

## New constructive methods for the ground-state energy of quantum fluids

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A new procedure for describing the ground-state-energy equation of state for quantum fluids is proposed. It begins with the well-known low-density expansions for the energy of a many-boson or -fermion system in terms of the two-body parameters. The latter can be expanded in powers of the two-body-attraction coupling parameter so that one is really then doing perturbation theory about the hard-sphere fluid. However, the energy as function of density for the latter system must be known accurately. We construct what we believe to be a good representation of this equation of state for bosons and then proceed to carry out perturbative corrections in the attraction up to fourth order. The case of liquid  $^4\text{He}$ , interacting via a pair hard-core-plus-attractive-square-well potential, is treated as an example. Saturation is achieved with second order, third and fourth order adding little binding energy at the saturation density. At the saturation minimum the attractive-coupling-constant perturbative series is a well-behaved one, as is attested to by the fact that different Padé approximants to it coincide with the series itself.

## I. INTRODUCTION

Among the most important successes of quantum many-body theory in its 50 or so years of existence is the application of quantum-field-theoretical techniques to sum partially, to infinite order, the perturbation series for the ground-state energy of a many-particle system.<sup>1</sup> This procedure, which applied to both the many-boson<sup>2</sup> as well as the many-fermion<sup>3</sup> systems, has led to nonregular (i.e., nonpower) series for the energy in terms of the density, about zero density. Unfortunately, only the very first few terms of these series have been evaluated. These are at best only asymptotic. That is, they are of zero radius of convergence in the limit as the number of particles,  $N \rightarrow \infty$ .

On the other hand, the use of constructive methods like Padé approximants have enjoyed considerable success in several branches<sup>4</sup> of physics and engineering in predicting the behavior of certain functions (which are originally only known very close to the origin) *well beyond* the range of validity of their meagerly known power-series expansions.

Finally, the application of perturbation techniques to the *classical* theory of fluids, in which the fluid of repulsive cores is taken as the unperturbed problem, have recently<sup>5</sup> provided successful representations of equations of state for these systems, even when going only up to second order in

the (attractive) perturbation.

We present here a new scheme for predicting ground-state equations of state for both many-boson and many-fermion systems ( $^4\text{He}$ ,  $\alpha$  matter, neutron and nuclear matter,  $^3\text{He}$ , the "spin-polarized quantum systems," etc.). It combines the three elements mentioned above, namely, (i) the known coefficients of the various low-density expansions, (ii) constructive methods (now generalized for non-power-series expansions), and (iii) perturbation theory of the attractive interparticle potential, taken as the perturbation, about the gas of repulsive particles (which in the quantum case has at present been carried out to fourth order).

To illustrate the essential ideas we limit ourselves here to an application to the liquid-helium ( $^4\text{He}$ ) many-boson system.<sup>6</sup> For this system, with identical particles of mass  $m$ , particle density  $\rho = N/\Omega$ ,  $\Omega$  being the volume, and with pair interactions giving rise to an  $S$ -wave scattering length  $a$ , the ground-state energy per particle is known to be given<sup>2</sup> by

$$\frac{E}{N} \underset{\rho a^3 < 1}{\sim} \frac{2\pi\hbar^2}{m} \rho a [1 + C_1(\rho a^3)^{1/2} + C_2 \rho a^3 \ln \rho a^3 + C_3 \rho a^3 + O((\rho a^3)^{3/2} \ln \rho a^3)],$$

$$C_1 \equiv \frac{128}{15\sqrt{\pi}}, \quad C_2 \equiv 8\left(\frac{4}{3}\pi - \sqrt{3}\right), \quad C_3 = \text{unknown} . \quad (1)$$

For illustrative purposes we pick the very simple two-body potential

$$v(r) = \begin{cases} +\infty & (r < c) \\ -v_0 & (c < r < R) \\ 0 & (r > R), \end{cases} \quad (2)$$

where  $r$  is the interparticle distance. (Generalization to more realistic potentials will be straightforward, but requiring numerical expansions.) An advantage in this choice (2) is that the scattering length is then just

$$\frac{a}{c} = 1 + \alpha \left[ 1 - \frac{\tan \sqrt{\lambda} c}{\sqrt{\lambda} c} \right], \quad (3)$$

$$\alpha \equiv \frac{R-c}{c}, \quad \lambda \equiv \frac{mv_0}{\hbar^2} (R-c)^2.$$

Using the values of parameters  $v_0$ ,  $c$ , and  $R$  obtained by Burkhardt<sup>7</sup> for helium, and by van der Spuy and Pienaar<sup>8</sup> for alphas, as well as the empirical saturation density  $\rho_{\text{sat}}$  for <sup>4</sup>He and a calculated value for  $\alpha$  matter,<sup>8</sup> one has

$$\begin{aligned} \alpha &= 2.264095, \quad \lambda = 1.719086, \\ \rho_{\text{sat}} c^3 &= 0.105 \quad ({}^4\text{He}), \\ \alpha &= 1.3529412, \quad \lambda = 3.6782231, \\ \rho_{\text{sat}} c^3 &= 0.393 \quad (\alpha \text{ matter}). \end{aligned} \quad (4)$$

Letting  $x \equiv (\rho c^3)^{1/2}$ , expanding (3) in powers of  $\lambda$  (valid for  $\lambda < \frac{1}{4}\pi^2 = 2.467\dots$ ), and substituting this result into (1) we have the *double series*, in  $x$  and  $\lambda$ , for the ground-state energy per particle

$$\frac{E}{N} \equiv \epsilon(x, \lambda) = \sum_{i=0}^4 \epsilon_i(x) \lambda^i + \dots, \quad (5)$$

where the coefficients  $\epsilon_i(x)$  would be known, for  $x \ll 1$ , up to  $i=4$  if we knew the value of  $C_3$  in (1) which multiplies the  $a^4$  term.

We remark that one can deduce some general properties of the  $\epsilon_i(x)$  from their explicit representations. If we write

$$\begin{aligned} H &= H_0 + V, \\ V &= \sum_{i < j} \Theta(r_{ij} - c) v(r_{ij}), \end{aligned} \quad (6)$$

where  $H$  is the Hamiltonian and  $\Theta(x)$  is the unit step function with  $\Theta(x) = 1$  for  $x > 0$  and  $\Theta(x) = 0$

for  $x < 0$ , and if we denote the wave function in the absence of any of the attractive part,  $V$ , of the complete potential as  $|\Phi\rangle$  then,

$$\lambda \epsilon_1(x) = \langle \Phi | V | \Phi \rangle \leq 0, \quad (7)$$

as  $V$  is a totally negative operator. Also, if  $P$  is a projector on  $|\Phi\rangle$ , then

$$\begin{aligned} \lambda^2 \epsilon_2(x) &= -\langle \Phi | [(H_0 - E_0)^{-1/2} (I - P) V]^+ \\ &\quad \times [(H_0 - E_0)^{-1/2} (I - P) V] | \Phi \rangle \leq 0. \end{aligned} \quad (8)$$

Both these inequalities are independent of statistics. From uncertainty principle argument, we expect that  $\epsilon_0$  is monotonically increasing as a function of  $x$ . We also expect  $\epsilon_1$  to be monotonically increasing as well, as with increasing density a greater amount of the wave function is crowded into the range of  $V$ .

Finally we remark that as no analytic singularities are expected to occur for small positive or negative  $\lambda$  we expect the expansion (5) to have a nonzero radius of convergence, and in fact to be analytically extendable right up to the phase boundary at the one-phase fluid region.

We shall discuss first the construction of  $\epsilon_0(x)$ , i.e., the energy per particle of the Bose hard-sphere system, and subsequently handle the  $\epsilon_i(x)$  for  $i = 1, 2, 3, 4$ .

## II. BOSE HARD-SPHERE FLUID

This system is described by (1) with  $a$  replaced by  $c$ , the hard-sphere diameter. We shall use (a) the fact that  $\epsilon_0(0) = 0$ , (b) the four Green's-function Monte Carlo (GFMC) energies at  $x = 0.407, 0.447, 0.494$ , and  $0.520$  of Ref. 9 for  $N = 256$  hard spheres, and (c) the existence in  $\epsilon_0(x)$  of an uncertainty principle (i.e., second-order) pole for some  $x > 0$  which can be associated with random-close-packing of our spheres. For a *classical* system of hard spheres the latter occurs<sup>10</sup> at about  $\rho = 0.86\rho_0$ , where  $\rho_0 \equiv \sqrt{2}/c^3$  is the density at which *regular* close-packing occurs in a face-centered-cubic (fcc) or hexagonal-close-packing (hcp) arrangement. Because of quantum mechanical diffraction effects the spheres appear larger,<sup>11</sup> we might expect a somewhat smaller value for the *quantum* random-close-packing density. At any rate, we shall *determine* this latter value subsequently, instead of assuming it to coincide with the classical value.

Using (1) with  $c$  replacing  $a$  we form the series

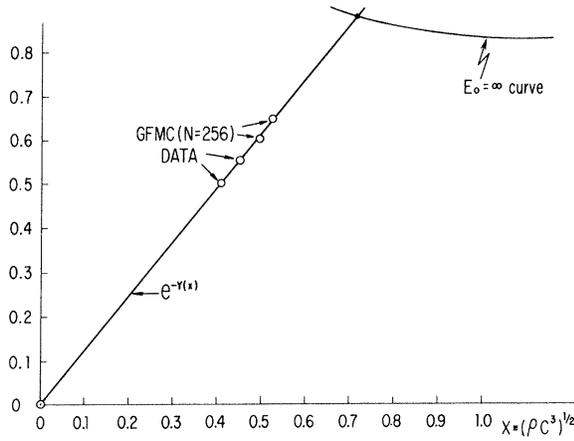


FIG. 1. Straight-line form constructed from the  $[1/1](x)$  generalized Padé approximant of Eqs. (10) and (11) which, when made to best-fit the Green's-function Monte Carlo (GFMC) data of Ref. 9 determines the up-to-now-unknown coefficient  $C_3$  as given in (14) and originally defined in (1). Also shown is the intersection with the infinite-energy curve (16), which gives the value of  $x_0$  of Eq. (17) corresponding to quantum random close packing of hard spheres of diameter  $c$ . The number density is  $\rho$ .

$$\left( \frac{4\pi x^2 \hbar^2}{2mc^2 \epsilon_0} \right)^{1/2} = 1 - \frac{1}{2} C_1 x - \frac{1}{2} C_2 x^2 \left[ \ln x^2 + \frac{1}{C_2} (C_3 - \frac{3}{4} C_1^2) \right] + o(x^2), \quad (9)$$

which we expect to vanish linearly at some  $x_0$ . Next, we construct to this the  $[1/1](x)$  generalized Padé approximant

$$\left[ \frac{4\pi x^2 \hbar^2}{2mc^2 \epsilon_0} \right]^{1/2} \simeq 1 - \frac{1}{2} C_1 x / \left[ 1 - \frac{2C_2}{C_1} x (\ln x + A) \right], \quad (10)$$

$$A \equiv \frac{1}{2C_2} (C_3 - \frac{3}{4} C_1^2) \quad (11)$$

and reduce the GFMC data by computing

$$Y(x) \equiv \left\{ \frac{1}{2} C_1 x / \left[ 1 - \left( \frac{4\pi x^2 \hbar^2}{2mc^2 \epsilon_0} \right)^{1/2} \right] - 1 \right\} \times \left[ \frac{2C_2}{C_1} x \right]^{-1} = -(\ln x + A). \quad (12)$$

Since

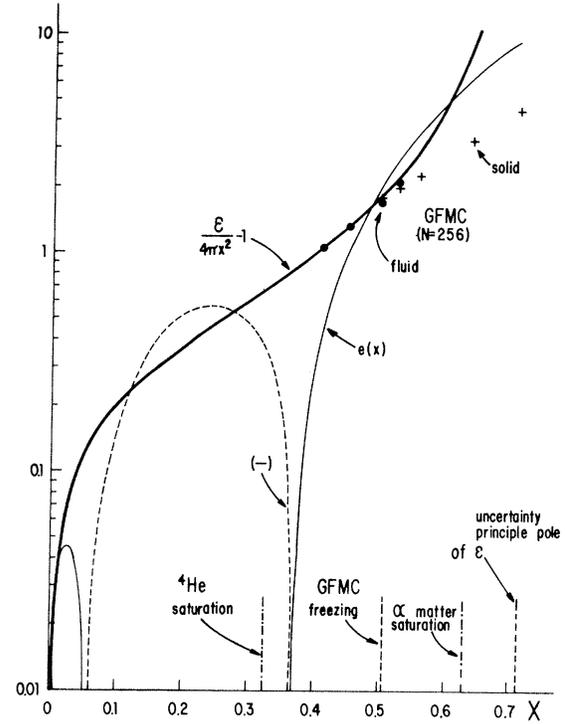


FIG. 2. Hard-sphere energy per particle (15) resulting from the  $[1/1](x)$  generalized Padé approximant (thick curve), compared with the truncated form (18) (thin curve, dashed portion of which is negative). Also shown are the GFMC data points for the "fluid" (dots) as well as the "solid" (crosses) phases of the 256 hard-sphere system, as determined in Ref. 9. Indicated on the  $x \equiv (\rho c^3)^{1/2}$  axis are the values at which (a) we determine random close packing to occur, Eq. (17), (b) liquid  $^4\text{He}$  saturates empirically, (c)  $\alpha$  matter saturates according to the calculations of Ref. 8, and (d) the 256 hard-sphere system freezes according to the GFMC calculations of Ref. 9.

$$e^{-Y(x)} = x e^A \quad (13)$$

we can expect a straight line to fit the GFMC data only if we have a good form. Figure 1 shows that this is indeed the case. The slope of 1.25 determines  $A=0.223$ , and from (11)  $C_3$  thus turns out to be

$$C_3 = 26.16. \quad (14)$$

Finally, squaring and inverting (10) we have our hard-sphere energy-per-particle extrapolant

$$\mathcal{E} \equiv 4\pi x^2 \times \left[ 1 - \frac{1}{2} C_1 x / \left[ 1 - \frac{2C_2}{C_1} x (\ln x + A) \right] \right]^{-2}. \quad (15)$$

We locate its pole at  $x_0$  by seeking the intersection of  $e^{-Y(x)}$  in Fig. 1 with the  $\epsilon_0 = \infty$  curve, i.e., with the curve

$$\exp \left[ -\left(\frac{1}{2}C_1x - 1\right) / \frac{2C_2}{C_1}x \right]. \quad (16)$$

The result is (quantum random-close-packing)

$$x_0 = 0.7082. \quad (17)$$

This density gives 55% of fcc-hcp close-packing density (for which  $x = 2^{1/4}$ ) and should be compared with the classical value of 1.1026 or 86%. We mention that in the GFMC method the difference in a data value between  $N=256$  and  $\infty$  particles is less<sup>14</sup> than an error bar, which in turn is less than the data-point circles on Fig. 1.

Figure 2 compares the newly constructed form (15) with the GFMC fluid points (dots) and with the truncated form

$$e(x) \equiv C_1x + C_2x^2 \ln x^2 + C_3x^2. \quad (18)$$

Also indicated are the values of  $x \equiv (\rho c^3)^{1/2}$  for which <sup>4</sup>He saturates,  $\alpha$  matter saturates,<sup>8</sup> and the hard-sphere system freezes<sup>9</sup> and the value  $x_0$  determined in (17).

Finally, Fig. 3 shows the energy per particle versus density (in units of the empirical liquid <sup>4</sup>He saturation values) of the [1/1] Padé (15) and the truncated form.

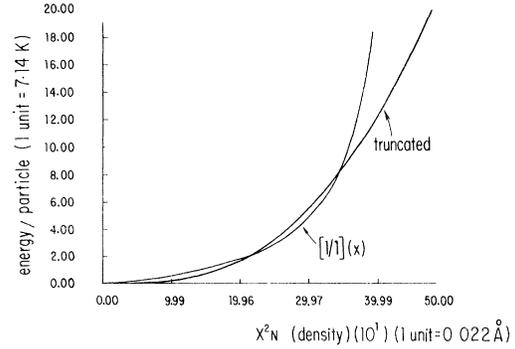


FIG. 3. Energy per particle (divided by  $2\pi$ ) vs density (times  $c^3$ ) (in units of the empirical saturation quantities for <sup>4</sup>He) for the [1/1] ( $x$ ) generalized Padé (15) and the truncated form  $e(x)+1$ , Eq. (18). The latter diverges only at  $x = \infty$  (as  $x^2 \ln x^2$ ) while the former at the value (17) as a second-order (uncertainty principle) pole.

### III. INCLUSION OF ATTRACTIVE FORCES

We now proceed to calculate the perturbation coefficients  $\epsilon_i(x)$ ,  $i=1,2,3,4$ , which appear in (5). For this task we note that

$$\epsilon_i(x) = \frac{1}{i!} \left[ \frac{\partial^i}{\partial \lambda^i} \epsilon(x, \lambda) \right]_{\lambda=0} \quad (i=1,2,3,4), \quad (19)$$

where  $\epsilon(x, \lambda)$  is given by (1), and  $a$  by (3). Using  $\partial/\partial \lambda = (da/d\lambda)\partial/\partial a$  we finally arrive at

$$\epsilon_i(x) = \frac{2\pi\hbar^2}{mc^2} d_i(\alpha)x^2 [1 + C_{1i}(\alpha)x + C_{2i}(\alpha)x^2 \ln x^2 + C_{3i}(\alpha)x^2 + o(x^2)] \quad (i=1,2,3,4), \quad (20)$$

where

$$d_1(\alpha) \equiv -\alpha/3, \quad d_2(\alpha) \equiv -2\alpha/15, \quad d_3(\alpha) \equiv -17\alpha/315, \quad d_4(\alpha) \equiv -62\alpha/2835 \quad (21)$$

and where

$$C_{11} = \frac{5}{2}C_1, \quad C_{12} = \frac{5}{16}(8-5\alpha)C_1, \quad C_{21} = 4C_2, \quad (22)$$

$$C_{22} = (4-5\alpha)C_2, \quad C_{31} = 3C_2 + 4C_3, \quad C_{32} = \left(3 - \frac{35}{4}\alpha\right)C_2 + (4-5\alpha)C_3,$$

$$C_{13} = \left[ \frac{7(25)}{6(8)(17)}\alpha^2 - \frac{3(5)(7)}{2(17)}\alpha + \frac{5}{2} \right] C_1, \quad C_{23} = \left[ \frac{4(5)(7)}{3(17)}\alpha^2 - \frac{8(21)}{17}\alpha + 4 \right] C_2, \quad (23)$$

$$C_{33} = \left[ \frac{5(7)(13)}{3(17)}\alpha^2 - \frac{3(7)(14)}{17}\alpha + 3 \right] C_2 + \left[ \frac{4(5)(7)}{3(17)}\alpha^2 - \frac{3(7)(8)}{17}\alpha + 4 \right] C_3,$$

$$\begin{aligned}
C_{14} &= \left[ \frac{5(5)(7)}{31(16)^2} \alpha^3 + \frac{5(7)(9)}{16(31)} \alpha^2 - \frac{9(127)}{8(31)} \alpha + \frac{5}{2} \right] C_1, \\
C_{24} &= \left[ -\frac{5(7)}{2(31)} \alpha^3 + \frac{4(7)(9)}{31} \alpha^2 - \frac{9(254)}{5(31)} \alpha + 4 \right] C_2, \\
C_{34} &= \left[ -\frac{5(7)(25)}{8(31)} \alpha^3 + \frac{7(9)(13)}{31} \alpha^2 - \frac{7(9)(127)}{5(62)} \alpha + 3 \right] C_2 + \left[ -\frac{35}{62} \alpha^3 + \frac{4(7)(9)}{31} \alpha^2 - \frac{9(254)}{5(31)} \alpha + 4 \right] C_3.
\end{aligned} \tag{24}$$

We now construct the following approximants, in  $x$ , to the expression ( $i=1,2,3,4$ )

$$(1 + C_{1i}x + C_{2i}x^2 \ln x^2 + C_{3i}x^2) \tag{25}$$

which appears in (20):

$$F_i^{(m,n)}(x) \equiv \left[ 1 + \frac{A_i x}{[1 + (B_i \ln x^2 + D_i)x]^m} \right]^n \quad (m, n = 1, 2, 3, \dots), \tag{26}$$

$$A_i \equiv \frac{C_{1i}}{n}, \quad B_i \equiv -\frac{C_{2i}}{mC_{1i}}, \quad D_i \equiv -\frac{C_{3i}}{mC_{1i}} + \frac{(n-1)}{2nm} C_{1i},$$

$$H_i^{(n)}(x) \equiv [1 - \alpha_i x - \beta_i x^2 (\ln x^2 + \gamma_i)]^{-n} \quad (n = 1, 2, 3, \dots), \tag{27}$$

$$\alpha_i \equiv \frac{C_{1i}}{n}, \quad \beta_i \equiv \frac{C_{2i}}{n}, \quad \gamma_i \equiv \frac{C_{3i}}{C_{2i}} - \frac{(n+1)}{2n} \left[ \frac{C_{1i}^2}{C_{2i}} \right],$$

$$J_i^{(m,n)}(x) \equiv \left[ 1 - \frac{a_i x}{[1 - b_i x (\ln x^2 + c_i)]^m} \right]^{-n} \quad (m, n = 1, 2, 3, \dots), \tag{28}$$

$$a_i \equiv \frac{C_{1i}}{n}, \quad b_i \equiv \frac{C_{2i}}{mC_{1i}}, \quad c_i \equiv \frac{C_{3i}}{C_{2i}} - \frac{(n+1)}{2n} \frac{C_{1i}^2}{C_{2i}},$$

$$K_i^{(n)}(x) \equiv \left[ 1 + \frac{C_{1i}x + C_{2i}x^2 \ln x^2}{(1 + b_i x)^n} \right] \quad (n = 1, 2, 3, \dots), \tag{29}$$

$$b_i \equiv - \left[ \frac{C_{3i}}{nC_{1i}} \right].$$

The coefficients of these approximants are defined so that the binominal expansion of the corresponding expression reproduces (25) exactly.

For  $\alpha = 2.264095$ , the range parameter given for  ${}^4\text{He}$ , we list in Table I the *minimum* value of exponents  $m$  and/or  $n$  required to avoid a pole in the approximants in the physical region of densities, i.e.,  $0 \leq x \leq x_0 \equiv 0.7082$ . We also report the value of  $x > x_0$  for which a pole first appears (if it appears at all for positive  $x$ ). Note that for the

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$K_i^{(n)}(x)$  approximant the pole occurs at  $x = -1/b_i \equiv nC_{1i}/C_{3i}$ . Also, for  $i=3$  and 4 this number is *negative*, namely,  $-0.2158$  and  $-0.0232$ , respectively.

Having thus a large (in fact, infinite) number of approximants for the  $\epsilon_i(x)$  coefficients, which moreover have no poles for  $0 \leq x \leq x_0$ , we turn to the construction of approximants to the (perturbation) power series in  $\lambda$  (5). We choose the usual Padé approximants<sup>4</sup>

TABLE I. Minimum value of the exponents  $m$  and/or  $n$  required to avoid a pole in the physical region of densities, that is  $0 \leq x \leq x_0 \equiv 0.7082$ , in the approximants to (26) given by Eqs. (27) and (30). Also given is the value of  $x > x_0$  for which a pole first appears, if it appears at all for  $x$  positive.

i	1	2	3	4
$F_i^{(m,n)}(x)$	$(m,n)=(4,3)$ 0.7305	$(m,n)=(64,1)$ 0.7368	$(m,n)=(1,1)$ 1.6583	$(m,n)=(1,1)$
$H_i^{(n)}(x)$	$n=1$	$n=1$	$n=1$	$290 < n < 300$ 0.7162
$J_i^{(m,n)}(x)$	$(m,n)=(6,13)$ 0.7186	$(m,n)=(15,1)$ 0.7701	$(m,n)=(1,1)$ 1.6583	$(m,n)=(1,1)$
$K_i^{(n)}(x)$	$n=9.6$ 0.71	$n=74.17$ 0.71	$n=1$	$n=1$

$$[N/M](\lambda) \equiv \sum_{i=0}^N p_i \lambda^i / \sum_{j=0}^M q_j \lambda^j. \quad (30)$$

With these we shall proceed to give the energy per particle versus density curves for  ${}^4\text{He}$  below.

#### IV. RESULTS

In units of liquid  ${}^4\text{He}$  saturation energy per particle (divided by  $2\pi$ ) and density values, we summarize our results in Figs. 4 and 5. We restrict ourselves only to the lowest  $m$  and/or  $n$  value(s) in the approximants for  $\epsilon_i(x)$  given in (26) to (29)

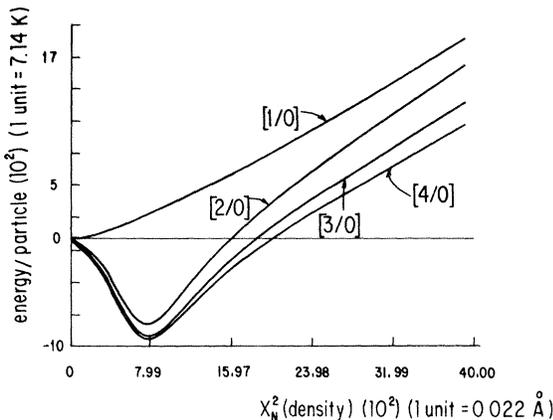


FIG. 4. Energy per particle vs density (same units as in Fig. 3) in first- [1/0], second- [2/0], third- [3/0], and fourth- [4/0] order perturbation theory (5) for  ${}^4\text{He}$ , with the interaction (2) and parameters given in (4) taken from Ref. 7. The extrapolants, in  $x$ , used for  $\epsilon_i(x)$ ,  $i=0,1,2,3,4$ , are respectively,  $\mathcal{E}$  Eq. (15),  $H_1^{(1)}$  Eq. (28),  $H_2^{(1)}$  Eq. (28),  $F_3^{(1,1)}$  Eq. (27), and  $F_4^{(1,1)}$  Eq. (27).

such that no poles appear in the physical region  $0 \leq x \leq 0.7082$ , in accordance with Table I. This still gives too many possible combinations and we further focus only on  $m$  and/or  $n$  values of unity. Noting that  $J_i^{(1,1)} \equiv F_i^{(1,1)}$  we thus have, for  $\epsilon_1, \epsilon_2, \epsilon_3$ , and  $\epsilon_4$  the combinations  $H_1^{(1)}, H_2^{(1)}, F_3^{(1,1)}, F_4^{(1,1)} \equiv HHFF, HHHF, HHKK, \text{ and } HHHK$ . An additional reason for selecting  $H_i^{(1)}$  for  $i=1,2$  is that these approximants automatically satisfy inequalities (7) and (8) in the physical region.

Figure 4 shows the typical case  $HHFF$ . We see that no binding is obtained in first-order perturbation theory (curve labeled [1/0]). Binding and saturation occur beginning with second order. Third

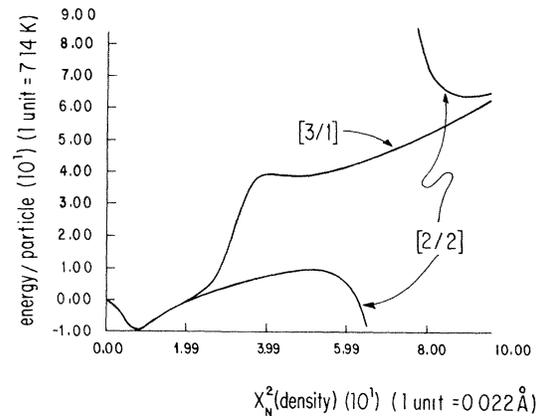


FIG. 5. Energy-per-particle vs density (same units as Fig. 3) given by the [3,1] ( $\lambda$ ) and [2/2] ( $\lambda$ ) Padé approximants (27), constructed from the perturbation series (5), for the  ${}^4\text{He}$  potential parameters (4). The first minimum coincides (to the scale of this graph) with the saturation minimum of [4/0] ( $\lambda$ ) of Fig. 4.

and fourth orders add very little binding. Furthermore, our perturbation series (in  $\lambda$ ) is a rapidly convergent one in the neighborhood of the saturation density, as is evident in Fig. 5 by the [3/1] ( $\lambda$ ) and [2/2] ( $\lambda$ ) Padé's coinciding there with the (truncated) [4/0] ( $\lambda$ ) curve shown in Fig. 4 only. (These two Padé approximants not only deviate at higher densities from the [4/0] ( $\lambda$ ) curve but also, as seen for the [2/2] case,<sup>12,13</sup> may develop singularities.) This rapid convergence is *not* to be expected for  $\alpha$  matter since the corresponding value of  $\lambda$  quoted in (4) is greater than  $(\pi/2)^2$ . Padé methods may thus be indispensable there.

We note, however, that both the predicted saturation energy per particle and density are *one-tenth* the empirical values for  ${}^4\text{He}$ , a result that could easily be attributable to the very simple two-body potential (2) chosen to illustrate the present methods.

It is interesting, however, to ask if the discrepancy with experiment could be reduced by varying the range parameter  $\alpha \equiv (R - c)/c$  somewhat, but correspondingly changing  $\lambda$  in (3) so that the scattering length  $a$ , upon which the energy solely depends, is kept fixed at the empirical value<sup>7</sup> for helium. The combinations *HHKK* and *HHHK* containing  $K$  gave overbinding by a factor of 2 with respect to the empirical value and at twice the empirical saturation density, even at the "physical" value of  $\alpha$  quoted in (4). This exaggerated saturation minimum was identified as a "spurious" one since it was coming mainly from the  $K_3$  extrapolant which eventually developed a singularity as  $\alpha$  was varied, i.e., diverged to minus infinity. Finally the case *HHHF* was studied in detail by varying  $\alpha$ . A second minimum shows up at higher density which predominates over the first one as  $\alpha$  is reduced to 2. As  $\alpha$  was reduced even further to 1.5,  $H_3$  (and thus  $\epsilon_3$ ) developed *two* singularities, and thus obliged us to discard *HHHF*. No such behavior was found for the first combination dis-

cussed here, the *HHFF*. This parameter study does indicate the expected existence of considerable sensitivity of the energy curve to the shape of the attraction and the care which must be taken with the density extrapolations of the  $\lambda$  coefficients  $\epsilon_i(x)$ .

## V. CONCLUSION

It is hoped that the use of more realistic (*ab initio*) two-body interaction potentials, like the ones of Aziz *et al.*,<sup>15</sup> for which in addition one possesses GFMC calculations<sup>16</sup> which agree remarkably well with experiment, will prove more accurate in predicting empirical properties, and such work is presently under progress.

It seems clear from the present study that *an appropriate smallness parameter for the microscopic description of quantum liquids is precisely the attractive strength of the two-body potential*, our  $\lambda$ . This is so not only because of its relative smallness compared to the central repulsion but mainly due to the well-known close similarity between the pair distribution function of the hard-sphere fluid and the corresponding liquid. This occurs not only in classical but also quantum systems and makes the hard-sphere fluid a reasonable starting point on which to base a perturbative treatment.

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