Aziz fermions and liquid $^3$He

Zhizhong Hu* and M. de Llano
Physics Department, North Dakota State University, Fargo, North Dakota 58105
E. Buendia and R. Guardiola
Departamento de Fisica Moderana, Universidad de Granada, E-18071 Granada, Spain
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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 $^3$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 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

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

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

$$V(|\mathbf{r}_{ij}|) \equiv V(|\mathbf{r}_{ij} - \mathbf{r}_{ij}|) = V_{\text{rep}} + \lambda V_{\text{at}}.$$

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, variational, or Monte Carlo (i.e., computer simulations). The approach here is perturbative and our starting point is the exact low-density expansion 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 (BH) and by Weeks, Chandler, and Andersen (WCA). The quantum version, called QTPT, for “quantum thermodynamic perturbation theory” was applied to a hard-core-plus-attractive-square-well pair potential modeling liquid $^4$He. A recent decisive, critical test of the QTPT method encouragingly materialized 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 $^4$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, and sound-velocity predictions for liquid $^4$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)
in predicting the properties of the liquid state it explicitly avoids 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 potential to fermions, and study the ground-state properties of liquid $^4$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, etc. The result finite, but nonanalytic, expansion for the ground-state energy per particle is then

$$\frac{E}{N} = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} \left[ 1 + C_1(k_F a) + C_2(k_F a)^2 + \left( \frac{C_3}{2a} + C_4 \frac{A_1(0)}{a^3} + C_5 \right) (k_F a)^3 + C_6(k_F a)^4 + O(k_F a)^5 \right],$$

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

$$\rho = \frac{v k_F^3}{6\pi^2},$$

with $v$ being the number of distinct fermion species. For the case of $^3$He, $v=2$ and, consequently, $C_6=0$. The symbols $a$, $R_0$, and $A_1(0)$ stand for the scattering parameters of effective-range theory 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 interrelated by effective-range theory with the scattering phase shift $\delta_l(k)$ in the $l$th partial wave through the low-energy ($\hbar^2 k^2/2m \to 0$) expressions

$$k^{2l+1} \cot \delta_l(k) \approx -\frac{1}{A_l(0)} + \frac{1}{2} R_l k^2 + O(k^4)$$

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

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

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


\[ u_1(r) = \frac{r^2}{\lambda} - \frac{A_1(0)}{r}, \]

if \( v(r) \) is short ranged. The integrals alluded to above are \(^{15,16}\)

\[ A_0(0) \equiv a = \int_0^\infty dr \, rv(r)u_0(r), \quad (7) \]

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

\[ A_1(0) = -\frac{1}{2} \int_0^\infty dr \, r^2 v(r)u_1(r). \quad (9) \]

On the other hand, the scattering parameter \( A_0^\prime(0) \) appearing in (3) in the (three-body) \( \rho^3 \) (i.e., \( k_p^3 \)) contribution to the energy, is potential-shape dependent and arises naturally from the various many-body selective infinite partial summations \(^{13,14}\) through the integral

\[ A_0^\prime(0) = -\frac{1}{2} \int_0^\infty dr \, r^3 \nu(r)u_0(r) . \quad (10) \]

As the pair potential \( V(r) \) is decomposed in QTPT into repulsive and attractive portions in (2), we can expand \( a, R_0, A_0(0), \) and \( A_0^\prime(0) \) numerically in powers of \( \lambda \),

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

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

\[ A_0(0) = t_0(1 + t_1 \lambda + t_2 \lambda^2 + \cdots + t_6 \lambda^6 + \cdots), \quad (11c) \]

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

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 \( k_p a_0 = x \) and expanding, leads to the ground-state energy rearranged as the double series, in \( x \) and \( \lambda \), given by

\[ \frac{E}{N} \approx \frac{3\hbar^2 x^2}{10ma_0} \left[ e_0(x) + \sum_{j=1}^{\infty} f_j x e_j(x) \lambda^j + \cdots \right] \]

\[ \approx E_0 + \lambda E_1 + \lambda^2 E_2 + \cdots , \quad (12) \]

where

\[ e_0(x) \equiv 1 + f_{10} x + f_{20} x^2 + f_{30} x^3 + f_{40} x^4 + \cdots , \quad (13) \]

\[ e_j(x) \equiv 1 + k_{1j} x + k_{2j} x^2 + k_{3j} x^3 + \cdots \]

\[ (j = 1, 2, \ldots, 6) , \quad (14) \]

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

The coefficients \( f_{ij} \) \((i = 1, \ldots, 5; j = 0, 1, \ldots, 6)\) were obtained \(^{11}\) (note that \( f_{4j} \equiv 0 \)) by using the computer-algebra packaged program called MACSYMA. \(^{18}\) 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-

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

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

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gram "sheet." In QTPT as implemented here, arrival at the equilibrium liquid point is explicitly achieved 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 $e_j(x)$ ($j = 1, 2, \ldots, 6$), Eqs. (13)–(15), to nonzero $x$ values. We denote these extrapolations by $e_0(x)$ and $e_j(x)$, respectively. Once obtained, (12) will become

$$\frac{E}{N} \approx \frac{3A^2 x^2}{10ma_0^2} \left[ e_0(x) + \sum_{j=1}^{6} f_{ij} x e_j(x) \lambda^j + \cdots \right]$$

$$\approx E_0 + \lambda E_1 + \lambda^2 E_2 + \cdots, \quad (16)$$

and is ready for the $\lambda$-series Padé analysis or extrapolation. The density-extrapolated functions $e_0(x)$ and $e_j(x)$, 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 $e_0(x)$ itself must therefore not decrease faster than $1/x^2$. (b) $e_0(x) \approx (x_0 - x)^2$ as $x \rightarrow x_0$, and (c) since the closest packing density $\rho = \sqrt[3]{2} \varepsilon_1$ for hard spheres of diameter $c$ is presumably the primitive-hexagonal regular packing density $\rho_0 = \sqrt{2} \varepsilon_1$, 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 to guide our analysis and selection of the optimum $e_0(x)$, 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 for two-species fermions interacting with the soft repulsive Bethe homework $e_0$ potential, which is the repulsive part of the $1^S_0$ 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 $e_0(x)$ 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 $e_0(x)$ 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 $e_0(x)$ at $x_F = 1.939 15$.

(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 $f_{ij} < 0$

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

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

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*aFrom the estimation procedure Eq. (21).

*bDeduced 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 \(\varepsilon_r(x)\) 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, \(\varepsilon_2(x_p), \varepsilon_3(x_p), \ldots\) should individually vanish. This requirement suggests itself, from the recent proof by Stell and Penrose,\(^{35}\) 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

\[
E \approx E_0 + \lambda E_1 \quad (x \to x_p) .
\]

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

\[
\varepsilon_2(x_p) = \varepsilon_3(x_p) = \cdots = 0 .
\]

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 \(\varepsilon_q(x)\), 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\(^{30}\) 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 \(v=2\) fermions

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

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 \(e_q(x)\), as \(x \to 0\). In the well-known method of Padé extrapolation,\(^{26,27}\) the Padé approximant \([L/M](x)\) to a given Taylor series \(f(x) = f_0 + f_1 x + f_2 x^2 + \cdots\) is defined as the ratio of two polynomials in \(x\), the numerator being of order \(L\) and the denominator of order \(M\), namely,

\[
[L/M](x) = \frac{1+p_1 x + p_2 x^2 + \cdots + p_L x^L}{1+q_1 x + q_2 x^2 + \cdots + q_M x^M} = \frac{P_L(x)}{Q_M(x)} ,
\]

such that \([L/M](x) - f(x) = O(x^{L+M+1})\). 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 \(\varepsilon_j(x)\) to (14) with \(j = 1\). Using the coefficients \(k_{ij}\) \((i = 1, 2, 3)\) 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 \(x \approx 0.5\) 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 \(^{1,28}\) for the attractive potential-energy contribution of the hard-core-square-well (HCSW) potential shape designed by Burkhardt\(^{29}\) 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

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

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

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

where \( \alpha = (R - c)/c = 2.046 \), if \( R = 5.5 \) \( \text{Å}, \) \( c = 1.685 \) \( \text{Å} \) 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 Padé approximant best represents \( \varepsilon_1(x) \). This approximant is defined such that, for small \( x \), it reproduces the three known coefficients of \( \varepsilon_1(x) \) in (14), and, in addition, satisfies the constraint

\[
[2/2](x_p) = \varepsilon(x_p) = \varepsilon_1^{\text{est}}(x_p) = 5.914 \text{901}
\]

determined from Eq. (21) for the Burkhardt HCSW, where, in accord with global constraint (5) above, \( x_p = 2.5 \) 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 finally plot in Fig. 4 the chosen extrapolants \( \varepsilon_i(x) \) (\( i = 2,3,\ldots,6 \)) 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.

**FIG. 3.** Two-point Padé extrapolants to \( \varepsilon_i(x) \) of Eq. (14) for the HCSW potential such that \( \varepsilon_i(x_p) = \varepsilon_1^{\text{est}}(x_p) = 5.825 \text{809} \), as calculated via Eq. (21), for \( x_p = 1.939 \text{15} \) which is the zero of the [3/1] approximant to \( \varepsilon_0^{1/2}(x) \), Eq. (13).

**FIG. 4.** Optimum approximants \( \varepsilon_i(x) \) to \( \varepsilon_i(x) \) (\( i = 2,3,\ldots,6 \)) 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.

**IV. ATTRACTION-COUPLING-SERIES ANALYSES**

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

\[
E \approx \frac{3\hbar^2 x^2}{10m\alpha^2} \varepsilon_0(x) \left( 1 + \sum_{j=1}^6 \frac{f_{j,x} \varepsilon_j(x)}{\varepsilon_0(x)} \lambda_j \right),
\]

where

\[
\lambda_j = \frac{1}{j!} \left( \frac{d^j}{dx^j} \varepsilon(x) \right)_{x=x_p}
\]

for \( j = 1,2,\ldots,6 \) and \( x_p \) is the optimum value found from a Padé approximant with BH decomposition. 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 λ series to extrapolate to nonzero λ values. Specifically, we can represent (22) in terms of Padé approximants in λ by writing

$$E/N = \frac{3\pi^2}{10m^2} \epsilon_0(x) [L/M](\lambda) \ (L + M \leq 6), \quad (23)$$

and investigate the “spread” at λ = λ_{physical} and at any given x value, of all the (L + M)th order energies. The value of λ_{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 \(\epsilon_i(x)\) (i = 0, 1, 2, ..., 6) stated before. In Fig. 5 we plot \(E/N\) versus x for the HCSW, with [0/0] representing (22) with λ = 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], ..., [6/0] stand for the energy-per-particle “straight” perturbation series in λ, from first to sixth order, respectively. The solid curve represents the fluid \(^3\)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 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-sphere \(\epsilon_0(x)\) 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 = (\(\rho a_0^3\))^{1/3} to \(\rho a^3\), where \(a = 2.556 \text{ Å}\). Perturbation results through sixth order are given for the attractive-coupling-constant λ series (22), and are labeled \([n/0](\lambda)\) (n = 1, 2, ..., 6) in Fig. 6. Also displayed are the GFMC data points listed in Table V,\(^{32}\) as well as the experimental curve.\(^{30}\) 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. 5](image_url)  
**Fig. 5.** Ground-state energy per particle as a function of x = \(k_Tc\) for the HCSW potential. Curves labeled \([L/M](\lambda)\) refer to the L/M Padé approximants to the L + M partial sum of the λ 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 \(^3\)He at zero absolute temperature.

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

![Fig. 7](image_url)  
**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 ±0.1 K.
the straight sixth-order perturbation λ series of Eq. (22), namely,

\[
\frac{E}{N} = \frac{3h^2}{10ma_0^2} x^2 \epsilon_\text{p}(x) [6/0](\lambda),
\]

and determine from this the saturation density \( \rho_s \) and binding energy \( E/N \), 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\(^{33}\) 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

\[
mc^2 = \frac{\partial P}{\partial \rho},
\]

where \( m \) is the \(^3\text{He} \) atomic mass [for which \( \hbar^2/m = 16.085\,775\,\text{K A}^2 \) (Ref. 16)], \( \rho \) is the number density, and the pressure \( P \) is given by

\[
P \equiv \rho^2 \frac{\partial(E/N)}{\partial \rho}.
\]

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)

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

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

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

<table>
<thead>
<tr>
<th>Expt. Ref. 30</th>
<th>GFMC Refs. 31 and 32</th>
<th>Variational calculation Ref. 33</th>
<th>QTPT (present work)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho_s ) (( \text{Å}^{-3} ))</td>
<td>0.016</td>
<td>0.0163</td>
<td>0.0166</td>
</tr>
<tr>
<td>( E/N ) (K)</td>
<td>-2.47</td>
<td>-2.37</td>
<td>-2.47</td>
</tr>
<tr>
<td>( \pm 0.01 )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( c ) (m/s)</td>
<td>182.9</td>
<td>176.7(^{a})</td>
<td>185</td>
</tr>
<tr>
<td>(</td>
<td>\rho - \rho_{\text{GFMC}}</td>
<td>/\rho_{\text{GFMC}} ) %</td>
<td>100%</td>
</tr>
<tr>
<td>(</td>
<td>E - E_{\text{GFMC}}</td>
<td>/E_{\text{GFMC}} ) %</td>
<td>100%</td>
</tr>
<tr>
<td>(</td>
<td>c - c_{\text{GFMC}}</td>
<td>/c_{\text{GFMC}} ) %</td>
<td>100%</td>
</tr>
</tbody>
</table>

\(^{a}\)From Eq. (30).
In order to compare with the GFMC result, we write

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

(28)

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

\[ a_2 = \frac{1}{2} mc^2. \]  

(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)

\[ c_{\text{GFMC}} \approx 176.7, \]  

(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\(^{10}\) to be the case for bosonic \(^4\)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 \(^3\)He, as found previously\(^{9,10}\) for the bosonic liquid \(^4\)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.

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\(^{*}\)Present address: Physics Department, Arizona State University, Tempe, AZ 85287.


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