1/2}(\alpha,A,x_i^{DMC})]^2 = -\sum_{i=1}^{N} 2[\epsilon_{0-DMC}^{-1/2}(x_i^{DMC}) - \epsilon_{0B}^{-1/2}(\alpha,A,x_i^{DMC})]\frac{d}{dA}\epsilon_{0B}^{-1/2}(\alpha,A,x_i^{DMC}) = 0$$

or

$$\sum_{i=1}^{N} 2[\epsilon_{0-DMC}^{-1/2}(x_i^{DMC}) - \epsilon_{0B}^{-1/2}(\alpha,A,x_i^{DMC})]\frac{(A/4\pi)^{-3/2}(1/12\pi)x_{rccp}^{1/3}(1 - K_2x_{rccp}^2\ln x_{rccp}^2 + \alpha x_{rccp}^2)[(x/x_{rccp})^2 - (x/x_{rccp})^3]}{1 - K_2x^2\ln x^2 + \alpha x^2} = 0. \tag{30}$$

Under the two conditions (29) and (30) we find an optimal $A \simeq 11.8715$ and an optimal $\alpha \simeq 169.516$, leading to $\beta \simeq 124.1$ and $\gamma \simeq -111.296$. This procedure gives the curve labeled B2 in Fig. 1. Note that the residue 11.8715 is now being associated with the *random* closest close-packing (rccp) density $0.86\rho_0$ of hard spheres. This value of A is somewhat smaller than the residue 15.667 at *regular* close-packing density ρ_0, though still within the rigorous range stated in Eq. (4).

Figure 2 compares the previous fluid branch expression XI (x), Eq. (17) of Ref. [24], with the present extrapolant (22) labeled B2, both as full curves. The dashed curve is the modified London (ML) formula (1) that connects smoothly with the crystalline branch. Open circles and squares are GFMC data for fluid and crystalline branches, respectively. Dots represent DMC [29] data spanning a wider range of densities in the fluid region than the GFMC data. The new expression B2 shows dramatically better agreement with DMC data for intermediate densities, as well as agreeing well with both DMC and GFMC data around the freezing transition mentioned in Table I of Ref. [12]. Figure 3 is an enlargement of Fig. 2 at low densities to show the remarkable agreement of B2 with the DMC data.

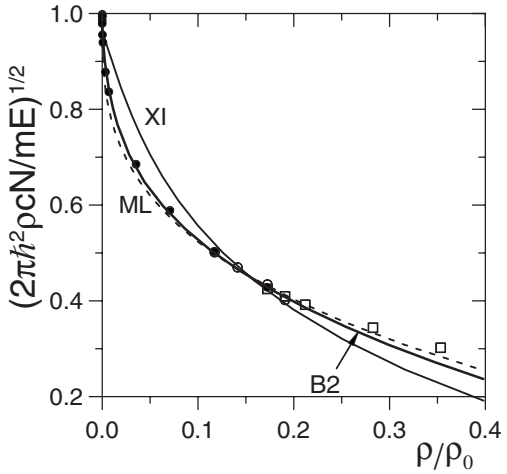

FIG. 2. The quantity $\epsilon_0^{-1/2} = \sqrt{2\pi\hbar^2\rho cN/mE} = [1 - (\rho/\rho_0)^{1/3}]\sqrt{1 + b(\rho/\rho_0)^{1/3}}$ as a function of ρ/ρ_0 for the boson hard-sphere system: XI is the fluid branch approximant of Ref. [24], Fig. 2; B2 refers to Eqs. (22) and (24) with $A \simeq 11.9$; ML is the modified London formula (1). Open circles and squares are GFMC data for the fluid and crystalline branches, respectively, and dots are DMC data points.

IV. FERMION HARD-SPHERE FLUID BRANCH

The ground-state energy per particle for fermion hard-sphere fluids (11) can be written as

$$E/N = \frac{3}{5}\frac{\hbar^2k_F^2}{2m}e_0(x), \quad x \equiv k_Fc \tag{31}$$

with

$$e_0(x) \equiv 1 + C_1x + C_2x^2 + (C_3/3 + C_4/3 + C_5)x^3 + C_6x^4\ln x + (C_7/3 - C_8/3 + C_9)x^4 + o(x^4) \tag{32}$$

for $x \equiv k_Fc \ll 1$, $\rho \equiv N/\Omega = \nu k_F^3/6\pi^2$ being the number of fer-

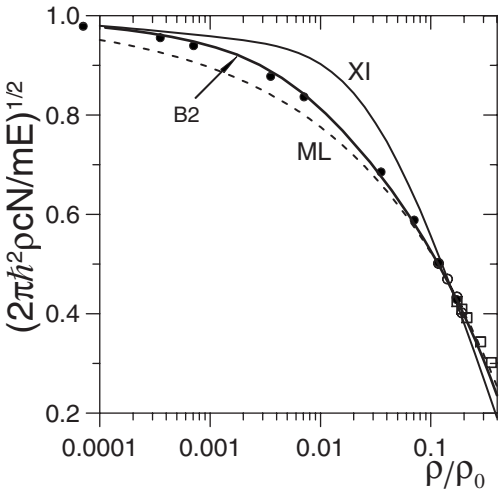

FIG. 3. Enlargement of Fig. 2 at low densities.

TABLE II. Coefficients D_i and F_i for $\nu=2$ appearing in Eqs. (33) and (34), respectively. Numbers in quotation marks were determined as indicated in text.

$\nu=2$	$i=1$	2	3	4	5
D_i	0.353678	0.185537	0.384145	−0.024700	"−0.265544"
F_i	−0.176833	−0.045863	−0.156677	0.109672	"0.130830"

mions N in the enclosed volume Ω. We shall examine both $\nu=2$ (corresponding to liquid ^{3}He and neutron matter) and $\nu=4$ (corresponding to nuclear matter).

A. Fermions with $\nu=2$

For $\nu=2$, $C_6=0$ [17] so that Eq. (32) simplifies to the pure power series

$$e_0(x) = 1 + D_1 x + D_2 x^2 + D_3 x^3 + D_4 x^4 + o(x^4), \quad (33)$$

where the C_i's have been determined in terms of the D_i's. As in the boson case, instead of $e_0(x)$ we consider the series

$$e_0^{-1/2}(x) = 1 + F_1 x + F_2 x^2 + F_3 x^3 + F_4 x^4 + F_5 x^5 + o(x^5), \quad (34)$$

where the F_i's depend algebraically on the D_i's in a simple manner, F_5 being unknown. Values of D_i and F_i are given in Table II. We use this simple power series to construct the usual Padé extrapolants. The approximants to Eq. (34) with four terms beyond the trivial unity were analyzed in Ref. [30], where it was concluded that the best approximant was the Padé $[0/4](x)$. However, this function does not have a zero in the region of physical interest, i.e., $0 \le \rho/\rho_0 \le 1$, which implies $0 \le x \equiv k_F c \le 3.47$ since $\rho = k_F^3/3\pi^2$. Accordingly, the energy does not manifest a close-packing density as it should. This deficiency made it advisable to introduce the fifth term $F_5 x^5$ in Eq. (34). Although in Fig. 1 of Ref. [31] only five of the six *two-point* Padé approximants $[L//M](x)$ with $L+M=5$ are shown, all six approximants were analyzed here to adjust F_5 so as to ensure a zero associated with a random close-packing in the physical region. The approximant $\epsilon_0(x)$ and the position of its zero were chosen in such way that the QTPT applied in Ref. [30] to calculate the ground-state energy of ^{3}He with the Aziz interatomic potential [32] reproduces the corresponding GFMC [34] data. [In this treatment, the Aziz potential was decomposed via the well-known Barker-Henderson (BH) [33] scheme as described in Ref. [30].] Eventually, the best extrapolant was found to be the *two-point* Padé approximant

$$e_0^{-1/2}(x) \doteq [3//2](x) \equiv \frac{N_0 + N_1 x + N_2 x^2 + N_3 x^3}{M_0 + M_1 x + M_2 x^2} \equiv \epsilon_0^{-1/2}(x), \quad (35)$$

where

$$N_0 = F_2 F_4 - F_3^2,$$

$$N_1 = F_4(F_3 + F_1 F_2) - F_2 F_5 - F_1 F_3^2,$$

$$N_2 = (F_3 - F_1 F_2) F_5 - F_4^2 + (F_1 F_3 + F_2^2) F_4 - F_2 F_3^2,$$

$$N_3 = (F_1 F_3 - F_2^2) F_5 - F_1 F_4^2 + 2 F_2 F_3 F_4 - F_3^3,$$

$$M_0 = F_2 F_4 - F_3^2, \quad M_1 = F_3 F_4 - F_2 F_5, \quad M_2 = F_3 F_5 - F_4^2.$$

The extrapolant (35) satisfies $[3//2](x=3.13)=0$. Hence the ground-state energy per fermion for $\nu=2$ becomes

$$E/N \doteq \frac{3}{5}\frac{\hbar^2 k_F^2}{2m}\{[3//2](x)\}^{-2} \quad (36)$$

with a random closest close-packing density $\rho_{rccp}/\rho_0 = 0.732$ only 15% smaller than the empirical [26] value $\rho_{rccp}/\rho_0 \simeq 0.86$. The coefficient F_5 is listed in Table II in quotation marks. In Fig. 4 we show the expression

$$\begin{aligned}\epsilon_0^{-1/2} &= [3\hbar^2(6\pi^2\rho/\nu)^{2/3}N/10mE]^{1/2} \\ &= 1 + [20\pi(\nu-1)/3\nu](2^{1/4}\nu/6\pi^2)^{2/3} \\ &\quad \times\{[(\rho/\rho_0)^{-1/3} - 1]^2[(\rho/\rho_0)^{-1/3} - b(\nu)](\rho/\rho_0)^{2/3}\}^{-1}\end{aligned} \quad (37)$$

as a function of ρ/ρ_0 for fermion hard spheres. Here $b(\nu)$ is as defined in Eq. (6). For $\nu=2$ the fluid branch $[3//2]$ (full curve) given by Eq. (35) is close to the ladder [35] (open squares), the variational Fermi hypernetted chain (VFHNC) [36] (plus-sign marks), and the so-called L-expansion data

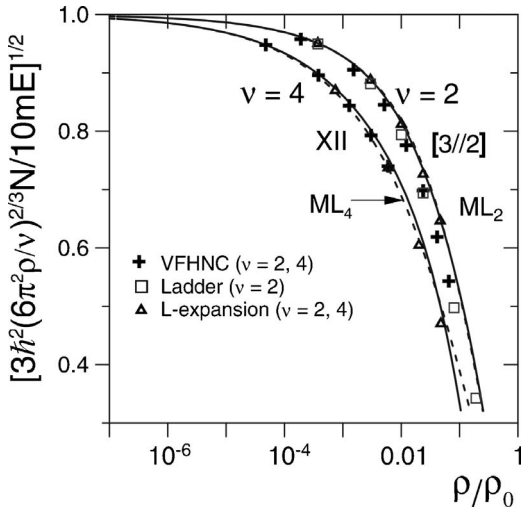

FIG. 4. The expression (37) as a function of ρ/ρ_0 for fermion hard spheres with $\nu=2$ labeled $[3//2]$ and with $\nu=4$ labeled XII (full curves). Dashed curves are the corresponding modified London ML_ν formulas, but note that the ML_2 dashed curve almost coincides with the full curve $[3//2]$.

TABLE III. The F_5 and F_6 coefficients for $\nu=2$ that follow from conditions (38) and (39) for all sixth-order Padé approximants with residue $A \simeq 15.667$ and random closest close-packing density $\rho_{rccp} \equiv 0.86\rho_0$.

Padé	F_5	F_6
[5/1]	−0.0272548	0.0038205
[4/2]	−0.20	no solution
[3/3]	−0.0130625	0.0039120
[2/4]	−0.0395076	0.0415222
[1/5]	−0.0115902	0.01887153
[0/6]	−0.1276	no solution

[37,38] (open triangles). Figure 4 shows good agreement over the entire range of available data.

In order to improve the many-fermion ground-state energy equation of state we include the next term in Eq. (34), i.e., F_6x^6, which is then used to generate all Padé approximants of order six to the series $\epsilon_0^{-1/2}(x)$. The lack of a logarithmic term $x^4 \ln x$ is due to the Pauli principle [17]. Such a term arises when there are *three* independent hole lines. But for $\nu=2$ there can be at most *two* lines of the same spin. Thus the Pauli principle reduces the size of the term by a factor of the density. We thus expect the first such term for $\nu=2$ to be $O(x^7 \ln x)$. The unknown coefficients F_6 and F_5 are determined from the two double-pole conditions (13) and (14), which become

$$\epsilon_0^{-1/2}(x) \underset{\rho\to\rho_{rccp}}{\to} (1 - x/x_{rccp})[5A/3(3\pi^2)^{2/3}]^{-1/2} \tag{38}$$

and

$$\epsilon_0(x) + \frac{x}{2}\frac{d\epsilon_0(x)}{dx} \underset{\rho\to\rho_{rccp}}{\to} \frac{5A/3(3\pi^2)^{2/3}}{(1 - x/x_{rccp})^3} \tag{39}$$

with $A \simeq 15.667$.

For each Padé approximant of order 6 we determined F_6 and F_5 as shown in Table III. Approximants [4/2] and [0/6] did not exhibit the double-pole conditions. The other four approximants are plotted in Fig. 5 together with the ladder [35] (open squares), the variational Fermi hypernetted chain (VFHNC) [36] (plus-sign marks), and the *L*-expansion [37] (open triangles) data for $\nu=2$, from which we conclude that the approximant [3/3](x) is the best. Figure 6 is a semilog enlargement of Fig. 5. In Fig. 7 we compare both the new improved expression [3/3](x) and the previous best energy expression, i.e., the two-point Padé approximant [3//2](x) reported in Ref. [24] and supported by ladder, VFHNC, and *L*-expansion data.

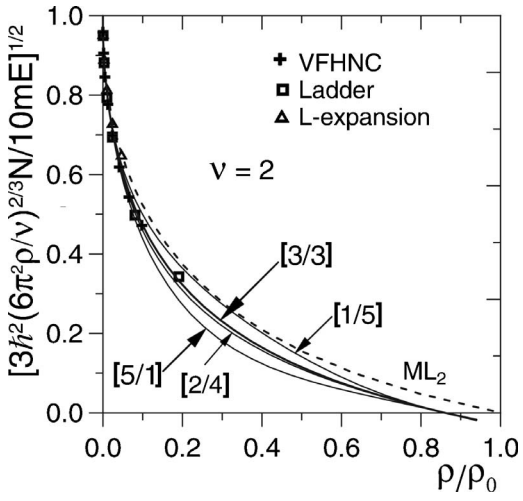

FIG. 5. Improved extrapolants for the many-fermion hard-sphere gas with $\nu=2$.

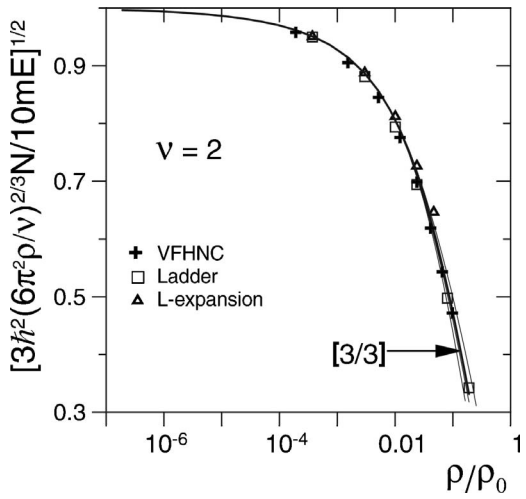

FIG. 6. Enlargement of Fig. 5 at low densities.

B. Fermions with $\nu=4$

For fermions with $\nu=4$ Eq. (32) becomes

$$e_0(x) = 1 + D_1x + D_2x^2 + D_3x^3 + D_4x^4 \ln x + D_5x^4 + o(x^4) \tag{40}$$

for $x \equiv k_Fc \ll 1$ and we recall that $\rho = \nu k_F^3/6\pi^2$. As for bosons or for fermions with $\nu=2$, we analyze

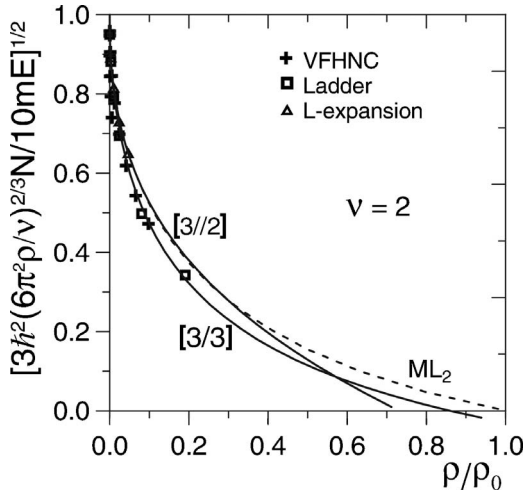

FIG. 7. Comparison of quantity (37) as a function of ρ/ρ_0 for many-fermion hard spheres with $\nu=2$, for the previously best approximant [3//2](x) [24] and the new improved one [3/3](x), full curves. Dashed curve is modified London formula.

TABLE IV. Coefficients D_i and F_i for $\nu=4$ appearing in Eqs. (40) and (41), respectively.

$\nu=4$	$i=1$	2	3	4
D_i	1.061033	0.556610	1.300620	−1.408598
F_i	−0.530517	0.143867	−0.5806558	−0.704299

$$e_0^{-1/2}(x) = 1 + F_1 x + F_2 x^2 + F_3 x^3 + F_4 x^4 \ln x + F_5 x^4 + o(x^4) \tag{41}$$

with all F_i $(i=1,2,3,4)$ known. Values of D_i and F_i are given in Table IV. Unlike the $\nu=2$ case, this series is not a pure power series as it contains logarithmic terms. Its so-called "tailing" [21] approximants are given in Table III of Ref. [28]. Of all the possible approximants using only the known coefficients, only the forms II and XII are free from flaws and have residues within the bounds (4). Of these two forms, form II has a residue less than that predicted in Ref. [7]. Hence we chose form XII, which is plotted in Fig. 4 as the full curve labeled XII.

In this case E/N can be written as

$$E/N = \frac{3\hbar^2 k_F^2}{10m}\epsilon_0(x), \tag{42}$$

where the series (41) is represented as

$$e_0^{-1/2}(x) \doteq \mathrm{XII}(x) \equiv \frac{1 + (F_1 - F_3/F_2)x + (F_2 - F_1F_3/F_2)x^2}{1 - (F_3/F_2)x - F_4 x^4 \ln x} \equiv \epsilon_0^{-1/2}(x).$$

We also plot the corresponding VFHNC data (plus-sign marks) and L-expansion data (open triangles). In terms of energy, our results are slightly below the VFHNC points, with agreement improving at lower densities. On the other hand, the XII approximant lies just above the L-expansion data over the range of densities where data are available.

In order to improve the $\nu=4$ many-fermion hard-sphere ground-state energy equation of state, the energy series (11) was written as

$$\frac{E}{N} - \frac{3}{5}\frac{\hbar^2 k_F^2}{2m} = \frac{3}{5}\frac{\hbar^2 k_F^3 c}{2m} e_0(x) = \frac{3}{5}\frac{\hbar^2 k_F^3 c}{2m}[D_1 + D_2 x + D_3 x^2 + D_4 x^3 \ln x + D_5 x^3 + D_6 x^4 \ln x + D_7 x^4 + \cdots], \tag{43}$$

where $x=k_F c$ and $\rho=\nu k_F^3/6\pi^2$. The suggested representation for $e_0(x)$ here is

$$e_0(x) = D_1 + D_2 x + D_3 x^2 + D_4 x^3 \ln x + D_5 x^3 + D_6 x^4 \ln x + D_7 x^4 + \cdots \tag{44}$$

which leads to

$$e_0(x)^{-1/2} = F_1 + F_2 x + F_3 x^2 + F_4 x^3 \ln x + F_5 x^3 + F_6 x^4 \ln x + F_7 x^4 + \cdots \tag{45}$$

with D_1 to D_4 known and equal to the values given in Table IV. The coefficients F_1–F_4 are different from those in Table IV, but they are derived simply from the D_i's and so are also known. They are

$$F_1 = 1/\sqrt{D_1}; \quad F_2 = -D_2/2D_1^{3/2};$$

$$F_3 = (3D_2^2 - 4D_1D_3)/8D_1^{5/2}; \quad F_4 = -8D_1^2D_4/16D_1^{7/2};$$

$$F_5 = (-5D_2^3 + 12D_1D_2D_3 - 8D_1^2D_5)/16D_1^{7/2};$$

$$F_6 = 32D_1^2(3D_2D_4 - 2D_1D_6)/128D_1^{9/2}.$$

We have also investigated the representation

$$\epsilon_0^{-1/2}(x) = \frac{F_1 + F_2 x + F_3 x^2 + bx^3}{1 - (F_4/F_1)x^3 \ln x + ax^3}$$

for which the two double-pole conditions (13) and (14) imply that

$$b = -x_{rccp}^{-3}[F_1 + F_2 x_{rccp} + F_3 x_{rccp}^2]$$

and

$$F_2 + 2F_3 x_{rccp} + 3bx_{rccp}^2 = -\left(\frac{3}{5x_{rccp}}\right)^{1/2}\left(\frac{3}{\pi\nu}\right)^{1/3}\left[1 - \frac{F_4}{F_1}x_{rccp}\ln x_{rccp} + ax_{rccp}^3\right].$$

The values of a and b so determined are −0.092 488 3 and 0.171 942, respectively. This representation is unsatisfactory because it has what applied mathematicians call a "defect." Unfortunately it is in the physical region $0<x<x_{rccp}$. The problem is not uncommon and stems from a pole and a zero lying very close to each other.

V. CONCLUSIONS

Based on known terms of field-theoretic perturbative low-density expansions we have constructed closed-form analytical expressions as functions of particle density using Padé and other approximants for the energy per particle of the fluid branches of both many-boson and many-fermion quantum hard-sphere systems. Improvements with respect to previous work (notably but not exclusively that of Ref. [24]) have been achieved by assuming (i) that the classical random closest close-packing hard-sphere densities are the ultimate fluid densities at which the energy diverges with a second-order pole, and (ii) proposing and imposing a value for the residue at the pole that is the same for either bosons or fermions as closest close-packing is approached and the hard spheres become distinguishable. Implementing these two conditions and taking advantage of recent diffusion Monte Carlo simulation data has allowed us to incorporate an additional term in the low-density expansion beyond that employed in Ref. [24]. The resulting determination of the best approximants has produced decidedly improved results for bosons as well as for two-component fermions, but not for four-component fermions.

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