

Aziz fermions and liquid  $^3\text{He}$ 

Zhizhong Hu\* and M. de Llano

*Physics Department, North Dakota State University, Fargo, North Dakota 58105*

E. Buendía and R. Guardiola

*Departamento de Física Moderna, Universidad de Granada, E-18071 Granada, Spain*

(Received 17 December 1990)

Starting from the well-known quantum-field-theory low-density expansion for the ground-state energy of a strongly interacting many-fermion assembly, we rearrange the series into a quantum-thermodynamic perturbation theory that is then applied to liquid  $^3\text{He}$ . Extrapolation to physical densities is implemented order by order via Padé and related approximants. We employ both the hard-core square-well potential and the Aziz pair potential with the Barker-Henderson (BH) and Weeks-Chandler-Andersen (WCA) potential-decomposition schemes familiar from classical fluid studies. The binding energy, saturation density, and sound velocity are calculated, *with no adjustable parameters*, and compared with Green-function Monte Carlo (GFMC) computer simulations, experimental data, and recent variational calculations. Our binding-energy and saturation-density results for the Aziz-WCA case, and the sound velocity result for the Aziz-BH case, are found to be within 2% of the GFMC data.

## I. INTRODUCTION

A long-standing problem in theoretical physics applied to condensed matter is that of calculating the equation of state of materials from first principles. Or, what is the relation among the macroscopic thermodynamic observables such as internal energy, pressure, entropy, density, temperature, etc., which arises from a given dynamic law at the microscopic, molecular level? Although some uncertainties remain for matter at moderate-to-high densities, significant progress<sup>1</sup> has been achieved over the past four decades in calculating the ground-state energy of a many-particle system with strong two-body interactions  $V(|\mathbf{r}_{ij}|)$  which are short-ranged attractive and repulsive at shorter ranges. The Hamiltonian is

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2 + g \sum_{i<j}^N V(|\mathbf{r}_{ij}|), \quad (1)$$

where  $0 \leq g \leq 1$  is a coupling parameter, with  $g=0$  corresponding to the ideal-gas case. Alternatively, instead of  $g$ , one can introduce  $0 \leq \lambda \leq 1$  such that

$$V(|\mathbf{r}_{ij}|) \equiv V(|\mathbf{r}_i - \mathbf{r}_j|) = V_{\text{rep}} + \lambda V_{\text{att}}. \quad (2)$$

Here  $\lambda$  is a “switching” parameter and the decomposition (2) into “repulsive” and “attractive” parts of the potential is still to be defined.

An important first step in understanding any liquid is to be able to determine from first principles its ground-state energy and equilibrium density at zero pressure, for which one needs to solve the Schrödinger equation for the system. Short of doing Monte Carlo simulations, it is customary to resort to some approximation scheme providing accurate results. Approaches to many-body theory in condensed-matter physics can be categorized as *perturbative*,<sup>2</sup> *variational*,<sup>3</sup> or *Monte Carlo*<sup>4</sup> (i.e., comput-

er simulations). The approach here is perturbative and our starting point is the exact low-density expansion<sup>5</sup> which includes, and systematically goes beyond, the Jastrow and Brueckner starting points of present-day variational and perturbative approaches, respectively. From the low-density expansion we derive a perturbative scheme picture based not on the *ideal-gas fluid* as the unperturbed or reference system, viz., Eq. (1), but rather on the nontrivial fluid of hard or soft spheres contained in the two-particle potential function, namely, Eq. (2). It is inspired in what is perhaps the most successful scheme for describing *classical* fluids, including liquids, based on an innovative idea of van der Waals for studying equations of state. The familiar van der Waals equation of state has been one outcome of this idea. Another is the thermodynamic perturbation theory (TPT) implemented by Barker and Henderson<sup>6</sup> (BH) and by Weeks, Chandler, and Andersen<sup>7</sup> (WCA). The quantum version, called QTPT for “quantum thermodynamic perturbation theory” was applied<sup>8</sup> to a hard-core-plus-attractive-square-well pair potential modeling liquid  $^4\text{He}$ . A recent decisive, critical test of the QTPT method encouragingly materialized<sup>9</sup> when one was able to work with a potential (2) for which “exact” ground-state results were available in the literature, viz., Green-function Monte Carlo (GFMC) simulations. Such is the case of liquid  $^4\text{He}$  modeled as a fluid of identical massive bosons interacting pairwise via either the traditional Lennard-Jones (6-12) or the more realistic Aziz potential, Fig. 1. Energy, density,<sup>9</sup> and sound-velocity<sup>10</sup> predictions for liquid  $^4\text{He}$  with either potential, based on the exact three-term, low-density expansion, proved to be within the statistical errors of the corresponding GFMC data.

We believe QTPT has two advantages over previous methods: (1) it exploits the maximum available rigorous many-body information for a given pair potential, and (2)

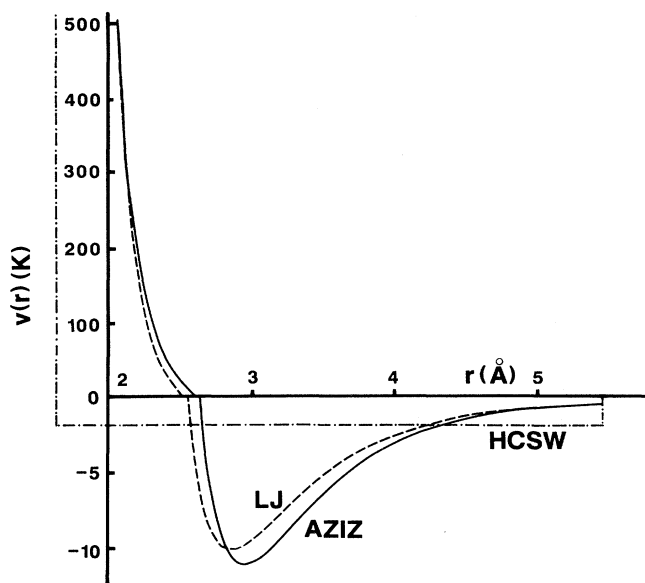


FIG. 1. Hard-core-square-well (HCSW), Aziz, and Lennard-Jones (LJ) pair potentials  $v(r)$  (in K) are compared. Note the drastic scale change between the positive and negative ordinate axes.

in predicting the properties of the liquid state it explicitly avoids<sup>11</sup> crossing phase boundaries, specifically the one separating the single-phase gas from the two-phase gas-liquid regions. (Of course, negative-pressure portions of the energy versus density curve must be discarded in the usual manner via the equivalent Maxwell construction.) In this paper we apply QTPT with a realistic pair poten-

$$\frac{E}{N} \cong \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} \left[ 1 + C_1(k_F a) + C_2(k_F a)^2 + \left[ C_3 \frac{R_0}{2a} + C_4 \frac{A_1(0)}{a^3} + C_5 \right] (k_F a)^3 + C_6 (k_F a)^4 \ln |k_F a| \right. \\ \left. + \left[ C_7 \frac{R_0}{2a} + C_8 \frac{A_0''(0)}{a^3} + C_9 \right] (k_F a)^4 + O(k_F a)^4 \right], \quad (3)$$

where the leading term is the ideal-Fermi-gas contribution and the dimensionless coefficients  $C_i$  are conveniently tabulated in Ref. 12. In (3),  $\hbar k_F$  is the Fermi momentum related to the particle density  $\rho \equiv N/\Omega$ , with  $\Omega$  the volume, through

$$\rho = \frac{\nu k_F^3}{6\pi^2}, \quad (4)$$

with  $\nu$  being the number of distinct fermion species. For the case of  ${}^3\text{He}$ ,  $\nu=2$  and, consequently,<sup>5</sup>  $C_6=0$ . The symbols  $a$ ,  $R_0$  and  $A_1(0)$  stand for the scattering parameters of effective-range theory<sup>13</sup> and are, respectively, the  $s$ -wave scattering length  $a$ , the  $s$ -wave effective range  $R_0$ , and the  $p$ -wave scattering length (cubed)  $A_1(0)$ —all of which characterize the potential assumed to act between pairs of particles in a shape-independent way. This is a consequence of the fact that these three parameters are

tial to *fermions*, and study the ground-state properties of liquid  ${}^3\text{He}$  modeled via the Aziz pair interaction. In Sec. II we rearrange the low-density ground-state energy expansion into QTPT form; Sec. III summarizes order-by-order density-series analyses; Sec. IV discusses the attractive-coupling-series Padé analysis; Sec. V gives our equation-of-state predictions compared with experiment, simulations, and with recent, very exhaustive, variational calculations; and Sec. VI presents our conclusions.

## II. REARRANGEMENT OF LOW-DENSITY EXPANSION

Every theoretical (nonsimulational) approach to the general many-body Schrödinger equation is necessarily an approximation of one kind or another. The most familiar *systematic* approximation scheme from elementary quantum mechanics is perturbation theory. In implementing this technique of quantum-field theory, one encounters the dilemma that perturbation theory leads, in general, for the fully interacting ground-state energy, to *infinite* terms in the series, when dealing with singular interactions. These divergences can be handled by applying infinite partial summation of selected Feynman diagrams which leave a finite *but nonanalytic expansion* in the density. The two most divergent sets of diagrams comprise the familiar “ladder” diagrams; when the next most divergent set is summed to this we have the so-called “complete” set of diagrams,<sup>5</sup> etc. The resultant finite, but nonanalytic, expansion for the ground-state energy per particle is then<sup>5</sup>

interrelated by effective-range theory with the scattering phase shift  $\delta_l(k)$  in the  $l$ th partial wave through the low-energy ( $\hbar^2 k^2/2m \rightarrow 0$ ) expressions<sup>14</sup>

$$k^{2l+1} \cot \delta_l(k) \cong -\frac{1}{A_l(0)} + \frac{1}{2} R_l k^2 + O(k^4) \quad (l=0, 1, 2, \dots). \quad (5)$$

Indeed, one can write these dynamical parameters as integrals over the pair interaction  $V(r) \equiv (\hbar^2/m)v(r)$  and reduced zero-energy radial wave function  $u_l(r)$ .<sup>15</sup> This function satisfies the zero-energy Schrödinger equation

$$u_l''(r) - \left[ v(r) + \frac{l(l+1)}{r^2} \right] u_l(r) = 0 \quad (6)$$

with  $u_l(0)=0$ . For  $r \rightarrow \infty$ , one must clearly have  $u_0(r) \rightarrow (r-a)$  and

$$u_1(r) \rightarrow \frac{r^2}{3} - \frac{A_1(0)}{r},$$

if  $v(r)$  is short ranged. The integrals alluded to above are<sup>15,16</sup>

$$A_0(0) \equiv a = \int_0^\infty dr r v(r) u_0(r), \quad (7)$$

$$R_0 = \frac{2}{a_0^2} \int_0^\infty dr [(r-a)^2 - u_0^2(r)], \quad (8)$$

$$A_1(0) = \frac{1}{3} \int_0^\infty dr r^2 v(r) u_1(r). \quad (9)$$

On the other hand, the scattering parameter  $A_0''(x)$  appearing in (3) in the (three-body)  $\rho^2$  (i.e.,  $k_F^6$ ) contribution to the energy, is potential-shape *dependent* and arises naturally from the various many-body selective infinite partial summations<sup>13,14</sup> through the integral

$$A_0''(0) \equiv -\frac{1}{3} \int_0^\infty dr r^3 v(r) u_0(r). \quad (10)$$

As the pair potential  $V(r)$  is decomposed in QTPT into repulsive and attractive portions in (2), we can expand  $a$ ,  $R_0$ ,  $A_1(0)$ , and  $A_0''(0)$  numerically in powers of  $\lambda$ :<sup>11</sup>

$$a = a_0(1 + a_1\lambda + a_2\lambda^2 + \cdots + a_6\lambda^6 + \cdots), \quad (11a)$$

$$R_0 = r_0(1 + r_1\lambda + r_2\lambda^2 + \cdots + r_6\lambda^6 + \cdots), \quad (11b)$$

$$A_1(0) = t_0(1 + t_1\lambda + t_2\lambda^2 + \cdots + t_6\lambda^6 + \cdots), \quad (11c)$$

$$A_0''(0) = p_0(1 + p_1\lambda + p_2\lambda^2 + \cdots + p_6\lambda^6 + \cdots). \quad (11d)$$

The Aziz potential can be decomposed via the two familiar BH (Ref. 6) and WCA (Ref. 7) schemes mentioned before and displayed in Fig. 2. In (11) the  $a_i$ ,  $r_i$ ,  $t_i$ ,  $p_i$  are reported for the Aziz-BH and Aziz-WCA cases in Ref. 17. Substituting (11a)–(11d) into (3), introducing the dimensionless variable  $k_F a_0 \equiv x$ , and expanding, leads to the ground-state energy rearranged as the double series, in  $x$  and  $\lambda$ , given by

$$\begin{aligned} \frac{E}{N} &\cong \frac{3\hbar^2 x^2}{10ma_0^2} \left[ e_0(x) + \sum_{j=1}^6 f_{1j} x e_j(x) \lambda^j + \cdots \right] \\ &\cong E_0 + \lambda E_1 + \lambda^2 E_2 + \cdots, \end{aligned} \quad (12)$$

where

$$e_0(x) \equiv 1 + f_{10}x + f_{20}x^2 + f_{30}x^3 + f_{50}x^4 + \cdots, \quad (13)$$

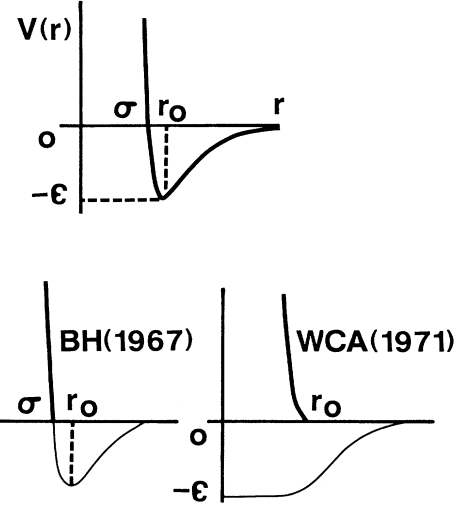


FIG. 2. Illustration of BH and WCA potential decompositions into repulsive and attractive parts of a typical interatomic potential like LJ or Aziz.

$$e_j(x) \equiv 1 + k_{1j}x + k_{2j}x^2 + k_{3j}x^3 + \cdots \quad (j=1, 2, \dots, 6), \quad (14)$$

$$k_{ij} = f_{i+1,j} / f_{1j} \quad (i=1, 2, 3). \quad (15)$$

The coefficients  $f_{ij}$  ( $i=1, \dots, 5$ ;  $j=0, 1, \dots, 6$ ) were obtained<sup>11</sup> (note that  $f_{4j} \equiv 0$ ) by using the computer-algebra packaged program called MACSYMA.<sup>18</sup> The values of  $f_{ij}$  for Aziz-BH and Aziz-WCA are listed in Tables I and II, and the  $k_{ij}$  defined in (15) are listed in Tables III and IV.

### III. DENSITY-SERIES ANALYSES

It is apparent that extrapolation to finite densities is the main task of *any* microscopic quantitative approach to the many-body fluid problem, whether it be variational or perturbative in technique. In extending a theory which is asymptotically exact in the *dilute*-gas region, to one expected to be suitable in the *dense*-liquid region, care must be exercised not to cross gas-to-liquid phase boundaries which may leave one in a spurious phase dia-

TABLE I. Coefficients  $f_{ij}$  of Eqs. (12) and (13) for Aziz-BH.

$j \setminus i$	1	2	3	4
0	0.353 678	0.185 537	0.384 776	-0.025 328
1	-0.359 101	-0.376 764	-2.134 120	0.655 874
2	-0.245 926	-0.066 752	-0.205 503	-0.234 123
3	-0.191 624	0.060 930	0.144 674	-0.392 697
4	-0.151 322	0.135 074	0.273 165	-0.563 786
5	-0.119 712	0.175 397	0.305 570	-0.742 253
6	-0.094 730	0.192 997	0.292 663	-0.918 767

TABLE II. Same as Table I but for Aziz-WCA.

$i \backslash j$	1	2	3	4
0	0.353 678	0.185 537	0.385 105	-0.025 515
1	-0.340 703	-0.357 461	-1.985 148	0.599 677
2	-0.233 038	-0.072 326	-0.215 569	-0.195 549
3	-0.183 273	0.043 242	0.104 304	-0.324 151
4	-0.146 443	0.112 138	0.228 562	-0.462 358
5	-0.117 293	0.151 645	0.266 870	-0.607 028
6	-0.093 983	0.171 001	0.262 989	-0.751 721

gram “sheet.” In QTPT as implemented here, arrival at the equilibrium liquid point is *explicitly* achieved<sup>11</sup> without crossing phase boundaries. Thus, QTPT is a “natural” way of correctly constructing the equation of state of a quantum liquid from first principles.

The primary specific task of the QTPT is extrapolation of the series  $e_0(x)$  and  $e_j(x)$  ( $j=1,2,\dots,6$ ), Eqs. (13)–(15), to nonzero  $x$  values. We denote these extrapolations by  $\varepsilon_0(x)$  and  $\varepsilon_j(x)$ , respectively. Once obtained, (12) will become

$$\begin{aligned} \frac{E}{N} &\cong \frac{3\hbar^2 x^2}{10ma_0^2} \left[ \varepsilon_0(x) + \sum_{j=1}^6 f_{1j} x \varepsilon_j(x) \lambda^j + \dots \right] \\ &\cong E_0 + \lambda E_1 + \lambda^2 E_2 + \dots, \end{aligned} \quad (16)$$

and is ready for the  $\lambda$ -series Padé analysis or extrapolation. The density-extrapolated functions  $\varepsilon_0(x)$  and  $\varepsilon_j(x)$ , to the series  $e_0(x)$  and  $e_j(x)$ , must satisfy the following global constraints or “boundary conditions.”

(1) Since, for a hard-sphere fluid, the energy increases with density up to an ultimate, finite (random or regular) packing density  $x_0$  at which, by the uncertainty principles, the energy *diverges* as a second-order pole, we expect that (a) the total energy by which (16) with  $\lambda=0$  is proportional to  $x^2 \varepsilon_0(x)$  implies that  $\varepsilon_0(x)$  itself must therefore *not decrease* faster than  $1/x^2$ . (b)  $\varepsilon_0(x) \propto (x_0 - x)^{-2}$  as  $x \rightarrow x_0$ , and (c) since the closest packing density  $\rho$  for hard spheres of diameter  $c$  is presumably the primitive-hexagonal regular packing density  $\rho_0 = \sqrt{2}/c^3$ , the value  $x_0$  must, by (10), be equal to  $(6\pi^2 \sqrt{2}/\nu)^{1/3}$  for  $\nu$ -species fermions, which is about 3.47

for  $\nu=2$ . However, in contrast to the boson hard-sphere fluid where accurate (GFMC) computer simulations are available<sup>19</sup> to guide our analysis and selection<sup>20</sup> of the optimum  $\varepsilon_0(x)$ , there are unfortunately no similar computer-simulation studies of *fermion* hard spheres. On the other hand, there is one valuable Jastrow Monte Carlo ( $J$ -MC) calculation<sup>21</sup> for two-species fermions interacting with the *soft* repulsive Bethe homework  $v_0$  potential, which is the repulsive part of the  ${}^1S_0$  Reid soft-core nucleon-nucleon potential. A Padé analysis of this fluid was reported in Ref. 22 giving energy very close to the  $J$ -MC data points and being everywhere *below* these (rigorous upper-bound) results, over the whole density range of the simulations. *One* optimum  $\varepsilon_0(x)$  was found which is a  $[0/4](x)$  approximant to  $e_0^{-1/2}(x)$ . We know of no previous many-body method—perturbative or (non-Monte Carlo) variational—which does not violate at some density the rigorous upper bound as provided by the benchmark variational Monte Carlo data of Ref. 21 to the ground-state energy of this many-fermion system, for which many calculations have been performed, and which are conveniently reviewed in Ref. 23. Thus, we adopt that  $\varepsilon_0(x)$  form here for the *soft*-cored Aziz interaction, but for the HCSW calculations we will use the  $[3/1](x)$  extrapolant to  $e_0^{-1/2}(x)$  found in Refs. 12, 22, and 24 which leads to a second-order pole in  $\varepsilon_0(x)$  at  $x_P = 1.939 15$ .

(2) Perturbation theory for a negative definite perturbation to the ground-state energy, as in (2), demands that both first- and second-order corrections to the energy  $E_1$  and  $E_2$  of (16) be *negative* for *all* densities. Since  $f_{1j} < 0$

TABLE III. Coefficients  $k_{ij}$  of Eqs. (14) and (15) for Aziz-BH.

$i \backslash j$	1	2	3	4
0	-0.176 839	-0.045 860	-0.156 998	0.110 158
1	1.049 186	5.942 949	-1.826 432	-6.417 795 <sup>a</sup>
2	0.271 431	0.835 626	0.952 007	-0.557 474 <sup>b</sup>
3	-0.317 966	-0.754 992	2.049 312	-4.725 388 <sup>b</sup>
4	-0.892 625	-1.805 189	3.725 743	
5	-1.465 157	-2.552 547	6.200 335	
6	-2.037 343	-3.089 462	9.698 816	

<sup>a</sup>From the estimation procedure Eq. (21).<sup>b</sup>Deduced through SP conditions.

TABLE IV. Same as Table III but for Aziz-WCA.

$j \setminus i$	1	2	3	4
0	-0.176 839	-0.045 860	-0.157 163	0.110 339
1	1.049 186	5.826 623	-1.760 115	-6.172 119 <sup>a</sup>
2	0.310 363	0.925 041	0.839 129	-0.529 121 <sup>b</sup>
3	-0.235 942	-0.569 113	1.768 672	-5.505 516 <sup>b</sup>
4	-0.765 745	-1.560 753	3.157 251	
5	-1.292 968	-2.275 234	5.175 294	
6	-1.819 493	-2.798 271	7.998 509	

<sup>a</sup>From the estimation procedure Eq. (21).

<sup>b</sup>Deduced through SP conditions.

for all  $j$ , this implies that both  $\varepsilon_1(x)$  and  $\varepsilon_2(x)$  should be *non-negative for all  $x$* .

(3) Furthermore, the first-order energy correction  $E_1$ , must *decrease monotonically* in  $\rho$ , or  $\varepsilon_1(x)$  must *not decrease* in  $x$  faster than  $1/x^3$ . This is because  $E_1$  is essentially an expectation value of the negative  $V_{\text{att}}$ , calculated with the many-body wave function of the fluid with repulsive potential  $V_{\text{rep}}$ .

(4) If the repulsion were a hard-core one, as close packing  $x_p$  is approached,  $\varepsilon_2(x_p)$ ,  $\varepsilon_3(x_p)$ ,  $\dots$ , should individually vanish. This requirement suggests itself, from the recent proof by Stell and Penrose,<sup>25</sup> based on the Gibbs-Bogoliubov inequalities, that *classical* thermodynamic perturbation theory becomes exact in first-order as close packing is approached. This is rigorous in one and two-dimensions, and has been conjectured to also hold in three dimensions. We assume that it further holds in the *quantum* case. The energy at close packing should then be given by

$$E \cong E_0 + \lambda E_1 \quad (\text{as } x \rightarrow x_p). \quad (17)$$

Therefore, in addition to having a second-order pole,  $E$  must depend *linearly* on the attractive well strength  $\lambda$ , as  $x \rightarrow x_p$ . In view of (16), this means that  $E_2 = E_3 = \dots = 0$ , as  $x \rightarrow x_p$ , implying that

$$\varepsilon_2(x_p) = \varepsilon_3(x_p) = \dots = 0. \quad (18)$$

We shall refer to these very important high-density relations (17) and (18) as the Stell-Penrose (SP) conditions.

(5) Since the Aziz potential to be used is a soft-cored potential, the choice of the optimum Padé-derived  $\varepsilon_0(x)$  suggested by the  $J$ -MC simulations on Bethe homework fermions, and stated at the end of condition (1) above, are in order. However, for the purpose of fixing the high-density behavior of  $\varepsilon_1(x)$  through  $\varepsilon_6(x)$ , we shall assume that, as close packing is approached, our soft-sphere fluid behaves, for all practical purposes, as a hard-sphere fluid with sphere diameter  $a_0$ , the  $s$ -wave scattering length of the repulsive part of the potential decomposed by either the BH or WCA scheme. More importantly, since no fermion hard-sphere fluid simulations are available, and in order to determine  $x_p$ , we postulate that any quantum fluid of identical hard spheres will develop an energy (and thus also, pressure) singularity at a universal density

value independent of statistics. This is reasonable since close packing implies perfect localization of the particles which, in turn, implies distinguishability. Since this density value  $\rho_p$  is known<sup>20</sup> for at least one quantum hard-sphere fluid, namely, bosons, to be  $\rho_p/\rho_0 = 0.371$  as extracted from GFMC (Ref. 19) data, Eq. (4) means that, for  $\nu=2$  fermions

$$x_p = (3\pi^2\rho_p)^{1/3}a_0 = [(3\pi^2\sqrt{2})(0.371)]^{1/3} \cong 2.5,$$

if  $\rho_0 = \sqrt{2}/a_0^3$  is used.

The five conditions just stated generally permit selection of a *single* density-series extrapolant from among a family of several possible ones, all of which, by construction, reproduce the exactly known initial series (13) and (14),  $e_0(x)$  or  $e_j(x)$ , as  $x \rightarrow 0$ . In the well-known method of Padé extrapolation,<sup>26,27</sup> the Padé approximant  $[L/M](x)$  to a given Taylor series  $f(x) = f_0 + f_1x + f_2x^2 + \dots$  is defined as the ratio of two polynomials in  $x$ , the numerator being of order  $L$  and the denominator of order  $M$ , namely,

$$[L/M](x) \equiv \frac{1 + p_1x + p_2x^2 + \dots + p_Lx^L}{1 + q_1x + q_2x^2 + \dots + q_Mx^M} \equiv \frac{P_L(x)}{Q_M(x)}, \quad (19)$$

such that  $[L/M](x) - f(x) \equiv O(x^{L+M+1})$ . Consequently, a binomial expansion of (19) about  $x=0$  generates a power series identical through order  $x^{L+M}$  to the original power series. The advantage of a *rational* approximant such as (19) is its ability to mimic nontrivial *zeros* and *poles* of the unknown function  $f(x)$ . Padé approximants have been shown to accurately reproduce a given function even out to values of  $x$  where the original Taylor series to the function no longer converges. They have even been found to be useful in representing functions with *diverging* Taylor series.

We now discuss in greater detail the approximants  $\varepsilon_1(x)$  to (14) with  $j=1$ . By using the coefficients  $k_{i1}$  ( $i=1,2,3$ ) for either Aziz-BH (Table III) or Aziz-WCA (Table IV), we set up and examine all third-order Padé approximants,  $[2/1](x)$ ,  $[1/2](x)$ , and  $[0/3](x)$ , plus the so-called non-Padé form  $(2/2)(x)$  introduced in Ref. 11 via the "tailing" method. We immediately discard forms  $(2/2)$  and  $[0/3]$  because they violate condition (3) above. Approximant  $[1/2]$  has a pole at  $x \cong 0.5$  so it, too, is dis-

carded. This leaves only  $[2/1](x)$  and  $[3/0](x)$ , the latter being the original series (14) for  $i=1$ . As a check on the high-density behavior of these two remaining forms, we consider the following rough estimate<sup>11,28</sup> for the attractive potential-energy contribution of the hard-core-square-well (HCSW) potential shape designed by Burkhardt<sup>29</sup> to be “phase-equivalent” to the He-He Lennard-Jones potential. It has a depth  $-V_0$ , range  $R$ , and hard-core diameter  $c$ . The estimate simply states that

$$\lambda E_1/N = -\frac{1}{2}V_0\left(\frac{4}{3}\pi R^3\rho_p - 1\right), \quad (20)$$

where the term in the parentheses is the number of hard-sphere centers between two concentric spheres of radii  $R$  and  $c$ , centered about a given particle (i.e., inside the attractive well of that particle’s HCSW potential). By equating the above to the  $j=1$  term in (6), one can obtain an estimate for the value of the first-order extrapolant at close packing, which depends on the parameters of the HCSW. From Eqs. (4), (16), and (20) and the fact that  $\lambda = mV_0(R-c)^2/\hbar^2$  for the HCSW problem as defined in Ref. 12, we obtain for this estimate of  $\varepsilon_1(x)$  at  $x_p$  the expression

$$\varepsilon_1^{\text{est}}(x_p) \equiv -\frac{5[4R^3x_p^3/9\pi c^3 - 1]}{3x_p^3 f_{11}\alpha^2}, \quad (21)$$

where  $\alpha = (R-c)/c = 2.264095$ , if  $R = 5.5 \text{ \AA}$ ,  $c = 1.685 \text{ \AA}$  as given in Ref. 29. For the  $\varepsilon_1(x)$  of the Aziz potential we found results very similar to those with the HCSW, Fig. 3, where we found that the  $[2//2](x)$  two-point fourth-order Padé approximant best represents  $\varepsilon_1(x)$ . This approximant is defined such that, for small  $x$ , it reproduces the three known coefficients of  $e_1(x)$  in (14), and, in addition, satisfies the constraint

$$[2//2](x_p) = \varepsilon(x_p) = \varepsilon_1^{\text{est}}(x_p) = 5.914901$$

determined from Eq. (21) for the Burkhardt HCSW, where, in accordance with global constraint (5) above,  $x_p \approx 2.5$  for  $\nu=2$  fermions.

The behavior of  $\varepsilon_2(x)$  for the Aziz potential (both BH and WCA) was again found similar to that of the HCSW potential. Since not approximant from the “small” family of third-order extrapolants shows acceptable Stell-Penrose behavior, we proceed to the “large” family of fourth-order approximants  $[L//M](x)$ , with  $L+M=4$ , which satisfy  $\varepsilon_2(x_p)=0$ , namely, the appropriate SP behavior. The two-point Padé extrapolants  $[2//2](x)$ ,  $[1//3](x)$ , and  $[3//1](x)$  all develop poles for  $x < 2$ , i.e., well within the physical interval of densities, and so we discard them. Only the  $[4//0](x)$  survives the global constraints (1)–(5) above and is thus chosen as the optimum representation.

As for  $\varepsilon_3(x)$ , it again differs little from the HCSW case, with  $[0/3](x)$  clearly being the best of the “small” family of extrapolants, albeit with an imperfect Stell-Penrose behavior because  $\varepsilon_3(x_p)$  does not quite vanish. This can be refined further if we go to the large family of two-point Padé approximants allowing us to impose the SP behavior approximant via the condition  $[2//2](x_p)=0$ . We

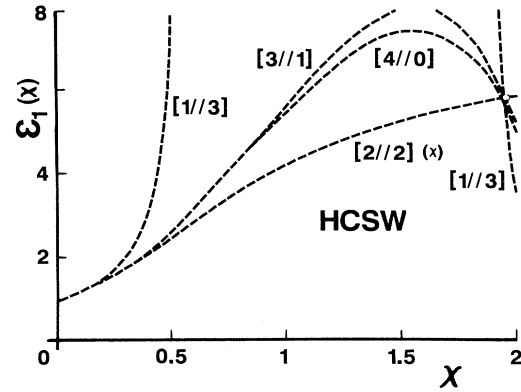


FIG. 3. Two-point Padé extrapolants to  $e_1(x)$  of Eq. (14) for the HCSW potential such that  $\varepsilon_1(x_p) = \varepsilon_1^{\text{est}}(x_p) = 5.825809$ , as calculated via Eq. (21), for  $x_p = 1.93915$  which is the zero of the  $[3/1]$  approximant to  $e_0^{-1/2}(x)$ , Eq. (13).

finally plot in Fig. 4 the chosen extrapolants  $\varepsilon_i(x)$  ( $i=2,3,\dots,6$ ) only for the Aziz-BH case since the Aziz-WCA case is very similar.

#### IV. ATTRACTIVE-COUPLING-SERIES ANALYSES

Having constructed good density extrapolants  $\varepsilon_0(x)$  and  $\varepsilon_j(x)$  to each of the series  $e_0(x)$  and  $e_j(x)$  in the QTPT energy expressions (12)–(15), the resulting series (16) for the ground-state energy per particle can be rewritten as

$$\frac{E}{N} \cong \frac{3\hbar^2 x^2}{10ma_0^2} \varepsilon_0(x) \left[ 1 + \sum_{j=1}^6 \frac{f_{1j} x \varepsilon_j(x)}{\varepsilon_0(x)} \lambda^j \right], \quad (22)$$

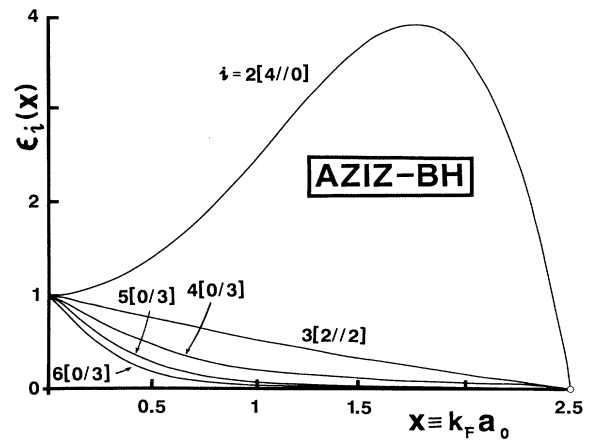


FIG. 4. Optimum approximants  $\varepsilon_i(x)$  to  $e_i(x)$  ( $i=2,3,\dots,6$ ) of Eq. (14) for the Aziz potential with BH decomposition, selected according to criteria set forth in the text. The open circle marks the value  $x_p = 2.5$  emerging from the postulate discussed under global constraint (5) of the text.

where the leading term refers to the hard-sphere fluid. This may now be analyzed as a  $\lambda$  series to extrapolate to nonzero  $\lambda$  values. Specifically, we can represent (22) in terms of Padé approximants in  $\lambda$  by writing

$$\frac{E}{N} \cong \frac{3\hbar^2 x^2}{10ma_0^2} \varepsilon_0(x) [L/M](\lambda) \quad (L+M \leq 6), \quad (23)$$

and investigate the “spread” at  $\lambda = \lambda_{\text{physical}}$  and at any given  $x$  value, of all the  $(L+M)$ th order energies. The value of  $\lambda_{\text{physical}}$  will be

$$mV_0(R-c)^2/\hbar^2 = 1.719086$$

for the Burkhardt HCSW and unity for the Aziz interaction. We use the chosen extrapolants  $\varepsilon_i(x)$  ( $i=0,1,2,\dots,6$ ) stated before. In Fig. 5 we plot  $E/N$  versus  $x$  for the HCSW, with  $[0/0]$  representing (22) with  $\lambda=0$ , or the energy per particle of the hard-sphere fluid. This lies everywhere above the ideal-Fermi-gas curve, as it should. The dashed curves marked  $[1/0],[2/0],\dots,[6/0]$  stand for the energy-per-particle “straight” perturbation series in  $\lambda$ , from first to sixth order, respectively. The solid curve represents the fluid  $^3\text{He}$  experimental data summarized in Ref. 30. Although our converged energy minimum is substantially far from the zero-pressure experimental binding energy, the QTPT scheme is seen to be converging quickly beyond third order. This serious discrepancy between the predicted versus the experimental energy-density equilibrium point is attributable to two possible sources: (a) the HCSW potential, even though it is phase equivalent to the more realistic He-He Lennard-Jones potential, is still inadequate for a many-body calculation, and/or (b) the extrapolant used to represent the hard-sphere fluid is inadequate in the relevant density range.

The more realistic Aziz interatomic potential alleviates difficulty (a) above, and we found that, using the soft-

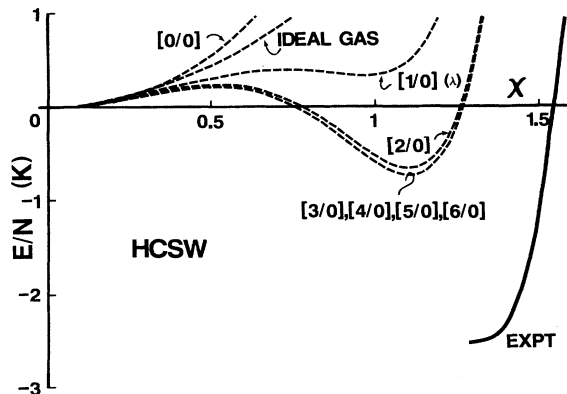


FIG. 5. Ground-state energy per particle as a function of  $x = k_F c$  for the HCSW potential. Curves labeled  $[L/M](\lambda)$  refer to the  $L/M$  Padé approximants to the  $L+M$  partial sum of the  $\lambda$  series, Eq. (23). The curve labeled  $[0/0]$  refers to the pure hard-sphere fluid using the  $[3/1]$  approximant of Ref. 24; the solid curve is the experimental result (Ref. 30) for liquid  $^3\text{He}$  at zero absolute temperature.

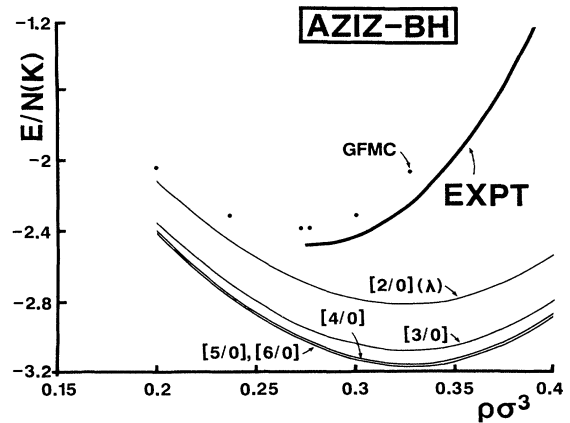


FIG. 6. Ground-state QTPT energy per particle as a function of  $\rho\sigma^3$  for the Aziz potential with BH decomposition. Here  $\sigma = 2.556 \text{ \AA}$  and  $\rho = k_F^3/3\pi^2$ , Eq. (4). The solid curve stands for the experimental results for liquid  $^3\text{He}$ , and the circles are the GFMC (computer-simulation) results.

sphere  $\varepsilon_0(x)$  discussed under global constraint (1) above succeeded nicely in avoiding difficulty (b). Results for the Aziz-BH case are shown in Fig. 6 where, in order to also compare with the computer- (GFMC) simulation results of Refs. 31 and 32, we change our density parameter from  $x \equiv (\rho a_0^3)^{1/2}$  to  $\rho\sigma^3$ , where  $\sigma = 2.556 \text{ \AA}$ . Perturbation results through sixth order are given for the attractive-coupling-constant  $\lambda$  series (22), and are labeled  $[n/0](\lambda)$  ( $n=1,2,\dots,6$ ) in Fig. 6. Also displayed are the GFMC data points listed in Table V,<sup>32</sup> as well as the experimental curve.<sup>30</sup> Figure 7 displays the Aziz-WCA, sixth-order QTPT results on an expanded scale. Agreement with the GFMC and experimental results in both energy and density in the saturation density region is better with the WCA than with the BH decomposition. We found that, at higher densities, the QTPT converged results tend to have smaller curvature than the simulation data—most probably a reflection of the inevitable

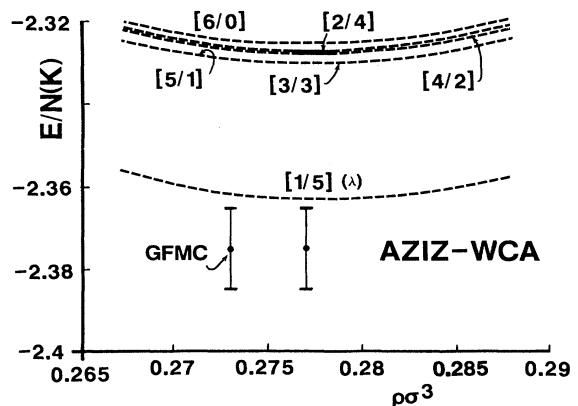


FIG. 7. Same as Fig. 6 but for the Aziz-WCA case and in an expanded scale. The error bar for the GFMC results is  $\pm 0.1 \text{ K}$ .

TABLE V. Results of fixed-node Green-function Monte Carlo calculations for 54  $^3\text{He}$  atoms interacting via the Aziz potential in a periodic box. All errors  $\delta$  are between 0.01 and 0.02 ( $\sigma = 2.556 \text{ \AA}$ ) [R. M. Panoff (private communication)].

$\rho\sigma^3$	$\frac{E}{N}$ (K)
0.200	$-2.030 \pm \delta$
0.237	$-2.300 \pm \delta$
0.273	$-2.375 \pm \delta$
0.277	$-2.375 \pm \delta$
0.300	$-2.300 \pm \delta$
0.327	$-2.050 \pm \delta$
0.377	$-1.160 \pm \delta$

breakdown of the assumption made in dealing with the series  $e_0(x)$ , where our Aziz interaction soft spheres have been regarded as hard spheres of diameter  $a_0$ . However, this approximation should be adequate at lower densities including, fortuitously, the saturation region of liquid  $^3\text{He}$ .

The “smallness parameter” which naturally emerges in the QTPT for the description of a quantum liquid is  $\lambda$ , the strength of the attractive interatomic potential. Its adequacy as a “smallness parameter” at the equilibrium density can be gauged from how small a “spread” will result at that density among the energy minima of *all* sixth-order Padé approximations—[6/0], [5/1], [4/2], [3/3], [2/4], and [1/5]—to the energy. If the [1/5] result were ignored, this spread is substantially smaller than the size as the GFMC uncertainty of  $\delta = \pm 0.01 \text{ K}$ .

## V. RESULTS AND DISCUSSION

Using the  $\varepsilon_i(x)$  ( $i = 1, 2, \dots, 6$ ) extrapolants chosen according to various physical constraints which follow from thermodynamic perturbation theory, we first calculate

the straight sixth-order perturbation  $\lambda$  series of Eq. (22), namely,

$$\frac{E}{N} \cong \frac{3\hbar^2 x^2}{10ma_0^2} \varepsilon_0(x) [6/0](\lambda), \quad (24)$$

and determine from this the saturation density  $\rho_s$  and binding energy  $(E/N)_s$  predicted for liquid  $^3\text{He}$ . In Table VI, we collect together the QTPT results at the saturation energy-density point, and compare with laboratory (expt.) and computer-simulation (GFMC) experiments, as well as with the recent variational results<sup>33</sup> based upon a Jastrow trial wave function with substantial further corrections to account for triplet, spin-dependent, and backflow correlations. Also included in Table VI are sound speed  $c$  results which are a very stringent test of the ground-state equation of state. The sound speed  $c$  is defined through

$$mc^2 = \frac{\partial P}{\partial \rho}, \quad (25)$$

where  $m$  is the  $^3\text{He}$  atomic mass [for which  $\hbar^2/m = 16.085775 \text{ K \AA}^2$  (Ref. 16)],  $\rho$  is the number density, and the pressure  $P$  is given by

$$P \equiv \rho^2 \frac{\partial(E/N)}{\partial \rho}. \quad (26)$$

Since the QTPT expression (24) for  $E/N$  is an explicit function of  $x$ , related to  $\rho$  through  $x = (3\pi^2\rho)^{1/3}a_0$ , which comes from (4), (25), and (26), it then yields (in m/s)

$$c = 17.5021 \left[ \frac{1}{x^2} \frac{\partial}{\partial x} \left[ x^4 \frac{\partial(E/N)}{\partial x} \right] \right]^{1/2}. \quad (27)$$

Using MACSYMA computer algebra we evaluated this expression at the calculated saturation densities determined for the HCSW, Aziz-BH, and Aziz-WCA cases.

TABLE VI. QTPT results for the density  $\rho$ , energy-per-particle  $E/N$ , and sound speed  $c$ , all at the equilibrium minimum, compared with experimental liquid  $^3\text{He}$  (expt), GFMC (fixed-node), and variational calculations. Percentage errors are against GFMC data.

	Expt. Ref. 30	GFMC Refs. 31 and 32	Variational calculation Ref. 33	QTPT (present work)		
				HCSW	Aziz BH	WCA
$\rho_s$ ( $\text{\AA}^{-3}$ )	0.016	0.0163	0.0166	0.0097	0.0195	0.0166
$E/N$ (K)	-2.47	-2.37 $\pm 0.01$	-2.47	-0.7516	-3.172	-2.33
$c$ (m/s)	182.9	176.7 <sup>a</sup>	185	118.1	173.2	150.8
		$\left  \frac{\rho - \rho_{\text{GFMC}}}{\rho_{\text{GFMC}}} \right $	1.5	40.6	19.9	1.5
		$\left  \frac{E - E_{\text{GFMC}}}{E_{\text{GFMC}}} \right $	4.2	68.3	33.8	1.7
		$\left  \frac{c - c_{\text{GFMC}}}{c_{\text{GFMC}}} \right $	4.7	33.2	2.0	14.7

<sup>a</sup>From Eq. (30).



In order to compare with the GFMC result, we write<sup>30</sup>

$$E/N = E_0 + \sum_{i=2}^5 a_i \left[ \frac{\rho - \rho_0}{\rho_0} \right]^i, \quad (28)$$

where, from (25) and (26), we can deduce that

$$a_2 = \frac{1}{2} mc^2. \quad (29)$$

First, we applied a least-squares method with the GFMC data listed in Table V to extract  $E_0$  and the  $a_i$  ( $i = 2, 3, 4, 5$ ) of (28). Then (29) gives (in m/s)

$$c_{\text{GFMC}} \cong 176.7, \quad (30)$$

which is the value cited in Table VI.

Lastly, as a convenient, though rough, comparison criterion, percentage errors are given in the table which are calculated against the corresponding GFMC central figure. We see that, for the WCA decomposition of the Aziz potential, the energy and density are both within 2% of the GFMC values as is the sound speed for the BH decomposition. The results can probably be improved by searching for a more suitable decomposition of the potential, perhaps intermediate between the BH and WCA ones, as already proved<sup>10</sup> to be the case for bosonic  ${}^4\text{He}$ .

## VI. CONCLUSIONS

Starting with the well-known, exact, low-density equation-of-state series for a many-fermion system, we rearrange the expansion into a double series (in density and attractive coupling) which is appropriately termed a quantum thermodynamic perturbation theory. Through the application of Padé approximants, the low-density terms in the perturbation expansion are extrapolated order by order to higher (i.e., physical) density.

Not surprisingly, the hard-core-square-well potential is too simple a model to yield reliable results. For the Aziz

interatomic potential, on the other hand, the predicted results are excellent both as regards saturation density and binding energy, but moderately good for sound speed, under the WCA potential decomposition, when compared against the GFMC (computer-simulation) data. On the other hand, for the BH potential decomposition, although both energy and density predictions are not as good as in the WCA case, the sound speed prediction is excellent. We conclude, in general, that QTPT is a convenient scheme to describe the ground-state equation of state of the fermion liquid  ${}^3\text{He}$ , as found previously<sup>9,10</sup> for the bosonic liquid  ${}^4\text{He}$ , but that, as in this latter case, an optimum potential decomposition may lie intermediate between the BH and WCA extremes dealt with here.

The results of this study are based on a very simple, inexpensive calculational scheme when compared with other intricate, complex methods, either of the variational or Monte Carlo kind—the latter, however, being used as benchmarks against which we compare our results. Finally, a “smallness parameter” emerges which is appropriate for describing the quantum liquid state in terms of a rapidly convergent scheme in a manner which explicitly avoids crossing gas-liquid phase boundaries.

## ACKNOWLEDGMENTS

One of us (Z. Hu) thanks Professor Christina Keller for invaluable help, and Professor Mark A. Ordal for aid with computers; another one of us (M. de Ll.) thanks Professor V. C. Aguilera-Navarro, Professor S. A. Moszkowski, Professor R. M. Panoff, and Professor M. A. Solís for discussions and/or correspondence. E.B. and R.G. acknowledge support from CICYT [Comisión Interministerial de Ciencia y Tecnología (Spain)] under Contract No. 969/87. Finally, M. de Ll. and R.G. acknowledge NATO (North Atlantic Treaty Organization) for support.

\*Present address: Physics Department, Arizona State University, Tempe, AZ 85287.

<sup>1</sup>A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971); D. J. Thouless, *The Quantum Mechanics of Many-Body Systems* (Academic, New York, 1972).

<sup>2</sup>B. Day, *Rev. Mod. Phys.* **50**, 495 (1978); *Springer Lectures in Physics* (Springer-Verlag, Berlin, 1981) Vol. 142, p. 169; *Comments Nucl. Part. Phys.* **11**, 115 (1983); A. D. Jackson, *Annu. Rev. Nucl. Part. Sci.* **33**, 105 (1983).

<sup>3</sup>J. W. Clark, *Prog. Part. Nucl. Phys.* **2**, 89 (1979); J. G. Zabolitzky, *Adv. Nucl. Phys.* **12**, 1 (1981).

<sup>4</sup>D. M. Ceperley and M. H. Kalos, in *Monte Carlo Methods in Statistical Physics*, edited by K. Binder (Springer, Berlin, 1979).

<sup>5</sup>G. A. Baker, Jr., *Rev. Mod. Phys.* **43**, 479 (1971).

<sup>6</sup>J. A. Barker and D. Henderson, *Rev. Mod. Phys.* **48**, 597 (1976).

<sup>7</sup>D. Chandler, J. D. Weeks, and H. C. Andersen, *Science* **220**,

787 (1983), and references therein.

<sup>8</sup>G. A. Baker, Jr., M. de Llano, and J. Pineda, *Phys. Rev. B* **24**, 6304 (1981).

<sup>9</sup>M. A. Solís, V. C. Aguilera-Navarro, M. de Llano, and R. Guardiola, *Phys. Rev. Lett.* **59**, 2322 (1987).

<sup>10</sup>Christina Keller, S. Z. Ren, M. de Llano, E. Buendía, and R. Guardiola, *Phys. Rev. B* **40**, 11 070 (1989).

<sup>11</sup>V. C. Aguilera-Navarro, R. Guardiola, C. Keller, M. de Llano, M. Popovic, and M. Fortes, *Phys. Rev. A* **35**, 3091 (1987).

<sup>12</sup>G. A. Baker, Jr., L. P. Benofy, M. Fortes, M. de Llano, S. M. Peltier, and A. Plastino, *Phys. Rev. A* **26**, 3575 (1982).

<sup>13</sup>P. Roman, *Advanced Quantum Theory* (Addison-Wesley, Reading, MA, 1965).

<sup>14</sup>E. Buendía, R. Guardiola, and M. de Llano, *Phys. Rev. A* **30**, 941 (1984).

<sup>15</sup>G. Gutiérrez, M. de Llano, and W. C. Stwalley, *Phys. Rev. B* **29**, 5211 (1984).

<sup>16</sup>L. P. Benofy, E. Buendía, R. Guardiola, and M. de Llano,

- Phys. Rev. A **33**, 3749 (1986).
- <sup>17</sup>E. Buendía, R. Guardiola, and M. de Llano, At. Data Nucl. Data Tables **42**, 293 (1989).
- <sup>18</sup>R. H. Rand, *Computer Algebra in Applied Mathematics: An Introduction to MACSYMA* (Pitman, London 1984); MACSYMA, 1976, 1984, Massachusetts Institute of Technology. Enhancements, 1984, Symbolics, Inc.
- <sup>19</sup>M. H. Kalos, D. Levesque, and L. Verlet, Phys. Rev. A **9**, 2178 (1974).
- <sup>20</sup>V. C. Aguilera-Navarro, Shirley Ho, and M. de Llano, Phys. Rev. A **36**, 5742 (1987).
- <sup>21</sup>D. Ceperley, G. V. Chester, and M. H. Kalos, Phys. Rev. B **16**, 308 (1977).
- <sup>22</sup>V. C. Aguilera-Navarro, G. A. Baker, Jr., L. P. Benofy, M. Fortes, and M. de Llano, Phys. Rev. A **36**, 4338 (1987).
- <sup>23</sup>J. M. Irvine, Prog. Part. Nucl. Phys. **5**, 1 (1981).
- <sup>24</sup>G. A. Baker, Jr., G. Gutiérrez, and M. de Llano, Ann. Phys. (N.Y) **153**, 283 (1984).
- <sup>25</sup>G. Stell and O. Penrose, Phys. Rev. Lett. **51**, 1397 (1983).
- <sup>26</sup>G. A. Baker, Jr., *Fundamentals of Padé Approximants* (Academic, New York, 1974); G. A. Baker, Jr. and P. Graves-Morris, in *Encyclopedia of Math and its Applications*, edited by G.-C. Rota (Addison-Wesley, Reading, MA, 1981), Vols. 13 and 14.
- <sup>27</sup>M. de Llano, Kinam **4**, 61 (1982).
- <sup>28</sup>Christina Keller, V. C. Aguilera-Navarro, and M. de Llano, J. Phys. A **21**, 715 (1988).
- <sup>29</sup>T. W. Burkhardt, Ann. Phys. (N.Y) **47**, 516 (1968).
- <sup>30</sup>R. A. Aziz and R. K. Pathria, Phys. Rev. A **7**, 809 (1973).
- <sup>31</sup>R. M. Panoff and J. Carlson, Phys. Rev. Lett. **62**, 1130 (1989).
- <sup>32</sup>R. M. Panoff (private communication).
- <sup>33</sup>M. Viviani, E. Buendía, S. Fantoni, and S. Rosati, Phys. Rev. B **38**, 4523 (1988).