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Thermodynamic perturbation theory of hard-core square-well bosons

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Abstract. We investigate a calculational scheme for an eventual first-principles description of the ground-state energy of the many-boson Schrödinger equation. We employ a model ^4He intermolecular pair potential consisting of a hard core surrounded by an attractive rectangular well. The study is based on the well known low-density expansion for such a system, where three coefficients are known. The first corrections to the fourth coefficient are determined on the basis of the rearranged series being a thermodynamic perturbation expansion, namely one representing perturbation not about the ideal gas but about the hard-sphere fluid. Padé approximants, and variations thereof, are employed to extrapolate to physical regimes in both resulting series, in density as well as in the attractive coupling constant.

1. Introduction

Quantum field theory and Rayleigh-Schrödinger perturbation theory applied to an ideal gas have produced for the ground-state energy per particle of a many-body system well known low-density expansions, with *three* coefficients thus far determined for bosons and *four* for fermions. The particular approach we have been implementing attempts [1] to ascertain how much can be achieved in constructing an accurate equation of state for several many-body Schrödinger systems, based only on the facts, namely the above-mentioned coefficients, and using extrapolation schemes such as Padé [2] and other generalisations.

For identical bosons of mass m , with pair interaction S-wave scattering length a and number density $n = N/V$, one has for the ground-state energy per particle [3]

$$\frac{E}{N} \approx \frac{2\pi\hbar^2}{m} na \{1 + C_1(na^3)^{1/2} + C_2 na^3 \ln(na^3) + C'_3 na^3 + O[(na^3)^{3/2} \ln(na^3)]\} \quad (1)$$

where $C_1 = 128/15\sqrt{\pi} = 4.814\,417\,78\dots$ and $C_2 = 8(4\pi/3 - \sqrt{3}) = 19.653\,915\,18\dots$. Here C'_3 is *unknown* but potential shape dependent since it involves three-body cluster diagrams. Expansions such as (1) were abandoned early, perhaps for two fundamental reasons: (i) for *negative* scattering length (namely most two-body potentials of interest in condensed matter science) *imaginary* terms appear on the RHS of (1) which are not easy to deal with and (ii) many-body systems such as liquid helium are definitely not low-density substances as (1) assumes. Difficulty (i) is bypassed very naturally by expanding (analytically or numerically)

$$a = a_0(1 + a_1\lambda + a_2\lambda^2 + \dots) \quad (2)$$

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where λ is some appropriate measure of the attraction of the two-body potential. Substitution into (1) then leads to

$$\frac{E}{N} = \frac{2\pi\hbar^2}{ma_0^2} x^2 \sum_{i=0}^{\infty} e_i(x)\lambda^i \quad x \equiv (na_0^3)^{1/2} \quad (3)$$

which is evidently *real* no matter how large λ is (and thus how negative a is). The 'rearrangement' (3) is nothing more than a perturbation scheme, but now about the gas of attractionless particles, i.e. the scheme recommended by van der Waals more than a hundred years ago for classical fluids. Difficulty (ii) can perhaps be surmounted with the extrapolation procedures mentioned above.

In general, the S-wave scattering length a has the integral representation

$$a \equiv \int_0^{\infty} r dr v(r)u_0(r) \quad (4)$$

where $v(r)$ is the central pair-potential interaction energy and $u_0(r)$ is the S-wave zero scattering energy radial wavefunction satisfying $u_0(0) = 0$. We restrict our present study to the hard-core square-well (HCSW) potential function:

$$v(r) = \begin{cases} \infty & (r < c) \\ -v_0 & (c < r < R) \\ 0 & (r > R). \end{cases} \quad (5)$$

In this instance, effective range theory [4] gives the analytical expression

$$a = c[1 + \alpha(1 - \tan\sqrt{\lambda}/\sqrt{\lambda})] \approx c[1 - \alpha(\frac{1}{3}\lambda + \frac{2}{15}\lambda^2 + \frac{17}{315}\lambda^3 + \frac{62}{2835}\lambda^4 + \dots)] \quad (6)$$

where we have defined the dimensionless range α and attractive strength λ parameters as

$$\alpha \equiv (R - c)/c \quad \lambda \equiv mv_0(R - c)^2/\hbar^2. \quad (7)$$

We shall also express the unknown coefficient C'_3 in (1) as

$$C'_3 \approx C_3(1 + C_{31}\lambda + C_{32}\lambda^2 + \dots) \quad (8)$$

with the coefficients C_{3i} ($i = 1, 2, \dots$) to be determined below via global physical constraints to be discussed later. Note that C_3 will be the coefficient of the n^2 term in the E/N low-density series for a fluid of boson hard spheres, a system which has been investigated [5] in the Green function Monte Carlo (GFMC) scheme. In general, the n^2 term in the energy in (1) is potential shape dependent since it corresponds to genuine three-body cluster diagrams which make their appearance for the first time in this order; such is *also* the case in the many-fermion [6] system with the k_F^6 term.

2. Rearranged perturbation scheme

In the rearranged perturbation series (3) we evidently have

$$e_0(x) \approx 1 + C_1x + C_2x^2 \ln x^2 + C_3x^2 + \dots \quad (9)$$

corresponding to the hard-sphere fluid. The extrapolant of (9), arrived at [7] by assuming that the corresponding energy per particle must have a second-order uncertainty principle pole at some *finite* (perhaps Bernal) density n_B , is the expression

$$\varepsilon_0(x) = \left(1 - \frac{\frac{1}{2}C_1x}{1 - (2C_2/C_1)x[\ln x + (C_3 - \frac{3}{4}C_1^2)/2C_2]} \right)^{-2}. \quad (10)$$

By definition, expansion of the RHS of (10) about $x = 0$ gives the series (9) through the order indicated. A global fit to the four GFMC data points of (10) determined [7] that

$$C_3 = 26.2 \quad \text{and} \quad x_B = (n_B c^3)^{1/2} = 0.7082. \quad (11)$$

The latter value means a packing density of about 0.35 times the ‘primitive hexagonal’ (FCC, HCP, etc) packing density $n_0 \equiv \sqrt{2}/c^3$ and is to be contrasted with the classical Bernal value of 0.86 as deduced through actual experiments [8] with steel ball-bearings. A *quantum* packing density *smaller* than the classical one is, of course, fully expected just from wave mechanical diffraction effects [1]. The form (10) thus obtained is very probably quite accurate over all physical densities, $0 < n < n_B$, since solving for $(\ln x + \text{constant})$ in (10) and exponentiating allowed a mapping of the GFMC data onto an almost straight line. The slope of this line fixes the value of the constant, and thus of C_3 , since C_1 and C_2 are known pure numbers.

The higher-order corrections to (10) will be, from (1), (3), (6) and (8), the infinite sequence of low-density non-power series:

$$e_i(x) \approx a_i(1 + C_{1i}x + C_{2i}x^2 \ln x^2 + C_{3i}x^2 + \dots). \quad (12)$$

Note that their structure is again identical to that of (1). Comparing (2) and (6) gives, for the a_i ,

$$a_1 = -\frac{1}{3}\alpha \quad a_2 = -\frac{2}{15}\alpha \quad \dots \quad (13)$$

while the coefficients C_{1i} and C_{2i} ($i = 1, 2, 3, 4$) are the polynomials in α given in [7]. Furthermore, C_{15} and C_{25} were found [9] by the computer-algebraic scheme called MACSYMA [10] and are

$$\begin{aligned} C_{15} &= (C_1/256a_5)[640a_5 + 960a_1a_4 + (960a_2 + 240a_1^2)a_3 + 240a_1a_2^2 - 40a_1^3a_2 + 3a_1^5] \\ C_{25} &= (C_2/a_5)[4a_5 + 12a_1a_4 + 12(a_2 + a_1^2)a_3 + 12a_1a_2^2 + 4a_1^3a_2]. \end{aligned} \quad (14)$$

Finally, the C_{3i} ($i = 1, 2, 3, 4, 5$) are to be determined by constraints on the first- and higher-order energy corrections which collectively reflect the hypothesis that in the *quantum* fluid case first-order van der Waals (also known as ‘thermodynamic’) perturbation theory is *exact* in the limit of *close* packing. This hypothesis has been proved rigorously in two [11] as well as one [12] dimensions for the *classical* statistical mechanical case at *closest* (primitive hexagonal) packing and conjectured [11] to occur as well in three dimensions. In our case, this amounts to saying that, as the packing density is approached from below, the many-boson energy (3) for HCSW particles must be *linear* in λ (or v_0). Specifically, in this limit the energy could be estimated by the simple result

$$\frac{E}{N} \xrightarrow{x \rightarrow x_B} \frac{A}{(x_B - x)^2} - \frac{1}{2}v_0\left(\frac{4}{3}\pi R^3 n_B - 1\right) \quad (15)$$

where the first (diverging) term follows from (10) and the second term arises as follows. As the density of close packing of spheres is approached the dependence on the attractive pair potential must be given simply by the number of sphere centres within the attractive range R , minus the central sphere (i.e. unity), times the attractive potential depth $-v_0$, with the customary factor of $\frac{1}{2}$ to avoid double counting. The constraint (15) thus obtained then demands, if $\epsilon_i(x)$ stand for the appropriate extrapolatants to the low-density forms $e_i(x)/a_i$ of (12), that

$$\epsilon_1(x_B) = \text{constant} \quad \epsilon_i(x_B) = 0 \quad (i = 2, 3, 4, \dots). \quad (16)$$

For the He-He HCSW potential deduced by Burkhardt [13] to be 'phase equivalent' to the He-He Lennard-Jones potential, one has $c = 1.685 \text{ \AA}$, $R = 5.5 \text{ \AA}$ and $v_0 = 1.899\,998\,65 \text{ K}$. Equations (6) and (7) then give (for $\hbar^2/m = 12.120\,904$, appropriate for ^4He)

$$\alpha = 2.264\,095 \quad \lambda = 2.281\,4165 \quad a = -36.2938 \text{ \AA}. \quad (17)$$

Hence, combining (3), (11), (15) and (16) yields

$$\varepsilon_1(x_B) = 2.955\,42. \quad (18)$$

The $e_i(x)/a_i$ ($i = 1, 2, 3, 4, 5$) series (12) through the known terms—that is, *without* the x^2 term—are plotted in figure 1. The open circle on the $x \equiv (nc^3)^{1/2}$ axis marks the packing density value $x_B = 0.7082$. We note that these 'raw' forms are not only far from conforming to the constraints (16) and (18) but also attain enormously large values compared with unity. Furthermore, first order violates the rigorous requirement [7] of positivity for all x . Finally, there is *no correlation* at all among the different orders, as would be expected in view of the almost perfect monotonicity in order $\varepsilon_i(x) > \varepsilon_{i+1}(x)$ observed in the *exact* calculations carried out [14] through fourth order for purely attractive fermions.

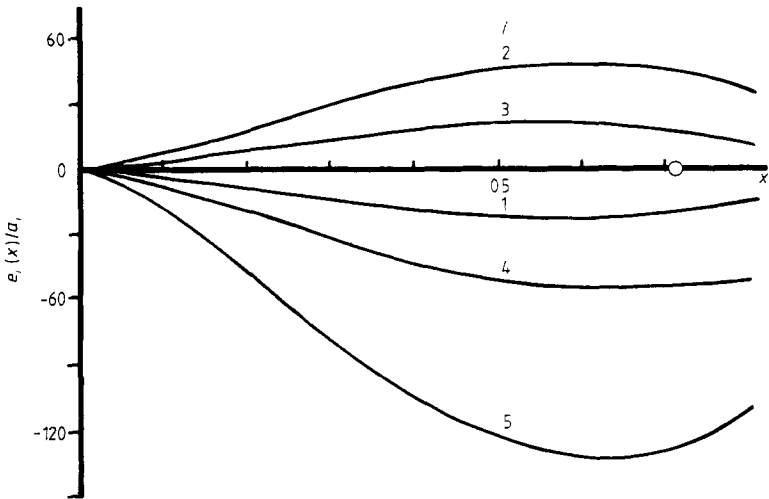


Figure 1. Plot of the known portion of low-density series, equation (12), namely $1 + C_{1i}x + C_{2i}x^2 \ln x^2$, for orders $i = 1-5$. Here $x \equiv (nc^3)^{1/2}$. Constants used appear in table 2. Note that the value of each curve at $x = 0$ is unity.

As a first attempt to 'tame' the functions $e_i(x)/a_i$, we assume values for the unknown C_{3i} in (12) such that the resulting series *do* conform to constraints (16) and (18). We designate these new truncated forms by $\varepsilon_i(x)_{\text{trun}}$; they are plotted in figure 2. Although the magnitudes have been damped down somewhat, one still has the first-order form violating positivity, as well as the absence of the expected correlation between orders. A more elaborate scheme is thus called for.

This extrapolation (or analytical continuation) of the $e_i(x)/a_i$ from $x = 0$ to physical values, say x_s (namely liquid ^4He saturation density), will be designated by

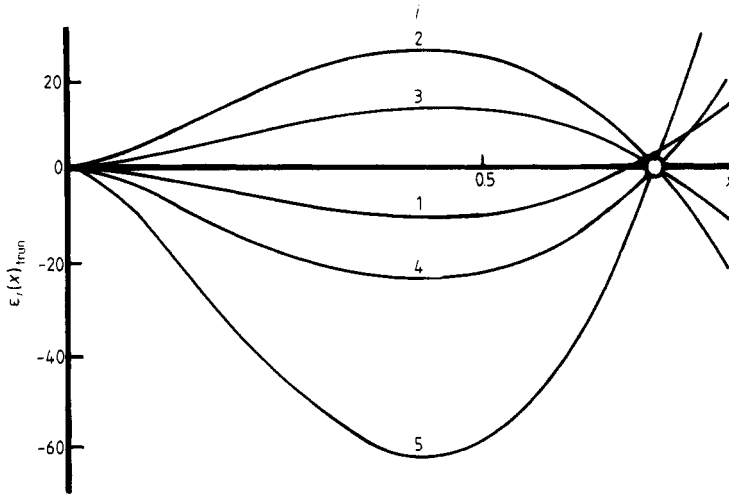


Figure 2. Same as figure 1 but with the first unknown term in (12), namely C_3x^2 , added and determined by imposing constraints (16) and (18). The open circle on the x axis locates the packing density constant at $x_B = 0.7082$. The value of each curve at $x = 0$ is unity.

$\epsilon_i(x)$. Once constructed, the $\epsilon_i(x)$ will permit expressing the ground-state energy (3) as

$$\frac{E}{N} \approx \frac{2\pi\hbar^2}{mc^2} x^2 \left[\epsilon_0(x) + \sum_{i=1}^{\infty} a_i \epsilon_i(x) \lambda^i \right]. \tag{19}$$

Afterwards, one might need to extrapolate the expression in large parentheses from $\lambda = 0$ to the physical $\lambda = \lambda_p$ (namely the value given in (17)). This latter step can be implemented, for example, by constructing the Padé approximants $[L/M](\lambda)$ to (19). We will work through fifth order so that $0 \leq L + M \leq 5$.

The two-step extrapolation just outlined—first in density, and then in attractive coupling—is in keeping with the trajectory described in [6, 9]. This particular path avoids crossing any gas–liquid phase boundaries in arriving at the desired equilibrium (zero-pressure) *liquid* state from the low-density *gaseous* phase. Thus, both our extrapolants $\epsilon_i(x)$ from the first step and the $[L/M](\lambda)$ from the second step must be singularity-free for $0 < x < x_B$ and $0 < \lambda < \lambda_p$, respectively. Note, however, that the $[L/M](\lambda)$ so constructed *may* develop poles in $0 < x < x_B$. These, however, are of no undesirable consequence as would be the case if we followed the trajectory defined by constant $\lambda = \lambda_p$ and x going from 0 to $x_s < x_B$.

3. Density series analysis

We apply the so-called ‘tailing’ method [9] of constructing generalised Padé approximants to the log-bearing series (12), which are simply rewritten as

$$1 + K_1x + K_2x^2 \ln x^2 + K_3x^2 + \dots \tag{20}$$

The method is inspired by the very common fact that series used in physical theories have the earlier coefficients known to higher accuracy than the later ones, occurring in the *tail* of the series. The idea is to split off from the tail of the original series the

smallest series that will admit a Padé-like representation. For example, (20) can be rewritten as

$$1 + K_1x + K_2x^2 \ln x^2 \left[1 + \frac{K_3}{K_2} \frac{1}{\ln x^2} + \dots \right] \tag{21}$$

and the bracketed expression Padé-represented by

$$\left[1 - \frac{K_3}{K_2} \frac{1}{\ln x^2} \right]^{-1}. \tag{22}$$

However, binomial expansion of this will generate unwanted terms $(\ln x^2)^{-n}$, n a positive integer, in the original series, and hence (21) is disqualified as a starting point. The next step is to rewrite (20) as

$$1 + K_1x \left[1 + \frac{K_2}{K_1}x \ln x^2 + \frac{K_3}{K_1}x + \dots \right] \tag{23}$$

and replace the bracketed expression by all possible Padé-like forms. The latter will be the *three* forms:

$$\frac{1 + (K_2/K_1)x \ln x^2}{1 - (K_3/K_1)x} \qquad \frac{1 + (K_3/K_1)x}{1 - (K_2/K_1)x \ln x^2} \qquad \frac{1}{1 - (K_2/K_1)x \ln x^2 - (K_3/K_1)x} \tag{24}$$

which upon binomial expansion reproduce the bracketed expression in (23). Finally, all possible Padé-like forms are constructed for the full expression (20); there turn out to be nine.

As such, the tailing method provides extrapolations to (20) with a general structure

$$M + N(x)/D(x) \tag{25}$$

with $M = 1$ or 0 , and where $N(x)$ and $D(x)$ are series with or without the log term. The left half of table 1 lists all possible extrapolants of the type (25) to the original series (20). We have deliberately listed twelve forms to emphasise that redundancies may occur easily in the course of tailing: namely, form V is identical to form I, for example, so that one really has only $3 + 8 = 11$ distinct extrapolants to (20). Tailing applied to other log-bearing series, such as the four-species fermion low-density series, leads [15] to a much larger number of extrapolants. The method can also be applied to *power* series, where it leads to all the standard Padé approximants plus a few new rational approximants [9].

Table 1 thus contains eleven distinct candidates for each $\varepsilon_i(x)$ ($i = 1, 2, \dots$) extrapolant to be used in the energy expression (19). The following global requirements will now be applied to each candidate and the latter rejected if it violates one or more of these conditions:

- (i) $\varepsilon_i(x)$ must have no poles in the physical interval ($0 < x < x_B = 0.7082$) for reasons given previously;
- (ii) $\varepsilon_i(x) > 0$, for all x in the physical interval, for $i = 1, 2$ (positivity) [7];
- (iii) $x^2\varepsilon_i(x)$ must increase monotonically in x . This is so because the first-order energy correction is equivalent to an expectation value, between the ground-state wavefunction of the hard-sphere fluid, of the attractive potential well summed over all pairs of particles. As such, this quantity can only *decrease* as the particles are packed closer together.

It is well known [16] that the ideal-gas-based perturbation series for bosons diverges as of third order, order by order, no matter how well behaved the interparticle

Table 1. List of possible members of (25) which, by definition, will reproduce (20) upon binomial expansion about $x = 0$. The right half of the table gives reasons for discarding a given approximant in each order, through fifth order, as explained in the text.

Form	M	N(x)	D(x)	Order				
				1	2	3	4	5
I	1	$K_1x + K_2x^2 \ln x^2$	$1 - (K_3/K_1)x$	Pole at $x = 0.067$	Pole at 0.015	Pole at 0.038	VP	Pole at 0.003
II	1	$K_1x + K_3x^2$	$1 - (K_2/K_1)x \ln x^2$		VP		Pole at 0.028	Pole at 0.005
III	1	K_1x	$1 - (K_2/K_1)x \ln x^2 - (K_3/K_1)x$				VP	Pole at 0.006
IV	0	$1 + (K_1 - K_3/K_1)x$	$1 - (K_3/K_1)x - K_2x^2 \ln x^2$		Pole at 0.034	Pole at 0.066	VP	VP
V	0	$1 + (K_1 - K_3/K_1)x + K_2x^2 \ln x^2$	$1 - (K_3/K_1)x$		Pole at 0.015	Pole at 0.038	VP	Pole at 0.003
VI	0	1	$1 - K_1x - K_2x^2 \ln x^2 - (K_3 - K_1^2)x^2$	NMI	NS	NS	NS	NS
VII	0	$1 + K_1x + K_2x^2 \ln x^2$	$1 - K_3x^2$	Pole at 0.7	NS	NS	NS	NS
VIII	0	$1 + K_2x^2 \ln x^2 + (K_3 - K_1^2)x^2$	$1 - K_1x$	Pole at 0.08	VMO	VMO	VP	VP
IX	0	$1 + K_1x + K_3x^2$	$1 - K_2x^2 \ln x^2$	NMI	Pole at 0.032	Pole at 0.043	VP	VP
X	0	$1 + K_1x$	$1 - K_2x^2 \ln x^2 - K_3x^2$	VP	NS	NS	NS	NS
XI	0	$1 + K_2x^2 \ln x^2$	$1 - K_1x - (K_3 - K_1^2)x^2$	Pole at 0.081	NS	NS	NS	NS
XII	0	$1 + (K_3 - K_1^2)x^2$	$1 - K_1x - K_2x^2 \ln x^2$	NMI	Pole at 0.03	Pole at 0.06		

VP: violates positivity.

NS: no solution.

NMI: non-monotonic-increasing.

VMO: violates monotonicity in order.

interaction. These divergences, in fact, necessitate the infinite partial summations yielding the renormalised, though non-analytic, result (1). It seems reasonable to expect that the hard-sphere-fluid-based perturbation corrections for bosons will have a general behaviour in many ways similar to that for fermions. The aforementioned exact fermion calculations [14] through fourth order suggest, for quantum particles in general, two characteristic properties as of third order for the $\varepsilon_i(x)$: (a) monotonicity in order for a given density, i.e. $\varepsilon_3(x) > \varepsilon_4(x)$ and (b) positivity, or $\varepsilon_3(x) > 0$ and $\varepsilon_4(x) > 0$. Through numerous applications in boson problems we found that, if these two latter properties were not imposed on the $\varepsilon_i(x)$ as of third order, we could not eliminate wildly behaving extrapolants and, worse still, an overall disruption developed in the expected convergence of the thermodynamic perturbation scheme beyond second order. With this *a posteriori* reasoning, we propose the two additional conditions:

(iv) $\varepsilon_i(x) > \varepsilon_{i+1}(x)$ ($i = 1, 2, 3, \dots$) (monotonicity in order);

(v) $\varepsilon_i(x) > 0$, for all x in the physical interval, for $i = 4$ and 5.

The right half of table 1 lists the reasons for elimination of a given extrapolant $\varepsilon_i(x)$, effected upon applying requirements (i)–(v), *after* imposing constraints (16) and (18). The designation ‘no solution’ (NS) in table 1 means that the condition $\varepsilon_i(x_B) = 0$ cannot determine the constant C_{3i} , since the latter constant appears only in the denominator of the corresponding extrapolant, which is finite for all finite x . In first order, as reported in table 1, two approximants survived: forms II and III. Both of these, however, are practically degenerate with each other in the physical interval $0 < x < x_B$. In figure 3 we graph their difference, which is at most 0.0075, or about 0.25% of the maximum value of $\varepsilon_1(x)$ which is given by (18). For definiteness we choose form II for $\varepsilon_1(x)$. It is perhaps significant that in first order the method yields virtually only *one* approximant which satisfies the necessary requirements. In second order only form III survives. The third order has *two* acceptable extrapolants for $\varepsilon_3(x)$; we have not been able to eliminate one in favour of the other and so must retain both. This will ultimately determine an uncertainty (which will be small) in the final equation of state. For both fourth and fifth orders form XII is the only extrapolant left from the elimination process. Figure 4 displays all the $\varepsilon_i(x)$ thus arrived at and

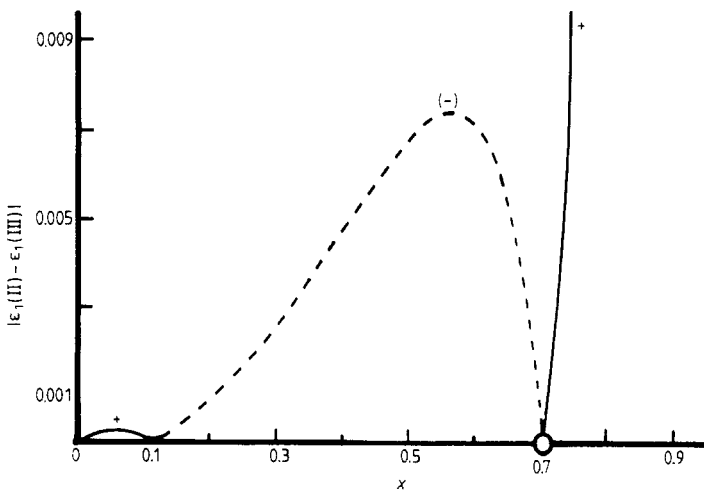


Figure 3. Difference of nearly degenerate forms II and III of table 1 of first-order energy extrapolants to (12).

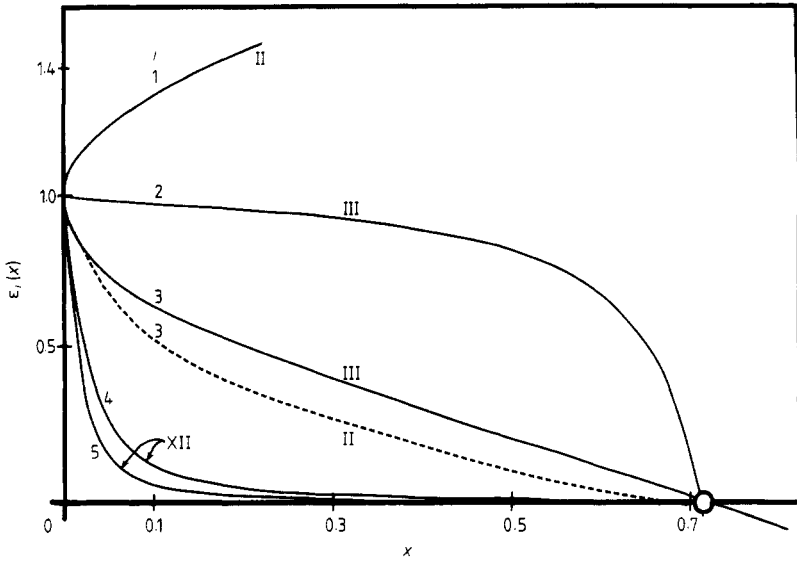


Figure 4. Graph of selected extrapolants to low-density series (12) for order $i = 1-5$. Roman numerals refer to specific approximants as listed in table 1.

Table 2. Numerical values of C_{1i} and C_{2i} ($i = 1, 2, \dots, 5$) in (12) for the Burkhardt HCSW model potential (5). The coefficients C_{3i} were determined in connection with the stated forms (Roman numerals) as selected from table 1 using constraints (16) and (18).

	i				
j	1	2	3	4	5
1	12.036 105	-4.955 702	-16.333 996	-21.296 272	-18.095 008
2	78.615 68	-143.876 079	-84.568 230	112.555 958	323.803 363
3	-0.651 64 (II)	-81.379 8 (III)	185.378 4 (III)	451.537 3 (XII)	325.435 5 (XII)
			16.025 5 (II)		

should be compared with figure 1 of [17] where the exact fermion results [14] mentioned before are plotted as a function of x .

Table 2 lists the numerical values of the coefficients C_{ji} ($j = 1, 2, 3; i = 1, 2, 3, 4, 5$) for the Burkhardt HCSW potential. We emphasise that the extrapolant forms $\epsilon_i(x)$ contain three- and higher-body correlation effects since expanding $\epsilon_i(x)$ about $x = 0$ produces an infinite series of terms, *in principle* reflecting n -body cluster effects even if imperfectly, as also occurs in conventional perturbative and variational schemes addressing the ground-state energy problem. Note the more than order-of-magnitude difference of C_{33} as given through forms II or III, which, however, will cause only a 7.5% uncertainty in the final saturation energy, to which we now turn.

4. Attractive coupling constant series analysis

We have arrived at what are believed to be reasonable representations for $\epsilon_i(x)$ over the greater part of the physical density interval. These are the generalised Padé forms

of table 1 corresponding, order by order, to the blank entries in the right half of the table, namely the forms plotted in figure 4. They are now used for the $\varepsilon_i(x)$ ($i=1-5$) in (19) for the ground-state energy of the many-boson Schrödinger equation. The λ power series through fifth order is, say,

$$\left(1 + \sum_{i=1}^5 a_i \frac{\varepsilon_i(x)}{\varepsilon_0(x)} \lambda^i\right) \equiv 1 + \sum_{i=1}^5 f_i(x) \lambda^i \quad (26)$$

a fifth-order polynomial in λ to be analysed in terms of all (standard) Padé approximants $[L/M](\lambda)$ with $0 \leq L+M \leq 5$. The form $[0/0](\lambda) \equiv 1$ will give in (19) the hard-sphere boson equation of state, while the form $[L/0](\lambda)$ will provide the 'straight' L th-order van der Waals perturbation corrections. All forms $[0/M](\lambda)$ are simple reciprocals of M th-order polynomials in λ with finite x -dependent coefficients. The latter are finite for all x and so $[0/M](\lambda)$ cannot be zero at any x for fixed λ ; hence they cannot provide energy minima. For illustration we display just one Padé form to (26), namely

$$[1/1](\lambda) = \frac{f_1(x) + [f_1^2(x) - f_2(x)]\lambda}{f_1(x) - f_2(x)\lambda} \quad (27)$$

Using form III for $\varepsilon_3(x)$, we plot in figure 5 all approximants with $0 \leq L+M \leq 5$, except the $[0/M](\lambda)$. Binding is already achieved in first order: the $[1/0]$ curve. The broken portion of each curve corresponds to the unstable and metastable segments eliminated by a standard 'convex hull construction' [18], of which the Maxwell rule of equal areas is an example. The experimental results for liquid ^4He are summarised [19] by the bold curve which represents an interpolation of the data. Figure 6 shows an enlargement of the saturation minima predicted by our calculations. The final predicted saturation energy in fifth order is about -15.10 ± 0.05 K, being bounded above by the $[2/3]$, and below by the $[4/1]$, Padé forms.

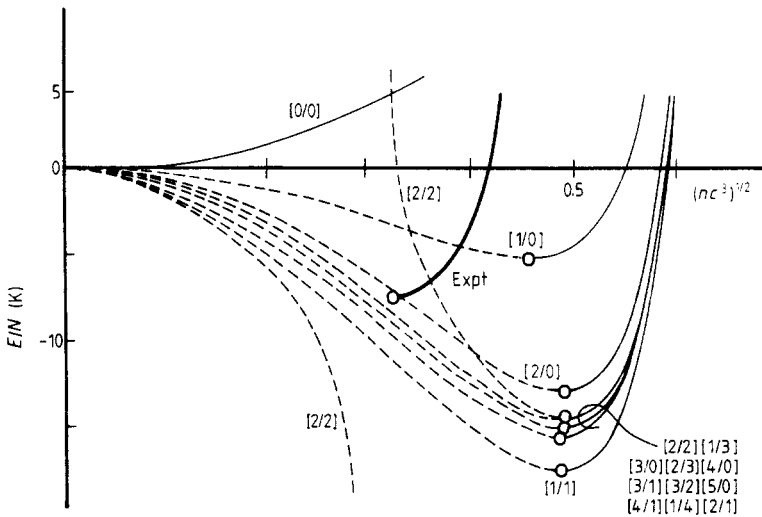


Figure 5. Energy per boson plotted against the $(nc^3)^{1/2}$ variable as given by Padé approximants $[L/M](\lambda)$ to λ expansion equation (19) using form III for $\varepsilon_3(x)$. The bold curve represents an interpolation of laboratory empirical liquid ^4He results. Open circles mark saturation minima. The broken curves refer to unstable branches of the equation of state, as explained in the text.

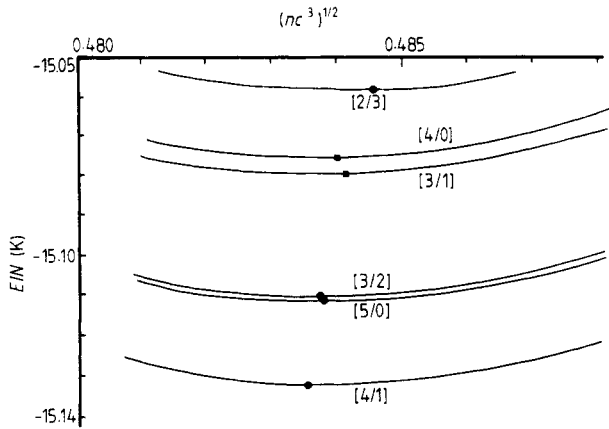


Figure 6. Same as figure 5, but enlarged. Energy minima: ■, $L + M = 4$; ●, $L + M = 5$.

On the other hand, form II for $\epsilon_3(x)$ gives the somewhat weaker-bound results of figure 7, with a saturation energy of about -14.070 ± 0.015 K. The net uncertainty due to the ambiguity of forms II and III in third order is thus only about 1.145 K out of 15.20 K, or about 7.5%.

We mention that all denominators of the $[L/M](\lambda)$ forms have been tested for possible zeros, at the fixed saturation x value, as λ goes from 0 to the value λ_p as given by (17). None were found, and thus all the λ Padé forms are singularity-free along the trajectory mentioned before, as required.

The somewhat large saturation density predicted—just over twice the empirical value of 0.022 \AA^{-3} —is probably attributable to the rather small core radius of 1.685 \AA of the Burkhardt HCSW. The larger core radius of 2.3 \AA of a more recent HCSW potential model [20], *not* constructed based on phase-equivalence criteria, however, would definitely reduce the saturation density discrepancy. In fact, it is easy to see that increasing c beyond the value of 1.685 \AA used here will (a) shift the experimental curve in figure 5 to the right and simultaneously (b) shift the calculated curves vertically

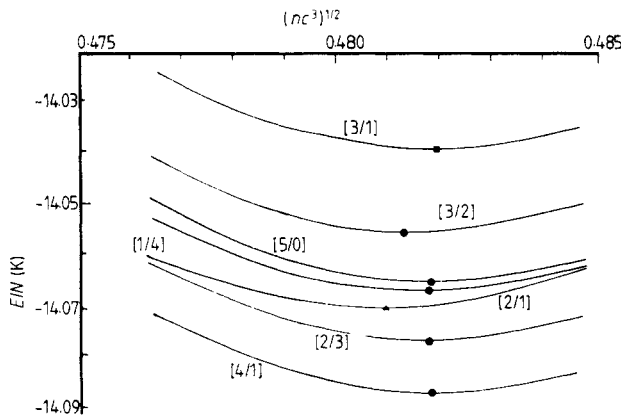


Figure 7. Same as figure 6, but using form II for $\epsilon_3(x)$. Energy minima: ▲, $L + M = 3$; ■, $L + M = 4$; ●, $L + M = 5$.

up, if λ and α are kept constant. Clearly, however, one should not insist too much on agreement with laboratory (as opposed to computer) experiments because of the simple nature of the model potential as well as, of course, the neglect of three- and higher-body forces in the whole calculation.

5. Conclusions

Starting from the well known low-density expansion for the ground-state energy of an interacting many-boson system we have rearranged the series into one whereby the unperturbed reference system is not the ideal Bose gas but rather the fluid of repulsive particles. We have limited ourselves for now to a model pair central potential of hard-core square-well shape.

The density dependence of the first five perturbation corrections to this fluid, due to attractions, was found to be violent and out of bounds. Little improvement was seen to ensue from direct imposition of physical constraints emerging from the assumption—known to be true in one and two dimensions in classical systems—that the present perturbation scheme is exact as close packing is approached. Extrapolation in density of the perturbation energies was then carried out via a new method called ‘tailing’ but based essentially on generalised Padé approximants. Together with the above-mentioned physical constraints, other general criteria were applied to the eleven distinct extrapolants thus constructed in each order. These conditions allowed the elimination of all but one acceptable form in each order, with the sole exception of third order, where two distinct and appreciably non-degenerate forms remained (which in the end left an uncertainty of about 7.5%). Moreover, the correlated behaviour in density of the energy corrections in all five orders was found to be very reasonable compared with exact calculations through fourth order that exist in the literature for purely attractive fermions.

A standard Padé analysis was then carried out in the remaining attractive coupling constant series through fifth order leading to a stable result in the ground-state energy of the many-boson Schrödinger equation.

Computer simulations, such as GFMC, for even the purely repulsive hard-sphere boson fluid at densities approaching the packing density would go a long way in testing the accuracy of our description of the reference unperturbed state. Of course, GFMC calculations for the full HCSW fluid would be ideal.

Applications like those presented here are planned for the same ^4He system but interacting via more realistic pair potentials for which there exist GFMC results [21]. For this purpose, extensive tables of the required λ expansion coefficients for several interparticle forces have been made available [22].

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