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A quantum thermodynamic perturbation study of spin-polarized boson fluids

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Received 14 September 1992

Abstract. With *no adjustable parameters* the ground-state properties of the spin-polarized bosonic fluids H^\downarrow and T^\downarrow are obtained via quantum thermodynamic perturbation theory. Here, perturbations are developed around the corresponding repulsive-sphere gas. The attractive and repulsive portions of the interatomic interaction potential (Lennard-Jones and Kolos–Wolniewicz) are decomposed as proposed by Barker and Henderson and by Weeks, Chandler and Anderson. The various density series for the energy are extrapolated, order by order, to physical densities via Padé and related approximants. The pressure and the sound velocity curves can be obtained from the energy. The difference between our results and variational results is only significant at higher densities, where our energy curves generally lie lower.

1. Introduction

The suggestion [1] of the possibility of extreme quantum behaviour in bulk spin-polarized hydrogen atoms, and later the experiment of Silvera and Walraven [2] showing this for hydrogen atoms by applying intense (~ 10 T) magnetic fields at low ($\sim 10^{-2}$ K) temperature, motivated increased efforts to stabilize these new ‘spin-polarized quantum systems’ at increasingly higher densities. In the particular case of spin-polarized atomic hydrogen H^\downarrow , even greater interest lies in the hope of eventually reaching densities high enough to observe a Bose–Einstein condensation (BEC) in this very weakly interacting quantum gas. However, the recombination of the hydrogen atoms on the container walls as well as in the bulk has thus far limited the prospects of this hope.

A great deal of work has been devoted to the theoretical problem of calculating the ground-state energy of a system of N bosonic particles described by a given Hamiltonian, when N tends to infinity [3–15]. These computations have mainly been standard variational or Monte Carlo variational ones. So, for example, in the pioneering works of Dugan and Eters [3] and Eters *et al* [4], the ground-state properties were obtained for spin-polarized hydrogen isotopes. The well known interaction potential between particles according to Kolos and Wolniewicz (KW), figure 1, was fitted by a Morse potential form. They then

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applied the variational Monte Carlo method for a finite number of particles inside a box whose volume corresponds to a choice of system density. To simulate the infinite system it was necessary to replicate the box and its contents in all directions by imposing periodic boundary conditions. They concluded that, unlike atomic hydrogen, tritium forms a liquid at 0 K. Nosanow *et al* [5] studied within the context of the quantum theorem of corresponding states the zero-temperature properties of systems obeying either Bose–Einstein or Fermi–Dirac statistics. This was applied by Miller and Nosanow [10] to the ground-state properties of N -body assemblies consisting of identical isotopes of spin-polarized hydrogen. Calculations of the ground-state energy were performed for the KW and Lennard-Jones (LJ) potentials, figure 1, as well as for a Morse function fit to the KW potential. The boson systems were treated variationally with a trial Jastrow-type wavefunction and the problem was reduced to obtaining the radial distribution function $g(r)$ generated by the trial wavefunction. They used $g(r)$ values from approximations such as the Born–Bogoliubov–Green–Kirkwood–Yvon (BBGKY), the Kirkwood superposition approximation (KSA) and hypernetted-chain (HNC) approximate integral equation, and confirmed that H^\downarrow can *never* form a liquid phase for $T = 0$ and zero pressure. We compare our results with the BBGKY ones. Stwalley and Nosanow [7] showed that spin-aligned isotopes exhibit *even more extreme* quantum behaviour than the helium isotopes: H^\downarrow was predicted to be a *gas* at all temperatures. Lantto and Nieminen [12] calculated the ground-state properties of H^\downarrow based on the variational Jastrow-type many-boson optimized wavefunction in the HNC approximation. The variational calculation of Ristig and Lam [14] is based on an optimized trial wavefunction with intra-atomic hyperfine mixing and interatomic spatial correlations. The respective radial distribution function $g(r)$ was calculated by employing the HNC procedure. More recently, Haugen and Østgaard [15] introduced a modified lowest-order constrained-variational method to calculate the ground-state properties of spin-polarized hydrogen isotopes for five different two-body potentials. Except for the work of Miller and Nosanow [10], Haugen and Østgaard [15] and Greef *et al* [16], all calculations thus far have been restricted to low values of density.

In a recent series of papers [17–31] the ground-state energy of several quantum many-body systems has been computed through a generalization of van der Waals’ original idea to describe classical fluids by separating the attractive part of the elementary two-body force from the short-range repulsions. This perturbative approach to quantum fluids—hereafter called quantum thermodynamic perturbation theory (QTPT)—has been applied in first-principles calculations [30, 31] of the ground-state energy of liquid helium-4 (^4He) and the results lie within the accuracy of GFMC simulations. This success has encouraged the present work.

In section 2 we present a brief review of the QTPT method for bosons; in section 3 we obtain the ground-state energies of spin-polarized hydrogen and tritium fluids interacting via the LJ and KW [32] potentials using both the Barker–Henderson (BH) [33] and the Weeks–Chandler–Anderson (WCA) [34] prescriptions to decompose the potential into a repulsive core plus an attractive tail. Section 4 gives the results and discussion; and section 5 states our conclusions.

2. Quantum thermodynamic perturbation theory for bosons

We consider an N -boson system in a volume Ω such that the particle density is given by $\rho = N/\Omega$. At low densities quantum-field-theoretic diagrammatic techniques employing

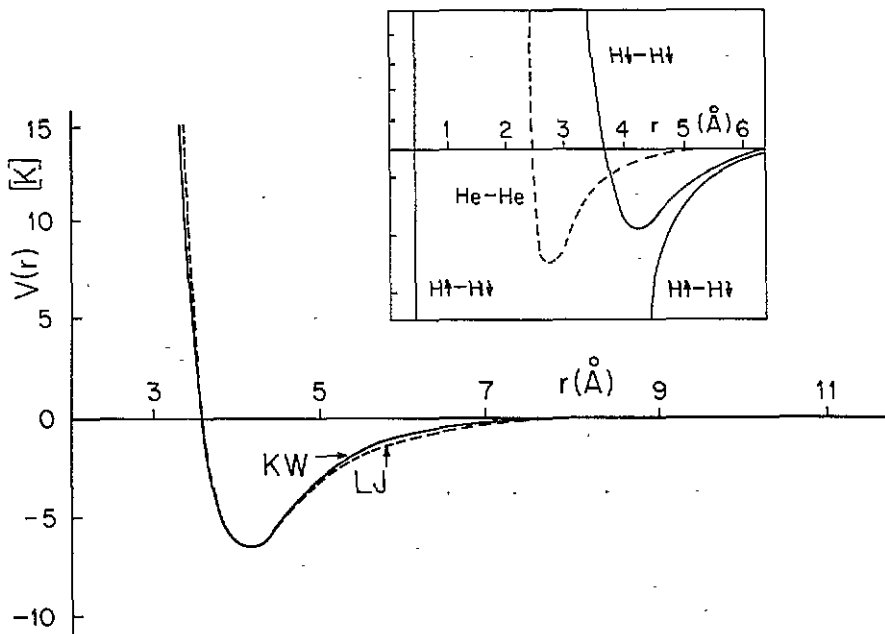


Figure 1. Lennard-Jones (LJ) and Kolos-Woyniewicz (KW) potentials between two hydrogen atoms in the triplet electronic state. Inset: the interaction in the singlet and triplet electronic states of hydrogen compared with that of two helium atoms.

infinite partial summations of successively less divergent terms give for the ground-state energy per particle of the boson system [35] the non-analytic infinite series

$$E/N = (2\pi\hbar^2/m)\rho a [1 + C_1(\rho a^3)^{1/2} + C_2\rho a^3 \ln(\rho a^3) + C_3\rho a^3 + O\{(\rho a^3)^{3/2} \ln(\rho a^3)\}] \tag{1}$$

where C_1 and C_2 are known dimensionless coefficients that do not depend on the potential. The coefficient C_3 and all successive coefficients are unknown and depend on the form of the interaction potential. Here a is the two-body S-wave scattering length which can be either positive or negative. Equation (1) is a complex quantity for most systems of interest where $a < 0$.

As described in [17]–[31] it is convenient to separate the pair potential $V(r)$ into the following repulsive and attractive parts:

$$V(r) = V_{\text{rep}}(r) + \lambda V_{\text{att}}(r) \quad 0 \leq \lambda \leq 1 \tag{2}$$

where $V_{\text{att}}(r)$ is negative and where $\lambda = 1$ corresponds to the full interaction, figure 2. The decomposition defined by (2) suggests an expansion of the scattering length a in powers of the attractive coupling λ :

$$a = a_0 + a_1\lambda + a_2\lambda^2 + \dots \tag{3}$$

where a_0 is manifestly positive, while $a_i < 0$ for all $i = 1, 2, \dots$. Inserting (3) into (1) yields the series

$$E/N = (2\pi\hbar^2/ma_0^2)x^2 \sum_{i=0}^{\infty} \alpha_i e_i(x)\lambda^i \quad \alpha_i \equiv a_i/a_0 < 0 \tag{4}$$

where each $e_i(x)$ is, in turn, a non-analytic infinite series in $x \equiv (\rho a_0^3)^{1/2}$, namely

$$e_i(x) = 1 + C_{1i}x + C_{2i}x^2 \ln x^2 + C_{3i}x^2 + \dots \tag{5}$$

The dimensionless coefficients C_{1i} and C_{2i} , $i = 1, 2, \dots, 6$, have been deduced [28] through the computer algebraic software package called MACSYMA [36], in terms of the $C_1, C_2, a_1, a_2, \dots, a_6$ of (1) and (3). In tables 1 and 2 we display these coefficients for both the LJ and KW potentials. Clearly, $C_{10} = C_1$ and $C_{20} = C_2$. (4) can be interpreted as a perturbation series about a reference (or unperturbed) system of repulsive spheres, and the energy is now real at all values of the attractive coupling λ . The appearance of the logarithmic term does not admit application of standard methods to accelerate convergence in power series such as Padé approximants. We therefore need a more general scheme of the form

$$e_i(x) \hat{=} \epsilon_i(x) \tag{6}$$

where $\epsilon_i(x)$ is a generalized extrapolant representing the series (5) subject to the constraint that, upon expansion about $x = 0$, it reproduces exactly the known coefficients C_{ij} of $e_i(x)$. Evidently, such a representation is not unique. The number of approximants $\epsilon_i(x)$ for each $e_i(x)$ will depend on the number of coefficients C_{ji} , $j = 1, 2, \dots$, we wish to reproduce in the series (5). So, to reproduce it with three terms there will be *four* so-called ‘tailing approximants’ [28, 37]

- Form (i) $1 + C_{1i}/(1 - C_{2i}x \ln x^2/C_{1i})$
- Form (ii) $(1 - C_{1i}x - C_{2i}x^2 \ln x^2)^{-1}$
- Form (iii) $(1 + C_{2i}x^2 \ln x^2)/(1 - C_{1i}x)$
- Form (iv) $(1 + C_{1i}x)/(1 - C_{2i}x^2 \ln x^2)$

which we have called the ‘small family’ of extrapolants. To reproduce up to the $C_{3i}x^2$ term of the series (5), *twelve* tailing approximants are possible which we designate form (I), form (II), ..., form (XII) and collectively call the ‘large family’ of extrapolants. A complete list of these for bosons is given in [31]. We use mainly the ‘small family’ approximants that reproduce the first two known coefficients in (5), but we needed to employ the ‘large family’ in order to deduce acceptable hard-sphere $\epsilon_0(x)$ and fourth-order $\epsilon_4(x)$ extrapolants for T^\dagger with the KW(BH) and KW(WCA) interactions, where the small family was found to be insufficient. Figure 3 shows a graph for H^\dagger with KW(BH) of the small family of extrapolants $\epsilon_1(x)$ to the series $e_1(x)$, labelled 0, given by (5) with $i = 1$.

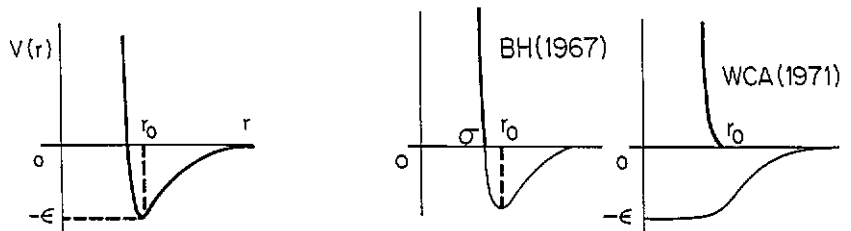


Figure 2. Barker–Henderson (BH) and Weeks–Chandler–Anderson (WCA) decomposition for the potential $V(r)$ into repulsive and attractive parts.

Table 1. Coefficients C_{ji} , $j = 1, 2$, $i = 1, \dots, 6$, of (5) for H^\downarrow for the LJ and kw potentials decomposed according to the BH and WCA methods.

		i						
		j	1	2	3	4	5	6
LJ	BH	1	12.036 05	-3.123 486	-10.964 71	-15.542 53	-16.449 92	-12.766 49
		2	78.615 66	-119.418 9	-75.178 03	21.016 6	133.402 7	224.524 7
	WCA	1	12.036 05	-2.450 462	-9.900 332	-14.470 9	-15.908 74	-13.506 00
		2	78.615 66	-110.627 0	-75.230 29	6.303 165	105.279 5	191.706 5
KW	BH	1	12.036 05	-2.271 039	-10.286 64	-15.207 43	-16.623 14	-13.686 29
		2	78.615 66	-108.283 1	-79.866 81	7.758 237	118.040 4	214.096 3
	WCA	1	12.036 05	-1.609 827	-8.959 857	-13.712 98	-15.647 01	-14.161 62
		2	78.615 66	-99.645 43	-77.068 1	-7.186 953	84.028 01	169.741 9

Table 2. As table 1, but for T^\downarrow .

		i						
		j	1	2	3	4	5	6
LJ	BH	1	12.036 05	-2.218 412	-9.604 303	-14.215 11	-15.807 07	-13.709 03
		2	78.615 66	-107.595 6	-75.569 14	2.155 968	98.345 87	184.280 3
	WCA	1	12.036 05	-1.669 831	-8.718 381	-13.274 98	-15.204 13	-13.976 85
		2	78.615 66	-100.429 3	-74.687 41	-7.995 518	77.273 70	157.570 0
KW	BH	1	12.036 05	-1.094 341	-8.478 799	-13.374 01	-15.562 41	-14.491 81
		2	78.615 66	-92.911 44	-78.482 18	-14.243 32	73.901 65	159.878 3
	WCA	1	12.036 05	-0.635 926 3	-7.430 579	-12.090 32	-14.522 28	-14.320 84
		2	78.615 66	-86.923 01	-74.615 66	-22.497 54	50.908 22	126.210 8

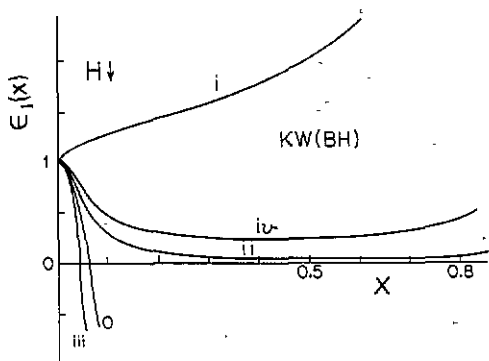


Figure 3. First-order approximants $\epsilon_1(x)$ for H^\downarrow for the kw(BH) potential. Roman numerals indicate the form of the approximant as defined below (6), and '0' refers to the original series (5) for $i = 1$.

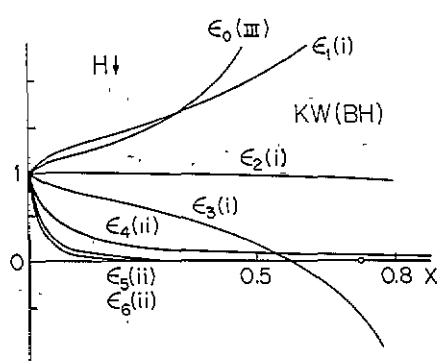


Figure 4. Optimum approximants $\epsilon_i(x)$, ($i = 1, \dots, 6$) for H^\downarrow from the analysis for the kw(BH) potential. The Roman numerals in parentheses specify the approximant used among the four defined below (6). Also displayed is the approximant $\epsilon_0(x)$ for the energy of the hard-sphere fluid (8). The close packing value of $x_B = 0.7245$ is also indicated by the open circle.

The available extrapolants in each order are constrained by the following global physical conditions:

- (i) For $i = 0$, the repulsive-sphere system $\epsilon_0(x)$ has a second-order pole, due to the

uncertainty principle, at some density $\rho = \rho_B$ and hence at $x = x_B$, corresponding to close packing.

(ii) $\epsilon_i(x)$ has no singularities in the physical region, i.e., in the region $x < x_B$.

(iii) From straightforward perturbation theory and due to the negativity of V_{att} , it can be shown [25] that for all $0 < x < x_B$

$$\epsilon_1(x) > 0 \quad \epsilon_2(x) > 0. \quad (7)$$

(iv) $\epsilon_1(x)$ must be monotonically increasing as can be argued from first-order perturbation theory.

The above constraints are rigorous; additional conditions can be imposed on physical grounds as follows:

(v) The ground-state energy of the hard-sphere system has been studied extensively. We therefore use a hard-sphere representation for $\epsilon_0(x)$ that has a characteristic close-packing density pole at some density, say ρ_B . A theorem [38] in classical thermodynamic perturbation theory suggests that $\epsilon_1(x_B) = \text{constant}$, while $\epsilon_i(x_B) \simeq 0$, for $i \geq 2$.

These constraints hopefully provide an essentially unique extrapolant for boson systems, to be designated the *optimal extrapolant*.

In [17] and [27] the optimal representation for the boson hard-sphere reference system has been obtained from (4) (setting $\lambda = 0$). The resulting approximant is

$$\epsilon_0(x) = \llbracket 1 - \frac{1}{2}C_{10}x / \{1 - (2C_{20}/C_{10})x[\ln x + (C_{30} - 3C_{10}^2/4)/2C_{20}]\} \rrbracket^{-2} \quad (8)$$

where C_{30} is the next term order contribution of (1) with $\lambda = 0$, i.e., the term of order ρa^3 , involving the unknown constant C_3 . A fit [27] to the available Green-function Monte Carlo (GFMC) data [39] for liquid ${}^4\text{He}$ yields the value $C_{30} = 25.11$, and the second-order pole apparently corresponding to a close-packing density is at $x_B = 0.7245$. The results for the ground-state energy of ${}^4\text{He}$ have been published recently [30, 31]. Here we merely note that QTPT gives agreement with the GFMC data within the statistical error of the simulations, as well as good agreement with laboratory experimental data, particularly with the more realistic Aziz interatomic potential.

3. Spin-polarized hydrogen and tritium

It is well known that the hydrogen molecule H_2 results from the interaction of two hydrogen atoms in their ground state through a comparatively attractive singlet potential. This contrasts with a predominantly repulsive electronic triplet potential, figure 1, inset. The singlet potential is responsible for the binding of H_2 . This fact has stimulated the study of hydrogen atoms interacting purely via the electronic triplet potential, in order to exhibit macroscopic quantum behaviour expected to be even more extreme than that observed with the helium isotopes. A strong magnetic field can produce spin-polarized hydrogen (H^\downarrow), deuterium (D^\downarrow) or tritium (T^\downarrow), of which H^\downarrow and T^\downarrow are boson particles. Theoretical calculations [10, 12, 14] have suggested that H^\downarrow does not form a liquid phase under either the LJ or the KW interactions, figure 1. In contrast, T^\downarrow is similarly expected to be a weakly bound liquid. Here we study the bosonic systems H^\downarrow and T^\downarrow , whose atoms interact via the spin-polarized triplet state (designated ${}^3\Sigma_u^+$) with either an LJ potential with $\sigma = 3.689 \text{ \AA}$ and $\epsilon = 6.464 \text{ K}$, or the KW potential with the Silvera [11] fit. The attractive and repulsive

parts of the potential are separated out as suggested by BH [33] and by WCA [34], figure 2. Depending on the potential between the particles and the mode of decomposition, we shall refer to the interaction as LJ(BH), LJ(WCA), KW(BH) or KW(WCA).

The QTPT method applied to these systems up to sixth order in λ with the constraints mentioned above yielded the following approximants to the $\epsilon_i(x)$ series in (4):

$\epsilon_i(x)$ forms for H^\downarrow							
Potential	$i=$	1	2	3	4	5	6
LJ(BH)		(i)	(i)	(i)	(ii)	(ii)	(ii)
LJ(WCA)		(i)	(i)	(i)	(ii)	(ii)	(ii)
KW(BH)		(i)	(i)	(i)	(ii)	(ii)	(ii)
KW(WCA)		(i)	(i)	(i)	(ii)	(ii)	(ii)

$\epsilon_i(x)$ forms for T^\downarrow							
Potential	$i=$	1	2	3	4	5	6
LJ(BH)		(i)	(i)	(i)	(iii)	(ii)	(ii)
LJ(WCA)		(i)	(i)	(i)	(ii)	(ii)	(ii)
KW(BH)		(i)	(i)	(i)	(III)	(ii)	(ii)
KW(WCA)		(i)	(i)	(i)	(III)	(ii)	(ii)

These sets of extrapolants have been chosen by analysis similar to that of [30]. For example, we summarize in tables 3 and 4 the results of analysis to obtain the energy coefficients for H^\downarrow with LJ(WCA) and T^\downarrow with KW(WCA), respectively. Figure 4 illustrates the optimum extrapolants $\epsilon_i(x)$ for H^\downarrow with KW(BH) for orders $i = 0-6$. The open circle on the x axis marks the location of $x_B = 0.7245$. Note that for the highest orders, $\epsilon_4(x)$, $\epsilon_5(x)$ and $\epsilon_6(x)$, good Stell–Penrose behaviour $\epsilon_i(x) \simeq 0$ is easily achieved. The possible $\epsilon_4(x)$ from the small family of approximants for T^\downarrow with KW(BH) and KW(WCA) did not satisfy the aforementioned constraints, so it was necessary to use the large family of approximants. This introduced the need to determine the unknown coefficients C_{34} requiring good Stell–Penrose behaviour at the close-packing density $x_B = 0.7245$. For both cases, KW(BH) and KW(WCA), the optimum approximant was found to be form (III), with $C_{34} = 151.224$ and 114.937 , respectively. It is clear that an accurate determination of the scattering length expansion parameters (3) is needed for each different two-body interaction describing the system. There exists a very precise (fourteen-digit accuracy) calculation of the low-energy scattering parameters (3) [40, 41] for the hydrogen and tritium isotopes interacting with the LJ, as well as with the KW, interaction.

In replacement of (4), the final expression for the energy is now given by

$$E/N = (2\pi\hbar^2/ma_0^2)x^2 \sum_{i=0}^6 \alpha_i \epsilon_i(x) \lambda^i \tag{9}$$

with the extrapolants $\epsilon_i(x)$ determined as discussed above. The particle masses m used are given by $\hbar^2/m = 48.133\,716 \text{ K \AA}^2$ for H^\downarrow , and $\hbar^2/m = 16.089\,71 \text{ K \AA}^2$ for T^\downarrow . The pressure $P(\rho)$ and the sound velocity $c(\rho)$ as functions of the density can be obtained from (9) through the following thermodynamic relations:

$$P(\rho) = \rho^2 d[E(\rho)/N]/d\rho \tag{10}$$

$$mc^2 = d[P(\rho)]/d\rho. \tag{11}$$

The derivatives were performed with the computer algebraic program REDUCE [42].

Table 3. For H^\downarrow , summary of density-series analyses to determine optimum approximants $\epsilon_i(x)$, marked with asterisks, for the LJ potential decomposed according to the WCA method. Abbreviations: VP \equiv violates positivity; NMI \equiv non-monotonically increasing; BSPB \equiv bad Stieltjes-Penrose behaviour.

Form	Approximant	ϵ_1	ϵ_2	ϵ_3	ϵ_4	ϵ_5	ϵ_6
0	$1 + K_1x + K_2x^2 \ln x^2$	VP	BSPB	BSPB	BSPB	BSPB	BSPB
(i)	$1 + \frac{K_1x}{1 + K_2/K_1x \ln x^2}$	—	—	—	BSPB	pole at $x = 0.02$	pole at $x = 0.01$
(ii)	$\frac{1}{1 - K_1x - K_2x^2 \ln x^2}$	NMI	pole at $x = 0.05$	pole at $x = 0.01$	—	—	—
(iii)	$\frac{1 + K_2x^2 \ln x^2}{1 - K_1x}$	VP	BSPB	BSPB	BSPB	BSPB	BSPB
(iv)	$\frac{1 + K_1x}{1 - K_2x^2 \ln x^2}$	NMI	pole at $x = 0.04$	pole at $x = 0.06$	BSPB	BSPB	BSPB

Table 4. As table 3 but for T^\downarrow and for the kw potential decomposed according to the WCA method. To obtain $\epsilon_4(x)$ it was necessary to use the ‘large family’ of $\epsilon_i(x)$; form (III) was chosen, with $K_3 = 114.937$. Abbreviations as table 3.

Form	Approximant	ϵ_1	ϵ_2	ϵ_3	ϵ_4	ϵ_5	ϵ_6
0	$1 + K_1x + K_2x^2 \ln x^2$	VP	BSPB	BSPB	BSPB	BSPB	BSPB
(i)	$1 + \frac{K_1x}{1 + K_2/K_1x \ln x^2}$	—	—	—	BSPB	BSPB	pole at $x = 0.01$
(ii)	$\frac{1}{1 - K_1x - K_2x^2 \ln x^2}$	NMI	pole at $x = 0.06$	pole at $x = 0.06$	BSPB	—	—
(iii)	$\frac{1 + K_2x^2 \ln x^2}{1 - K_1x}$	VP	BSPB	BSPB	(III) ^a	BSPB	BSPB
(iv)	$\frac{1 + K_1x}{1 - K_2x^2 \ln x^2}$	NMI	pole at $x = 0.06$	pole at $x = 0.07$	pole at $x = 0.1$	BSPB	BSPB

^a With $K_3 = 114.937$.

4. Results and discussion

Figure 5 illustrates how rapidly QTPT converges with KW(BH) for H^\downarrow as of second order in the λ series (9). The notation $[L/0]$ refers to the L th partial summation of the λ series (9), and comes from the more general notation $[M/N]$ for the Padé approximant of order $M+N$. Use of these approximants in λ was necessary in liquid ^4He [30, 31], where the attractive interaction is comparatively much stronger than in H^\downarrow . As expected, figure 5 shows that QTPT is in good agreement with the variational calculations of Miller and Nosanow [10], denoted by open circles in the figure. The figure is an amplification of the energy curves where the difference in energy between orders 4 and 5 in λ is at most 0.001 K. In figure 6 we show optimum $\epsilon_i(x)$, $i = 1, 2, \dots, 6$ for T^\downarrow with the KW(WCA) potential. Lower-case Roman numerals refer to the form of the extrapolant of the ‘small family’ and capital Roman numerals refer to the ‘large family’. When we introduce in (9) the corresponding $\epsilon_i(x)$ for T^\downarrow with the potential KW(BH), we obtain the energies per particle (9), given by $[L/0]$, $L = 0, 1, \dots, 6$, figure 7. Their convergence becomes very acceptable beyond fourth order in λ . Figure 8 is a scale amplification of figure 7. In both figures filled circles refer

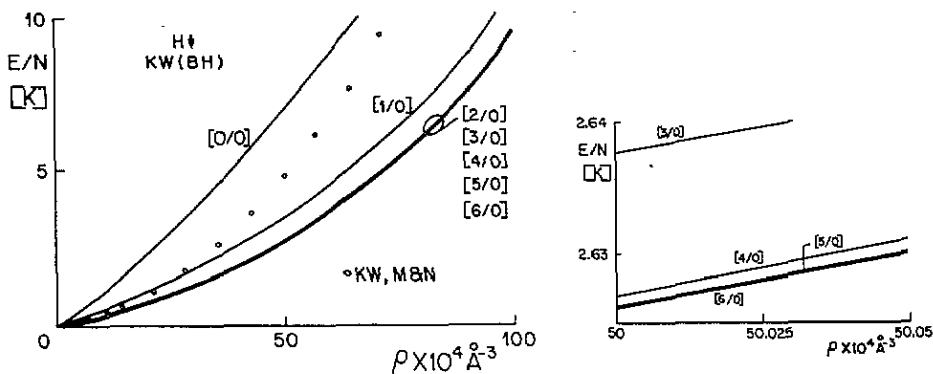


Figure 5. First seven partial sums $[L/0]$, $L = 0, 1, \dots, 6$, of (9) for E/N , the energy per particle, as a function of density, for the $kw(BH)$ potential. Open circles are the kw variational results of Miller and Nosanow. Inset: expanded scale showing convergence rate from third to sixth order of QTPT.

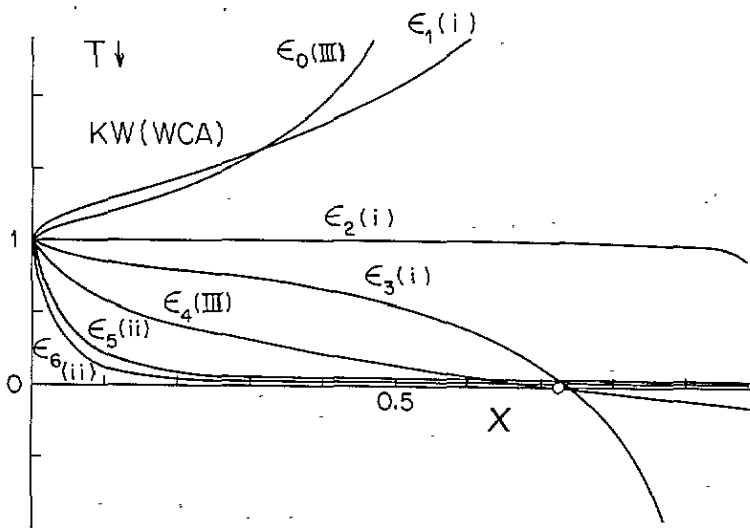


Figure 6. As figure 4, but for T^\downarrow with potential $kw(WCA)$.

to the results of Miller and Nosanow [10], with which we again have good agreement.

We summarize all our results in figure 9, where energy per particle versus density curves for H^\downarrow as well as T^\downarrow are displayed, using the interactions $LJ(BH)$, $LJ(WCA)$, $kw(BH)$ and $kw(WCA)$. We also include variational results obtained recently by other authors. Our curves refer to results obtained by substitution of the series $e_i(x)$ in (4) with the optimal representations $\epsilon_i(x)$ in (9). For H^\downarrow , our results show a systematic trend towards a softer equation of state (EOS) as compared with the variational calculations of Miller and Nosanow [10], Haugen and Østgaard [15], Ristig and Lam [14], Eters *et al* Monte Carlo (MC) [4] and Lantto and Nieminen [12]. However, at higher densities, our EOS becomes more rigid due to the hard-sphere reference system described by (8). Thus, most of our energy curves lie *below* those of the variational calculations. In contrast, the agreement with the T^\downarrow calculations of Miller and Nosanow is very good for this self-bound liquid boson system, the agreement with those of Haugen and Østgaard is only moderately so.

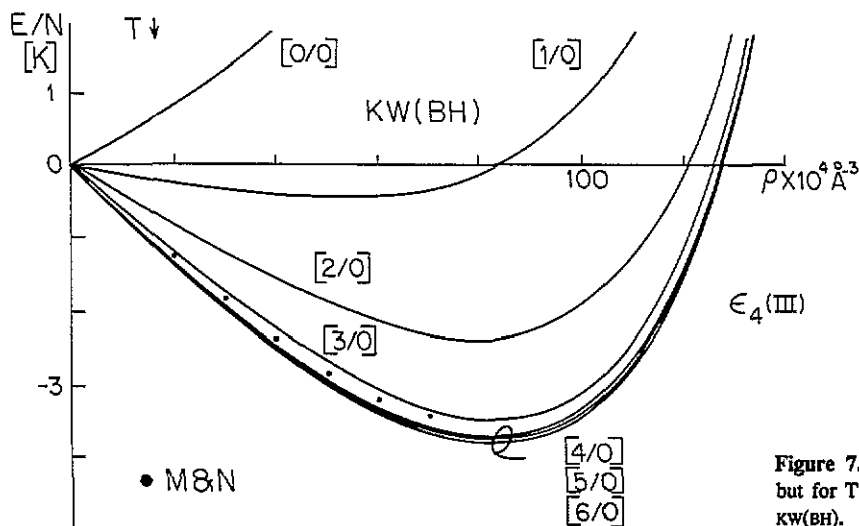


Figure 7. As figure 5, but for T^\downarrow with potential $KW(BH)$.

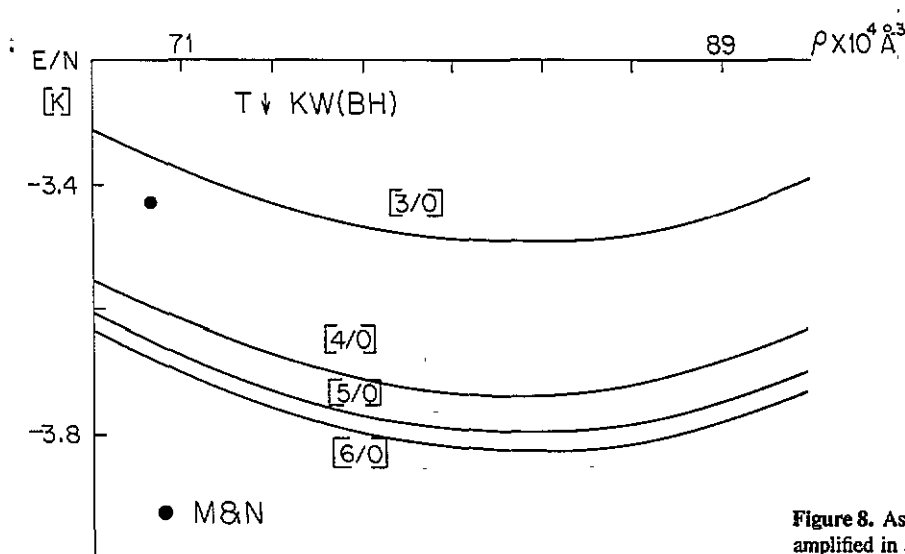


Figure 8. As figure 7, but amplified in scale.

At the saturation density (zero pressure) our results predict the following T^\downarrow equilibrium densities, binding energies, and sound velocities, depending on the interactions:

Interaction	ρ (\AA^{-3})	E/N (K)	c (m s^{-1})
LJ(BH)	0.0079 ± 0.00004	-4.22 ± 0.02	15.97 ± 0.1
LJ(WCA)	0.0075 "	-4.26 "	16.04 "
KW(BH)	0.0082 "	-3.83 "	14.63 "
KW(WCA)	0.0073 "	-3.21 "	14.11 "

The 'errors' quoted in the energy per particle, the density and the sound velocity correspond to the calculated *spread* in the sixth-order Padé curves in λ , namely [6/0], [5/1], [4/2], [3/3], [2/4], and [1/5].

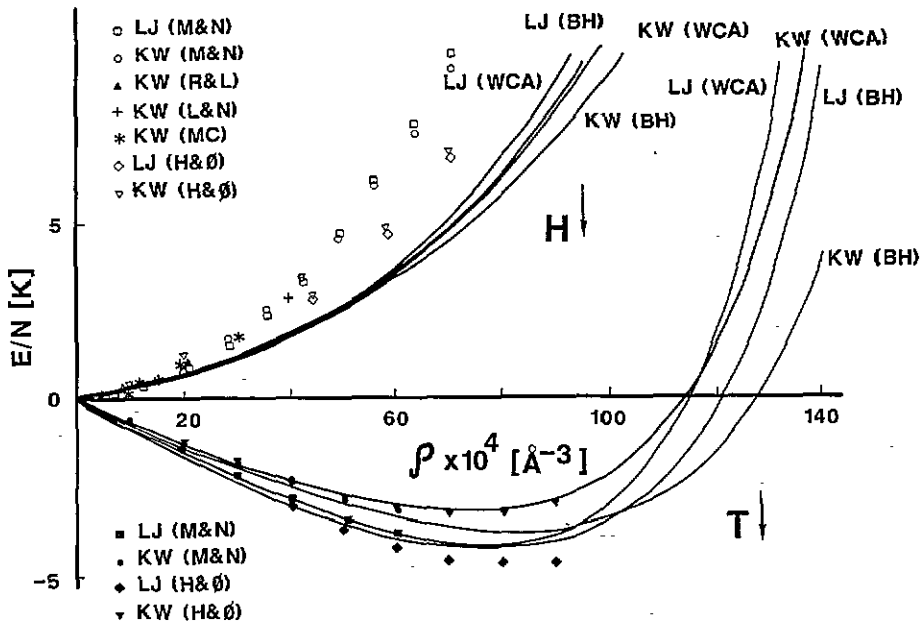


Figure 9. Our results (full curves) for the sixth-order ground-state energy per particle as function of the density, for H^\downarrow and T^\downarrow . Also, shown are the variational energies calculated for these two fluids by several authors as detailed in the text.

5. Conclusions

We have obtained the ground-state energy for the boson fluids H^\downarrow and T^\downarrow , for a wide density range. The pressure and the sound velocity can also be obtained but are not reported here. Our results agree at very low densities with all variational calculations carried out on these bosonic fluids, and at higher densities generally lie below them in energy for H^\downarrow .

The QTPT is again found to be a simple, inexpensive, reliable and accurate method for the calculation of the ground-state properties of quantum fluid systems. Since it exactly reproduces the first known coefficients of the low-density expansions for these fluid systems, it incorporates the maximum amount of rigorous information, and can furthermore be made more precise as higher-order coefficients in these expansions become available.

No adjustable parameters were used, even though results are sensitive to the way the pair potential is split; this also occurs in the TPT of classical fluids, considered to be the best theory of classical liquids. For example, our condition (ii) above is strictly a mathematical property of the first-order energy only, and is consistent with the general expectation that the total energy will likely possess a singularity below saturation density. But this density region cannot be trusted in its entirety from this or any other calculation that starts from low-density information. Also, the Bernal density for hard spheres will not be the correct value for a soft-sphere fluid (since such a density value would be strictly infinite here), but aids in 'taming' the density approximants at the higher-density end, which is much too high compared with physical saturation densities anyway. Explicit justification of the validity of QTPT at liquid densities is sketched in [28].

Finally, a definitive test of all calculations would be provided by benchmark GFMC simulations for these systems.

Acknowledgments

M de Ll and MAS gratefully acknowledge the hospitality of the Universidad de Valencia; M de Ll and RG acknowledge a NATO research grant. WCS thanks the Instituto de Física, UNAM, for its hospitality and acknowledges a National Science Foundation Grant.

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