The Correlated Basis Function Method and its Application to Liquid ^{3}He, Nuclear Matter and Neutron Matter

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The method of correlated basis functions is studied and applied to the Fermi systems: liquid ^{3}He, nuclear matter and neutron matter. The reduced cluster integrals $x_{ijkl...}$ and so the subnormalization integrals $I_{ijkl...}$ are generalized to coinciding quantum numbers out of the set $\{i, j, k, l, \ldots\}$. This generalization has an important consequence for the radial distribution function $g(r)$ (and then for the liquid structure function); $g(r)$ has no contributions of the order $O(A^{-1})$. For ^{3}He the state-independent two-body correlation function $f(r)$ is calculated from the Euler-Lagrange equation (in the limit of $r \to 0$) for the unrenormalized two-body energy functional. For nuclear matter and neutron matter we adopt the three-parameter correlation function of Bäckman et al. Then the energy expectation values are calculated by including up to the three-body terms in the un-renormalized and renormalized version of the correlated basis functions method. The experimental ground-state energy and density of liquid ^{3}He can be well reproduced by the present method with the Lennard-Jones-(6–12) potential. The same method is applied to the nuclear matter and neutron matter calculations with the OMY-potential. The results of the energy expectation values indicate a practical superiority of the unrenormalized cluster expansion method over the renormalized one.

1. Introduction

A general method of describing many-body systems (for example, nuclei, nuclear matter, neutron matter and liquid He) of particles interacting through potentials with short-ranged, strong repulsion is based on the use of correlated wave functions of the type:

$$\Psi = F\,\Phi\,. \tag{1}$$

Here Φ is a model wave function (especially for the ground-state) of the system in the absence of the repulsive part of the interaction and embodies the statistics and symmetry properties of the system. In the case of a uniform, infinitely extended system of fermions in the normal phase, Φ is the Slater determinant constructed from one-particle plane-wave functions. The symmetrical correlation operator $F(1, 2, \ldots, A)$ must fulfill some boundary conditions and describes the strong short-range correlations between the particles due to the repulsive part of the potential.

We assume that the interaction between the particles in the considered many-body system is characterized by simple two-body forces. Therefore, the Hamiltonian,

$$H = -\sum_{i=1}^{A} (\hbar^2/2\,m)\,\nabla_i^2 + \sum_{1 \le i < j \le A} v(i\,j)\,, \tag{2}$$

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describes a system of A identical particles with mass m (in our case, A fermions) in the volume Ω. The potential $v(i\,j)$ which is mostly obtained in a phenomenological way contains the above mentioned short-range repulsions (which sometimes include a "hard core").

Our investigation of the equilibrium properties of Fermi-systems starts with the Ansatz (1) with $--1 \leqq n \leqq A--$

$$F(1, 2, 3, \ldots, n) = \prod_{1 \le i < j \le n} f(r_{ij}) \tag{3}$$

which is known as the Bijl-Dingle-Jastrow Ansatz [1] and extended by Feenberg and coworkers [2], and with the "independent-particle" Φ. Then we estimate the energy expectation value

$$E = \langle \Psi \,|\, H \,|\, \Psi \rangle / \langle \Psi \,|\, \Psi \rangle \tag{4}$$

by referring to the factor-cluster formalism of Clark and Westhaus [3] which makes it possible to evaluate E without respect to the perturbation theory in a "linked hole-line expansion". These cluster-expansion techniques – originally developed for the calculation of the partition function of a classical imperfect gas and adapted to the quantum-mechanical many-body problem by Iwamoto and Yamada [4] – have recently been generalized by Clark et al. [5] (in due course, the Iwamoto-Yamada expansion has been renormalized).

Specializing the general state-dependent set of correlation operators $\{F(1,2), F(1,2,3), \ldots, F(1,2,3\ldots,n);\ n=4,5,\ldots,A\}$ we are able to deduce, in the framework of the factor-cluster formalism, well-known many-body methods such as Brueckner's reaction-matrix approximation [6] for a uniform, extended system or the unitary transformation method [7]. Therefore, it is of special interest to compare the results of the renormalized and unrenormalized Iwamoto-Yamada expansions for dense Fermi systems with those obtained by other alternative approaches; especially with the Brueckner method. It is known [8] that the lowest order Brueckner approximation is not suitable to describe such systems as ^{3}He and neutron matter at high densities. Therefore the inclusion of higher-order cluster contributions (at least the Bethe-Faddeev-term) is necessary. In his ^{3}He calculations Østgaard [9] includes three-body effects in a somewhat approximate way.

On the other hand, the correlated basis function method developed by Feenberg [2] and the Iwamoto-Yamada method have been suitably adapted for calculating the expectation values of physical operators in dense systems. In addition, the numerical treatment of the higher-order cluster contributions are much simpler. For liquid Helium the Feenberg expansion is most appropriate.

Comparing the renormalized and unrenormalized Iwamoto-Yamada expansions, we want to settle the question of higher renormalization effects in the cluster expansion of the energy expectation value. In Section 2 we briefly refer to the basic formalism of the method of correlated basis functions (unrenormalized and renormalized versions) and study the simplest approximants of the expansions of the energy expectation value and define the so-called "ordering"- and "smallness"-parameters [3, 10, 11] which characterize the Iwamoto-Yamada expansion. With the Bijl-Dingle-Jastrow [1, 12] Ansatz of the correlation operator $F(1, 2, \ldots, A)$ we explicitely present the effective two- and three-body potentials as well as the two- and three-particle correlation matrix elements.

In Section 3 we study the normal phase of liquid ^{3}He. We connect the finding of a suitable short-range two-body correlation operator with the solution of the Euler-Lagrange equation for the unrenormalized energy functional in the two body approximation. We compare our numerical results for ^{3}He with those of other authors as well as with the experimental data.

The final section, Section 4, is devoted to the application of the formalism developed in Section 2 to symmetrical nuclear matter and neutron matter, where the OMY-potential [13] is used. It has turned out that in our approach the unrenormalized ground-state energy expansion gives a better numerical convergence than the renormalized one. This might be due to the cancellation phenomenon of the Iwamoto-Yamada expansion in the Jastrow case [14,15]. Whether the practical advantage (the better convergence) of unrenormalized expansion over renormalized one persists in higher orders or not is still open to question.

2. Basic Formalism

2.1. Correlated Basis Functions

The method of correlated *b*asis *f*unctions [2, 3] (CBF) is a powerful tool for constructing theories of quantum mechanical systems with strong short-range interaction. Dealing with Fermi systems in this paper, we start with the "extended Jastrow" Ansatz [16, 17] (1) for the trial ground-state wave function. The correlation operator F is defined for an arbitrary number n of particles ($1 \leqq n \leqq A$) and is required to possess the cluster property [18]. Here, the "cluster property" means a sufficiently rapid factorization

$$F(1,\ldots,l,m,\ldots,n) \to F(1,\ldots,l)\ F(m,\ldots,n)\,; \quad F(1)=1 \tag{5}$$

as the particle group $\{1,\ldots,l\}$ is moved from the particle group $\{m,\ldots,n\}$, far enough compared with the range of the interaction of the particles. It would be necessary to symmetrize the right-hand side of Equation (5). We, however, suppressed those terms which do not contribute to the expectation value in the thermodynamic limes (particle number $A\to\infty$, volume $\Omega\to\infty$, density $\varrho = A/\Omega = \text{const}$). Special examples fulfilling the above-mentioned requirements are the Jastrow Ansatz [3, 12] and the unitary-model-operator Ansatz [7, 19]. The expectation value (4) can be evaluated with the help of the "*f*actorized" version of the *I*wamoto-*Y*amada (FIY) expansion and leads to

$$E = E_0 + (\Delta E)_1 + \ldots + (\Delta E)_n + \ldots + (\Delta E)_A\,, \tag{6}$$

where the terms are arranged according to the number n of involved particles, and $(\Delta E)_n$ is called the n-body cluster or "n-hole-line" contribution. E_0 is the ground-state energy of the non-interacting system. The approximation of E by the first n terms of (6) is denoted $E_U^{[n]}$. A complete classification and decomposition of each $(\Delta E)_n$ into proper n-body parts and (reducible and irreducible) combination terms is given in a detailed analysis of the FIY expansion in Reference 5. This analysis starts with the generalized normalization integral

$$I(\beta) := \langle \Psi \,|\, \exp\{\beta(H-E_0)\} \,|\, \Psi \rangle \tag{7}$$

from which we easily recover the energy expectation value through

$$E = E_0 + \frac{\partial}{\partial \beta} \ln I(\beta)_{|\beta=0}. \tag{8}$$

Successive definition of subnormalization integrals

$$\begin{aligned}
I_i(\beta) &:= \langle i \,|\, F^+(1) \exp\{\beta[t(1) - \varepsilon_i]\} F(1) \,|\, i \rangle = 1, \\
I_{ij}(\beta) &:= \langle ij \,|\, F^+(12) \exp\{\beta[t(1)+t(2)+v(12) - \varepsilon_i - \varepsilon_j]\} F(12) \,|\, ij \rangle_a, \\
I_{ijk}(\beta) &:= \langle ijk \,|\, F^+(123) \exp\{\beta[t(1)+t(2)+t(3)+v(12)+v(23) \\
&\qquad +v(31) - \varepsilon_i - \varepsilon_j - \varepsilon_k]\} F(123) \,|\, ijk \rangle_a, \\
&\vdots \\
I^{(q)}(\beta) &:= \langle i_1 \ldots i_A \,|\, a_q^+ F^+[1,\ldots,(A-1)] \exp\left\{\beta\left(\sum_{i<j}^{A-1}[t(i)-\varepsilon_i] + \sum_{i<j}^{A-1} v(ij)\right)\right\} \\
&\qquad \cdot F[1,\ldots,(A-1)] a_q \,|\, i_1 \ldots i_A \rangle_a, \\
I_{1\ldots A}(\beta) &\equiv I(\beta) = \langle i_1 \ldots i_A \,|\, F^+(1,\ldots,A) \exp\{\beta(H - E_0)\} F(1,\ldots,A) \,|\, i_1 \ldots i_A \rangle_a
\end{aligned} \tag{9}$$

and a factor-cluster decomposition of these integrals

$$\begin{aligned}
I_i &= Y_i, \\
I_{ij} &= Y_i Y_j Y_{ij}, \\
I_{ijk} &= Y_i Y_j Y_k Y_{ij} Y_{jk} Y_{ki} Y_{ijk}, \\
&\vdots \\
I_{1\ldots A} &= \prod_i Y_i \prod_{i<j} Y_{ij} \prod_{i<j<k} Y_{ijk} \ldots Y_{1\ldots A}
\end{aligned} \tag{10}$$

result in a general expression for the energy expectation value

$$E = E_0 + \sum_{i<j} \frac{\partial}{\partial \beta} \ln Y_{ij}(\beta)_{|\beta=0} + \sum_{i<j<k} \frac{\partial}{\partial \beta} \ln Y_{ijk}(\beta)_{|\beta=0} + \ldots \tag{11}$$

Comparison of Eqs. (6) and (11) leads to the simple relation (12):

$$(\Delta E)_n = \sum_{i_1<\ldots<i_n} \frac{\partial}{\partial \beta} \ln Y_{i_1 \ldots i_n}(\beta)_{|\beta=0} \tag{12}$$

between the n-body cluster contribution $(\Delta E)_n$ and the factor-cluster integral $Y_{i_1\ldots i_n}(\beta)$. The explicit representation of $(\Delta E)_n$ in the leading order $O(A^1)$ (thermodynamic limes) is [5]:

$$\begin{aligned}
(\Delta E)_1 &= 0, \\
(\Delta E)_2 &= \frac{1}{2!} \sum_{ij} w_{ij}(\beta)_{|\beta=0}, \\
(\Delta E)_3 &= (\Delta E)_3{}^{(2)} + (\Delta E)_3{}^{(3)}, \\
(\Delta E)_3{}^{(3)} &= \frac{1}{3!} \sum_{ijk} w_{ijk}(\beta)_{|\beta=0}, \\
(\Delta E)_3{}^{(2)} &= -\sum_{ijk} \eta_{ij}(\beta)\, w_{ik}(\beta)_{|\beta=0}, \\
(\Delta E)_4{}^{(2)(1)} &= \sum_{ijkl} (\eta_{ik}\eta_{il} + \eta_{ik}\eta_{kl})\, w_{ij}(\beta)_{|\beta=0}, \\
&\vdots
\end{aligned} \tag{13}$$

We note that $(\Delta E)_3{}^{(2)}$ and $(\Delta E)_4{}^{(2)(1)}$ belong to the dispersion contributions considered in a standard (unrenormalized) Brueckner approximation. The new quantities of Eq. (13) are defined as follows:

$$\begin{aligned}
w_{ij} &:= \langle ij \,|\, \tfrac{1}{2} F^+(12)\ [t(1)+t(2), F(12)]\ + \tfrac{1}{2} F^+(12)\, v(12)\, F(12)\ + \text{adj.} \,|\, ij \rangle_a, \\
w_{ij} &= :\langle ij \,|\, w_2(12;0) \,|\, ij \rangle_a,\ \eta_{ij} = \langle ij \,|\, [F^+(12)\, F(12) - 1] \,|\, ij \rangle_a = :\langle ij \,|\, \eta(12;0) \,|\, ij \rangle_a, \\
\eta_{ijk} &:= \langle ijk \,|\, \{F^+(123)\, F(123) - [F^+(12)\, F(12) + \text{cycl.}] + 2\} \,|\, ijk \rangle_a, \\
w_{ijk} &:= \langle ijk \,|\, \tfrac{1}{2} F^+(123)\ [t(3), F(123)]\ + \tfrac{1}{2} F^+(123)\, v(12)\, F(123) - \tfrac{1}{2} w_2(12;0) + \text{cycl.} + \text{adj.} \,|\, ijk \rangle_a.
\end{aligned} \tag{14}$$

The definition of the generalized n-body correlation matrix elements $\eta_{i_1\ldots i_n,\ j_1\ldots j_n}$ and the generalized effective or induced many-body potentials $w_{i_1\ldots i_n,\ j_1\ldots j_n}$ deduced from these matrix elements are given in Reference 20.

In studying the expansion (11) which is valid for any particle number A we are now interested in terms of order $O(A^0)$. The knowledge of these terms is necessary to see the asymptotic behavior of the radial distribution function $g(r)$ (see below). We define a function

$$G(\beta) := \ln I(\beta) = \sum_{i<j} \ln Y_{ij} + \sum_{i<j<k} \ln Y_{ijk} + \dots \quad (15)$$

and from G the quantities:

$$\begin{aligned} G^1(\beta)/A &:= \lim_{A\to\infty} G(\beta)/A\,, \\ G^0(\beta) &:= \lim_{A\to\infty} [G(\beta) - G^1(\beta)]\,, \\ G^{-1}(\beta) &:= \lim_{A\to\infty} \{A[G(\beta) - G^1(\beta) - G^0(\beta)]\}\,, \\ G^{-2}(\beta) &:= \lim_{A\to\infty} \{A^2[G(\beta) - G^1(\beta) \\ &\qquad - G^0(\beta) - G^{-1}(\beta)]\}\,. \end{aligned} \quad (16)$$

Now we are ready to write G as:

$$G(\beta) = G^1(\beta) + G^0(\beta) + G^{-1}(\beta) + G^{-2}(\beta) + \dots \quad (17)$$

where $G^n(\beta)$ is of order $O(A^n)$. It can be shown [20] that $G^0(\beta)$ vanishes. This result has several important consequences for the behavior of the radial distribution function [20]:

a) $g(r)$ does not contain contributions of order $O(A^{-1})$,

b) $$\lim_{A\to\infty} \{A[g(\infty) - 1]\} = 0\,. \quad (18)$$

The property b) is discussed in Section 3.

2.2. Renormalized FIY-Expansion and Energy Functional in the Three-Body Approximation

In this Section we briefly review the main steps of the renormalization of the FIY-expansion [5, 20–22]. The aim is to find a suitable partial resummation of the expansion (6). Thereby we pay attention to the close connection of the FIY scheme with the theories of classical statistical mechanics, especially with the cluster expansion of thermodynamic quantities [23] in powers of the fugacity of an imperfect fluid.

Wu and Feenberg [2, 24, 25] found the connection between the subnormalization integrals ($I^{(q)}(\beta)$, $I^{(qi)}(\beta)$, ... for the $(A-1)$-, $(A-2)$-, ... subsystems) and the generalized normalization integral $I(\beta)$:

$$I(\beta) = I^{(q)} + \sum_i x_{qi} I^{(qi)} + \sum_{i<j} x_{qij} I^{(qij)} + \dots \quad (19)$$

Introducing a generalized "true" distribution function

$$z_q{}^0(\beta) := \frac{I^{(q)}(\beta)}{I(\beta)}\Big|_{A\to\infty} \quad (20)$$

and assuming the following relations of a certain number of subnormalization integrals (limes $A\to\infty$):

$$\begin{aligned} \frac{I^{(q_1)}}{I} &= \frac{I^{(q_1 q_2)}}{I^{(q_1)}} + O(A^{-1})\,, \\ \frac{I^{(q_1 q_2)}}{I^{(q_1)}} &= \frac{I^{(q_1 q_2 q_3)}}{I^{(q_1 q_2)}} + O(A^{-1})\,, \\ \frac{I^{(q_1 q_2 q_3)}}{I^{(q_1 q_2)}} &= \frac{I^{(q_1 q_2 q_3 q_4)}}{I^{(q_1 q_2 q_3)}} + O(A^{-1})\,, \\ &\vdots \end{aligned} \quad (21)$$

we can write series (19) in the thermodynamic limes (providing a rapid convergence) into:

$$1 = z_q{}^0 \{1 + \sum_i x_{qi} z_i{}^0 + \sum_{i<j} x_{qij} z_i{}^0 z_j{}^0 + \dots\} \quad (22)$$

or (by omitting contributions of order $O(A^{-1})$) into:

$$1 = z_q{}^0 \{1 + \sum_i x_{qi} z_i{}^0 + \frac{1}{2!} \sum_{ij} z_i{}^0 z_j{}^0 x_{qij} + \dots\}\,. \quad (23)$$

Iteration of Eq. (23) yields the (unrenormalized) expansion $z_q{}^0$ as

$$z_q{}^0 = 1 - \sum_i x_{qi} - \frac{1}{2!} \sum_{ij} x_{qij} + \sum_{ij} (x_{qj} + x_{ij}) x_{qi} + \dots \quad (24)$$

which can be regarded as the FIY expansion of the occupation number-operator $a_q{}^+ a_q$ if the correlation operators $F(1, \dots, n)$ are required to fulfill the exact Pauli condition [26]. Now we obtain the renormalized representation of the energy expectation value with the aid of $z_q{}^0$ as:

$$E = E_0 + \left[\frac{1}{2!} \sum_{ij} z_i{}^0 z_j{}^0 \frac{\partial}{\partial\beta} x_{ij} + \frac{1}{3!} \sum_{ijk} z_i{}^0 z_j{}^0 z_k{}^0 \frac{\partial}{\partial\beta} x_{ijk} + \dots\right]_{|\beta=0}\,. \quad (25)$$

To construct the analogy to the classical statistical mechanics [23, 27] of imperfect fluids we define a functional [28]

$$\Xi(z_q, \beta, \Omega) := 1 + \sum_i z_i + \frac{1}{2!} \sum_{ij} z_i z_j I_{ij} + \dots \quad (26)$$

which depends on the independent function z_q, the volume Ω and on the parameter β. The sub-

normalization integrals in (26) are also defined for coincident quantum numbers [20]. The analog to the particle-number equation of the classical theory is then given by:

$$1 = z_q \frac{\delta[\Omega\chi(z_q,\beta)]}{\delta z_q} \tag{27}$$

with

$$\Omega\chi(z_q,\beta) := \ln \Xi(z_q,\beta,\Omega)\,. \tag{28}$$

Expanding the logarithms we get the explicit form of the functional $\Omega\chi(z_q,\beta)$:

$$\Omega\chi(z_q,\beta) = \sum_i z_i + \frac{1}{2!}\sum_{ij} z_i z_j x_{ij} + \frac{1}{3!}\sum_{ijk} z_i z_j z_k x_{ijk} + \ldots \tag{29}$$

The solution of the (nonlinear) integral Eq. (27) gives the weight factor $z_q{}^0$ in Equation (22). Furthermore it is easy to see that E in Eq. (25) is generated by differentiation of $\Omega\chi(z_q,\beta)$ with respect to β:

$$E = E_0 + \frac{\partial}{\partial\beta}[\Omega\chi(z_q,\beta)]\,\Big|_{\substack{z_q=z_q{}^0\\ \beta=0}}\,. \tag{30}$$

Here we introduce the notation necessary for presenting some numerical results. We denote the n-particle approximation of $\Omega\chi(z_q,\beta)$ with

$$\Omega\chi^{[n]}(z_q,\beta) := \sum_i z_i + \frac{1}{2!}\sum_{ij} z_i z_j x_{ij} + \ldots + \frac{1}{n!}\sum_{i_1\ldots i_n} z_{i_1}\ldots z_{i_n}\, x_{i_1}\ldots{}_{i_n} \tag{31}$$

and the energy expectation value and the weight-function approximation deduced from (31) with

$$E_{\mathrm{R}}{}^{[n]} := E_0 + \frac{\partial}{\partial\beta}\,\Omega\chi^{[n]}(z_q,\beta)\,\Big|_{\substack{z_\alpha=z_\alpha{}^0\\ \beta=0}} \tag{32}$$

and

$$1 = z_q{}^{[m]}\frac{\delta\Omega\chi^{[m]}}{\delta z_q}\,\Big|_{\beta=0}\,, \tag{33}$$

respectively. The approximate energy obtained for z_q replaced by $z_q^{0[m]}$ [solution of Eq. (33)] in $E_{\mathrm{R}}^{[n]}$ is written as $E_{\mathrm{R}}^{[n,m]}$.

With the B-D-J Ansatz (3) we can easily evaluate the effective potentials as

$$\begin{aligned} w(12;0) &= \frac{\hbar^2}{m}\left(\frac{\mathrm{d}f}{\mathrm{d}r}\right)^2 + f^2(r_{12})\,v(12)\,,\\ w(123;0) &= [f^2(13)\,f^2(23) - 1]\,w(12;0) \\ &\quad + \frac{\hbar^2}{4m} f^2(12)\,\nabla_3 f^2(13)\,\nabla_3 f^2(23) + \mathrm{cycl.} \end{aligned} \tag{34}$$

Other quantities necessary for the estimation of $E_{\mathrm{R}}^{[2]}$, $E_{\mathrm{U}}^{[2]}$, $E_{\mathrm{R}}^{[3]}$, $E_{\mathrm{U}}^{[3]}$ and of $z_q^{0[2]}$ and $z_q^{0[3]}$ are the operators $\eta(12;0)$ and $\eta(123;0)$ as well as the correlation matrix elements $\eta_{ij}(0)$ and $\eta_{ijk}(0)$:

$$\begin{aligned} \eta(12;0) &= f^2(12) - 1\,; \qquad \eta_{ij}(0) = \langle ij\,|\,[f^2(12) - 1]\,|\,ij\rangle_a\,,\\ \eta(123;0) &= f^2(12)f^2(13)f^2(23) - [f^2(12) + f^2(13) + f^2(23)] + 2\,,\\ \eta_{ijk}(0) &= \langle ijk\,|\,\eta(12;0)\,\eta(13;0)\,\eta(23;0) + \eta(12;0)\,\eta(13;0) + \eta(12;0)\,\eta(23;0) \\ &\quad + \eta(13;0)\,\eta(23;0)\,|\,ijk\rangle_a\,. \end{aligned} \tag{35}$$

The FIY- and IY-expansions are characterized by the following three parameters [3, 10, 11]:

$$(1)\qquad \xi := \frac{1}{A}\sum_{ij}\eta_{ij}(0)\,, \tag{36}$$

$$(2)\qquad \varkappa := \frac{1}{A}\sum_{ij}\langle ij\,|\,[F^+(12) - 1]\cdot[F(12) - 1]\,|\,ij\rangle_a\,, \tag{37}$$

$$(3)\qquad \zeta := \frac{1}{A}\sum_{ij}\langle ij\,|\,[F(12) - 1]\,|\,ij\rangle_a\,. \tag{38}$$

The smallness of ξ, which is known as the "smallness parameter" in the (F)IY approach, is often considered to be a guarantee for good convergence of Eq. (6); if ξ is much less than unity (as in the case of low density nuclear (neutron) matter) the convergence is assumed to be "reasonable". The parameter $\varkappa$ is the analog to the "smallness parameter" in the Brueckner-Bethe-Goldstone [29, 30] expansion. The parameter ξ is equal to $\varkappa$ when the correlation factor $F(12)$ satisfies the "average Pauli condition", i. e. $\zeta = 0$.

3. The Normal Phase of Liquid ^{3}He

3.1. Pair-Correlation-Function

Several authors [9, 31–36] have made much effort to calculate the ground-state energy of liquid ^{3}He. In order to compare our results with those of other authors [32–34, 36] we assume in our calculations the Lennard-Jones-(6 – 12) potential

$$v(r) = 4\varepsilon\{(\sigma\,|\,r)^{12} - (\sigma\,|\,r)^6\} \tag{39}$$

with the de Boer-Michels parameters [37]

$$\varepsilon = 10.22\ ^\circ\mathrm{K}\,, \quad \sigma = 2.556\ \text{Å}\,. \tag{40}$$

Then we obtain the pair-correlation function $f(r)$ [cf. Eq. (3)] for small distances (i. e. $r \to 0$) be-

tween the ^{3}He atoms from the Euler-Lagrange equation for the unrenormalized energy-functional in the two-body approximation:

$$\frac{\hbar^2}{m r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{(\mathrm{d}f/\mathrm{d}r)}{f(r)}g^{[2]}(r)\right)=\tilde{w}(r)\,g^{[2]}(r) \quad (41)$$

with

$$\tilde{w}(r):=v(r)+\frac{\hbar^2}{m}\frac{(\mathrm{d}f/\mathrm{d}r)^2}{f^2(r)}\,. \quad (42)$$

The function $g^{[2]}(r)$ is the familiar two-body cluster approximant of the radial distribution function of a Fermi liquid:

$$g^{[2]}(r)=f^2(r)\{1-\tfrac{1}{2}\,l^2(r\,k_\mathrm{F})\}\,,$$
$$l(x)=(3/x^3)\{\sin x-x\cos x\}\,. \quad (43)$$

Solving Eq. (41) in the above-mentioned limit we get

$$f(r)=f_0(r)\exp\{-\mu_1(\sigma\,|\,r)^5\}\,, \quad (44)$$

where μ_1 has the value 0.8151 for the parameter set (40) and where the function $f_0(r)$ has to fulfill the following conditions:

$$f_0(r)\neq 0 \text{ for all } r\,,$$
$$\lim_{r\to 0} f_0(r)<\infty\,, \quad (45)$$
$$\lim_{r\to\infty} f_0(r)=1\,.$$

The validity of solution (44) has been proved by Krotscheck [32] for the exact Euler-Lagrange equation at $r\approx 0$. Since the conditions (45) do not uniquely define $f_0(r)$ we have some freedom in its choice. As a first approach we chose $f_0(r)\equiv 1$. The resulting pair-correlation function

$$f_\mathrm{SV}(r)=\exp\{-\mu_1(\sigma\,|\,r)^5\} \quad (46)$$

(μ_1 now is a variational parameter)
has been used by McMillan [38] for the calculation of the ground-state energy of liquid ^{4}He and by Schiff and Verlet [33] also for liquid ^{3}He. In the relatively accurate Monte Carlo calculation or in molecular-dynamics methods the correlation function (46) has been successfully used but it is not suitable for our (F)IY-cluster expansions; in the relevant density region ($k_\mathrm{F}=0.73114\,\text{Å}^{-1}-0.81077\,\text{Å}^{-1}$) the absolute magnitude of ξ turned out to be between 1.5 and 4.0, which suggests a rather poor convergence of our energy expansions. In the whole considered density region the three-body energy approximation $E_\mathrm{R}^{[3,3]}$ calculated with $f_\mathrm{SV}(r)$ leads to no binding because

$$\xi_3:=(1/A)\sum_{ijk}\eta_{ijk}(0) \quad (47)$$

is too large (between 7.0 and 30.0). In addition, the "average Pauli condition" (PC) cannot be fulfilled with the correlation function (46).

A very important and difficult problem is embedded in the treatment of long-range correlations in the (F)IY cluster scheme. Since a truncated (renormalized) (F)IY expansion of the energy expectation value including long-range correlations ($f\to 1/r^n$; $r\to\infty$, $n=1, 2, 3$) does not converge, we make for $f(r)$ the specified and parametrized Ansatz:

$$f(r)=\exp\{-\mu_1(\sigma\,|\,r)^m\}\,[1+\lambda\,(1-\exp\{-\mu_2\,(\sigma\,|\,r)^n\})]\,, \quad (48)$$

where m and n are integers greater than or equal to 4. This Ansatz enables us to describe accurately the behavior of the short-range ($m=5$) correlations, and by choosing $n=4$ we can adjust a long-range behavior of $f(r)$ which is compatible with our cluster expansion. In the following we take $m=5$, $n=4$ and $\mu_1=\mu_2=:\mu$ (C 2), and at each k_F we determine λ by the "average Pauli condition". The parameter μ is found by minimizing $E_\mathrm{R}^{[3,3]}(\mu)$ at an arbitrarily chosen density ϱ_0 [$\varrho_0=k_\mathrm{F}^{0^3}/(3\pi^2)$], and we denote the energy minimum by $E_\mathrm{R}^{[3,3]}(k_\mathrm{F}^0,\mu_0)$. Then for other densities ($k_\mathrm{F}\neq k_\mathrm{F}^0$) μ is determined to reproduce the previously obtained asymptotic value of the renormalized approximant $g_\mathrm{R}^{[3,3]}(k_\mathrm{F}^0, \mu_0, \infty)$ of the radial distribution function

$$g(r):=\frac{1}{\varrho^2}\,A(A-1)\,\frac{\sum_{\{\sigma\}\{\tau\}}\int|\Psi|^2\,\mathrm{d}^3r_3\ldots\mathrm{d}^3r_A}{\sum_{\{\sigma\}\{\tau\}}\int|\Psi|^2\,\mathrm{d}^3r_1\ldots\mathrm{d}^3r_A} \quad (49)$$

i.e. $g_\mathrm{R}^{[3,3]}(k_\mathrm{F}^0,\mu_0,\infty)=g_\mathrm{R}^{[3,3]}(k_\mathrm{F},\mu,\infty)$.

For example, choosing k_F^0 equal to the experimental equilibrium density $k_\mathrm{F}^{\mathrm{exp.}}=0.786\,\text{Å}^{-1}$ we get: $E_\mathrm{R}^{[3,3]}(\mu_0, k_\mathrm{F}^{\mathrm{exp.}})=-2.368\,^\circ\mathrm{K}$ and $g_\mathrm{R}^{[3,3]}(k_\mathrm{F}^{\mathrm{exp.}},\mu_0,\infty)=0.899$, or choosing $k_\mathrm{F}^0=0.81077\,\text{Å}^{-1}$ we obtain $g_\mathrm{R}^{[3,3]}(k_\mathrm{F}^0,\mu_0,\infty)=0.876$. The deviations of $g_\mathrm{R}^{[3,3]}(k_\mathrm{F}^0,\mu_0,\infty)$ from unity [exact asymptotic value of $g(r)$] indicate the importance of higher order cluster contributions in the renormalized energy expansion.

The results given in Tables 1 and 2 refer to the above mentioned two asymptotic values of $g_\mathrm{R}^{[3,3]}$. These Tables show only those quantities which are almost independent of the density.

Table 1. $g_R^{[3,3]}(\infty)=0.899$. The "averaged" weight factors $z_Q^{[3]}$ and $z_Q^{[3]}$ are defined by $z_Q^{[m]} := (\sum_q z_q^{0[m]})/A$, and $g_Q^{[n,m]}(\infty)$ are the "averaged" approximants of $g(r)$ obtained when $z_Q^{[m]}$ is inserted in $g_R^{[n,m]}(\infty)$.

$\varkappa, \xi$	ξ_3	$z_Q^{[2]}$	$z_Q^{[3]}$	$g_Q^{[3,3]}(\infty)$	$g_Q^{[4,3]}(\infty)$
0.605	0.061	0.703	0.699	0.902	1.004

Table 2. $g_R^{[3,3]}(\infty)=0.876$.

$\varkappa, \xi$	ξ_3	$z_Q^{[2]}$	$z_Q^{[3]}$	$g_Q^{[3,3]}(\infty)$	$g_Q^{[4,3]}(\infty)$
0.6725	0.120	0.686	0.678	0.880	1.001

As can be seen the smallness-parameter $\varkappa$ and ξ become relatively large as compared with the results $\varkappa=\xi=0.474$ which correspond to the density $k_F^0=0.73114$ Å^{-1} and $g_R^{[3,3]}(k_F^0, \mu_0, \infty)=0.942$ and $E_R^{[3,3]}(k_F^0, \mu_0)=-1.936$ °K], whereas the averaged three-body effects ξ_3 remain small. Further results will be given in the next Section.

3.2. Comparison and Discussion

The ground state properties of liquid ^{3}He have been the subject of many theoretical studies. We compare our results with those of Schiff and Verlet [33] (SV), Massey and Woo [34] (MW), Pandharipande [39] (P) and of Krotscheck [32] (K). All these authors used the L-J-(6 – 12) potential in their variational calculations.

In Table 3 we compare some characteristic equilibrium properties of liquid ^{3}He obtained by different authors: the saturation density $\varrho_{eq.}$, saturation energy (per particle) $E_{eq.}$, unit radius r_0, the maxima of the structure function and the radial distribution function *. The unit radius is defined by

$$\tfrac{4}{3}\, r_0^3\, \varrho = 1 . \qquad (50)$$

At equilibrium density, r_0 is a few percent less than the He-He atomic potential core radius σ. The quantities r_m and k_m are the arguments of the maxima of the radial distribution function and static structure function, respectively.

We found good agreement with experiment as far as the position of the maximum of $S(k)$ ($k_m \approx 2.0$ Å^{-1}) is concerned. The maximum value of the structure function itself, however, differs from the experimental value in all cases.

The situation for the distribution function $g(r)$ is very similar: the r_m-values lie between 3.6 – 3.8 Å which is very close to the experimental value 3.6 Å. But the maximum $g(r_m)$ of $g(r)$ becomes too low. For $\varrho_{eq.}$ and $E_{eq.}$ a number of different results have been published. Pandharipande and Krotscheck used simple variational methods constrained by "reasonable" auxiliary conditions. K combines the FIY-expansion of the energy expectation value with a variational procedure which takes into account the short-range behavior of the state-independent pair-correlation function. P's treatement in the

Table 3. Comparison of ^{3}He results.

Authors	ϱ_{eq} [Å^{-3}]	E_{eq} [°K]	r_0 [Å]	r_m [Å]	$g(r_m)$	k_m [Å^{-1}]	$S(k_m)$
Schiff and Verlet (SV)	0.0142	−1.27 (−1.35)	2.562	3.783 at $\varrho=$ 0.0164 Å^{-3}	1.128	1.995 at $\varrho=$ 0.0164 Å^{-3}	1.146
Massey and Woo (MW)	0.0140	−0.20	2.574	comparable with the results of Schiff and Verlet			
Pandharipande (P)	0.0204	−2.87	2.270	—	—	—	—
Krotscheck (K) ($\lambda_K=2.5$)	0.0204	−1.75	2.270	3.60 at $\varrho=$ 0.0164 Å^{-3}	1.113	2.05 at $\varrho=$ 0.0164 Å^{-3}	1.122
Here unrenormalized	0.0164	−2.595	2.442	3.80	1.17	1.95	1.12
(renormalized)	(0.0172)	(−2.415)	(2.403)	(4.20)	(1.05)	(2.0)	(1.09)
Experiment (Achter and Meyer)	0.0164	−2.52	2.442	3.60	1.238	1.95	1.247

* Further discussions on the liquid structure function $S(k)$ and radial distribution function will be given in our forthcoming paper.

lowest cluster-order (two-body approximation) with state-dependent correlation overestimates the saturation energy of ^{3}He. The imposed constraints are rather arbitrary and severe and lead to a correlation function without overshoot. In a more recent work [36] P has improved his results by including a class of higher-order cluster contributions of the direct matrix elements (and, in addition, certain higher-order exchange contributions; HNC/4). For further comparison it would be interesting to know P's results for the liquid structure function, especially in the range of low momenta.

Table 4. ^{3}He results: C2 and PC with $g_R^{[3,3]}(\infty)=0.899$.

k_F [Å^{-1}]	μ	λ	$(\Delta E)_2$ [°K]	$(\Delta E)_3^{(2)}$ [°K]	$(\Delta E)_3^{(3)}$ [°K]
0.73114	1.35	0.713	−4.308	5.202	−5.073
0.74562	1.23	0.725	−4.857	5.878	−5.711
0.75956	1.12	0.738	−5.373	6.485	−6.230
0.77300	1.03	0.750	−5.815	7.028	−6.632
0.78600	0.95	0.761	−6.181	7.473	−6.868
0.79858	0.88	0.772	−6.449	7.805	−6.916
0.81077	0.815	0.784	−6.593	7.966	−6.693

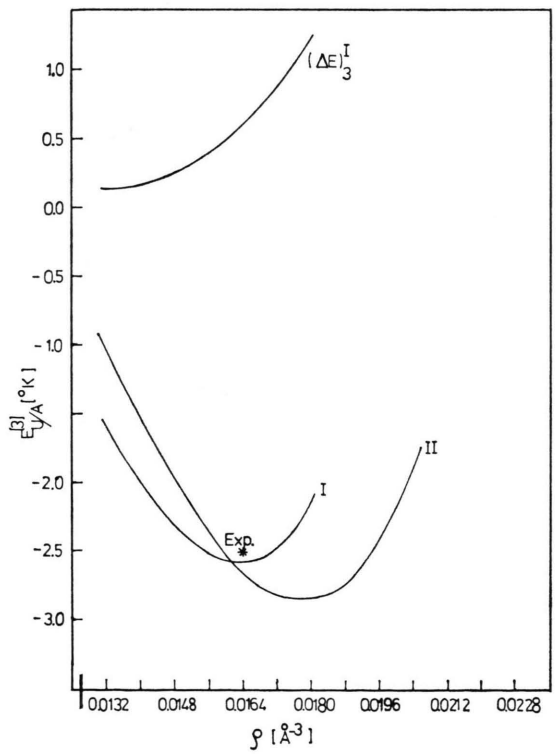

Fig. 1. ^{3}He. The unrenormalized energy $E_U^{[3]}$ per particle in dependence of k_F for two different asymptotical values — I) $g_R^{[3,3]}(\infty)=0.899$ and II) $g_R^{[3,3]}(\infty)=0.876$ — of the approximated radial distribution function. * denotes the experimental equilibrium energy per particle.

The comparison of the SV and MW calculations are made in Reference 34. The major discrepancy of their equilibrium energies $E_{eq.}$ comes essentially from the difference of 0.86 °K of the energies they obtained for the hypothetical boson ^{3}He system. Inclusion of a perturbation correction in the second order might bring better results.

Our detailed results are given in Tables 4 and 5. The saturation energies are in the neighbourhood of the experimental value.

Table 5. ^{3}He results: C2 and PC with $g_R^{[3,3]}(\infty)=0.876$.

k_F [Å^{-1}]	μ	λ	E_{kin} [°K]	$(\Delta E)_2$ [°K]	$(\Delta E)_3^{(2)}$ [°K]	$(\Delta E)_3^{(3)}$ [°K]
0.75956	1.31	0.721	2.783	−4.947	6.655	−6.468
0.77300	1.20	0.733	2.883	−5.498	7.385	−7.138
0.78600	1.105	0.744	2.980	−5.998	8.050	−7.691
0.79858	1.025	0.755	3.077	−6.429	8.644	−8.119
0.81077	0.95	0.766	3.171	−6.790	9.117	−8.351
0.81920	0.905	0.773	3.237	−6.991	9.401	−8.426
0.8448	0.780	0.795	3.443	−7.268	9.791	−7.853

We note the following features:

(1) The two-body contribution to the energy, $(\Delta E)_2$, is always negative and decreases with increasing k_F. Within the considered density region the energy approximants $E_U^{[2]}$ and $E_R^{[2,2]}$ do not lead to saturation.

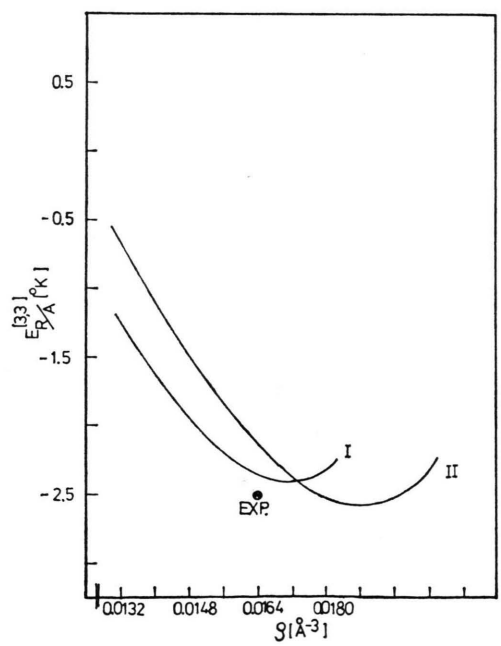

Fig. 2. ^{3}He. The renormalized energy $E_R^{[3,3]}$ per particle in dependence on k_F.
I) $g^{[3,3]}(\infty)=0.899$ and II) $g_R^{[3,3]}(\infty)=0.876$.

(2) The two-body combination term $(\Delta E)_3^{(2)}$ is positive throughout all densities and increases with k_F. On the other hand the proper three-body part $(\Delta E)_3^{(3)}$ is negative and has a minimum. The point to be stressed here is that there is a cancellation between $(\Delta E)_3^{(2)}$ and $(\Delta E)_3^{(3)}$. This phenomenon is a general feature[15] of the cluster expansion method with the Jastrow wave function describing the uniform extended Fermi liquid. Above all, however, the three-body part, $(\Delta E)_3$, of the energy approximation gives rise to finding saturation energies (see Figure 1).

4. Nuclear Matter and Neutron Matter

4.1. Potential and Procedure

A uniform extended system of nucleons with the same number of neutrons and protons is referred to as symmetrical nuclear matter and is characterized by the two, empirically known data:

(a) the equilibrium energy

and

(b) the equilibrium density.

As reference data we adopt the values suggested by Bethe[40]: the energy per particle of -16 MeV and the equilibrium density of $k_F^{eq.} = 1.36\,\mathrm{fm}^{-1}$ ($r_0 = 1.12$ fm).

The properties of pure neutron matter are of great interest, especially because of the existence of neutron stars. One wants to know the transport properties and one also wishes to answer the question whether the interior of a neutron star is solid[41] or liquid.

For our nuclear matter (or neutron matter) calculations we use the OMY[13] (IY) potential. It is a central nucleon-nucleon potential with a state-independent hard core of radius $r_c = 0.6$ fm and is adjusted (in the presence of the core) to fit the low-energy singlet and triplet scattering parameters and effective ranges. For the even-parity states the OMY potential has an attractive shape (outside of the hard cure):

$$\begin{aligned} {}^1V_c^+(r_{ij}) &= -397.31\,\mathrm{MeV} \\ &\quad \exp\{-2.6272\,(r_{ij}-r_c)\}, \\ {}^3V_c^+(r_{ij}) &= -947.02\,\mathrm{MeV} \\ &\quad \exp\{-3.6765\,(r_{ij}-r_c)\}, \\ {}^1V_c^-(r_{ij}) &= {}^3V_c^-(r_{ij}) = 0 \quad (r_{ij} \geqq r_c)\,. \end{aligned} \tag{51}$$

In this special case the effective two-body potentials are

$$\begin{aligned} {}^3W_c^+(r) &:= \frac{\hbar^2}{m}\left(\frac{df}{dr}\right)^2 + f^2(r)\,{}^3V_c^+(r)\,, \\ {}^1W_c^+(r) &:= \frac{\hbar^2}{m}\left(\frac{df}{dr}\right)^2 + f^2(r)\,{}^1V_c^+(r) \end{aligned} \tag{52}$$

for the even states, and

$${}^1W_c^-(r) = {}^3W_c^-(r) := \frac{\hbar^2}{m}\left(\frac{df}{dr}\right)^2 \tag{53}$$

for the odd states. Instead of using the potentials (52) and (53) to evaluate the energy per particle it is more convenient to use the effective potentials $W_D(r)$ and $W_A(r)$ which are defined as

$$\begin{aligned} W_D(r) &:= 3\,{}^3W_c^+ + 9\,{}^3W_c^- + 3\,{}^1W_c^+ + {}^1W_c^-, \\ W_A(r) &:= -3\,{}^3W_c^+ + 9\,{}^3W_c^- - 3\,{}^1W_c^+ + {}^1W_c^-. \end{aligned} \tag{54}$$

For neutron matter we have

$$\begin{aligned} W_D(r) &:= ({}^1V_c^+ + 3\,{}^3V_c^-)f^2 + 4\,\frac{\hbar^2}{m}\left(\frac{df}{dr}\right)^2, \\ W_A(r) &:= (-{}^1V_c^- + 3\,{}^3V_c^-)f^2 + 2\,\frac{\hbar^2}{m}\left(\frac{df}{dr}\right)^2. \end{aligned} \tag{55}$$

There are two main reasons for choosing the OMY potential in our calculations:

(a) There have already been extensive nuclear matter studies[14, 42] with the use of this potential.

(b) For the OMY (and also for the IY) potential, the parameters ξ and $\varkappa$ are uncomfortably large (about twice that for the realistic Reid soft-core potential). Therefore we can expect a significant effect of the renormalization procedure.

As pair-correlation function $f(r)$ of Eq. (3) we adopt the three-parameter form:

$$f(r) = \begin{cases} 0 \quad (r \leqq r_c)\,, \\ [1-\exp\{-\mu_1(r-r_c)\}] \\ \cdot[1+\lambda\exp\{-\mu_2(r-r_c)\}]\,. \end{cases} \tag{56}$$

To see the influence of the average Pauli condition on the equilibrium energy of the nuclear matter system we choose two different procedures to determine the three parameters μ_1, μ_2 and λ. In the second procedure we disregard the average Pauli condition.

First procedure

a) The class of correlation functions is restricted by choosing $\mu_1 = \mu_2 =: \mu$.

b) The parameter λ is determined so as to fulfill the average Pauli condition.

c) Then, we find μ by minimizing $E_R^{[3.3]}(k_F, \mu)$ with respect to μ in the density region $k_F = 1.2 - 1.4\,\mathrm{fm}^{-1}$ (at higher densities we can not find an energy minimum). For these densities, the obtained values of $g_R^{[3,3]}(\infty)$ are in the vicinity of 0.981. Therefore, we finally re-determine μ at all densities ($k_F = 1.2 - 1.8\,\mathrm{fm}^{-1}$) by requiring $g_R^{[3,3]}(k_F, \mu, \infty) = 0.981$.

The conditions a) – c) uniquely define the three parameters in $f(r)$.

Second procedure

α) Again we restrict the class of correlation functions by choosing $\mu_1 = \mu_2 = : \mu$.

β) The parameter μ is fixed by requiring $g_R^{[3,3]}(k_F, \infty) = 1.000$.

γ) The parameter λ is obtained by finding the minimum of $E_R^{[3,3]}(k_F, \lambda)$ for each k_F.

We note that in the second procedure the conditions $\alpha) - \gamma)$ can be almost completey fulfilled for all density values $k_F = 1.2 - 1.8\,\mathrm{fm}^{-1}$ with a fixed parameter set, for example $\mu = 2.10$ and $\lambda = 1.45$. This is a case of special interest: The correlation functions now do not depend on the density and therefore the single-particle energies (see Ref. 20) do fulfill the theorem of Hugenholtz-Van Hove [43]. On the other hand we violate the average Pauli condition with the second procedure. But as we can see from Table 9 this violation is insignificant.

For neutron matter we proceed as follows:

(1) We choose $\mu_1 = \mu_2 = : \mu$.

(2) The parameter λ is determined by the average Pauli condition.

(3) We use the parameter μ to get $g_R^{[3,3]}(k_F, \infty) = 1.000$.

4.2. Results and Discussion

(a) Nuclear Matter

The results for the binding energy per particle are displayed in Figs. 3 and 4 and in Tables 6 and 7. In Tables 8 and 9 we show the results of the quantities most important for the (F)IY-expansions.

Table 7. Nuclear Matter: C2 and $\mu = 2.10$, $\lambda = 1.45$ and $g_R^{[3.3]}(\infty) \approx 1.000$.

k_F [fm^{-1}]	μ	E_0 [MeV]	$(\Delta E)_2$ [MeV]	$(\Delta E)_3^{(2)}$ [MeV]	$(\Delta E)_3^{(3)}$ [MeV]	$(\Delta E)_3$ [MeV]
1.20	2.10	17.915	−27.91	5.783	−6.58	−0.79
1.30	2.10	21.025	−32.85	8.893	−9.89	−1.00
1.40	2.10	24.384	−37.81	13.050	−14.08	−1.03
1.50	2.10	27.992	−42.69	18.380	−19.08	−0.70
1.54	2.10	29.505	−44.58	20.862	−21.27	−0.40
1.60	2.10	31.849	−47.35	24.969	−24.69	0.28
1.70	2.10	35.955	−51.69	32.848	−30.59	2.26
1.80	2.10	40.309	−55.61	41.982	−32.29	5.69

We note that the binding energies of the unrenormalized energy approximations reproduce the empirical value (−16 MeV) fairly well. For the renormalized expansion this agreement is valid only for the second procedure. But in both procedures the equilibrium densities are too high ($k_F^{eq.} = 1.58 - 1.60\,\mathrm{fm}^{-1}$). One can imagine that one of the reasons for this deviation is the missing tensor component of the potential. A certain simulation of the tensor force by a relatively large hard core radius, density-dependent effective potentials and a strong triplet-even attraction is not sufficient.

From Fig. 3 we see the reason for the divergence in the high-density region of the unrenormalized energy curves corresponding to the two different procedures. In the second procedure the three-body effects are essentially less attractive and become

Table 6. Nuclear Matter: C2 and PC with $g_R^{[3,3]}(\infty) = 0.981$.

k_F [fm^{-1}]	μ	E_0 [MeV]	$(\Delta E)_2$ [MeV]	$(\Delta E)_3^{(2)}$ [MeV]	$(\Delta E)_3^{(3)}$ [MeV]	$(\Delta E)_3$ [MeV]	$E_R^{[3,2]}$ [MeV]	$E_R^{[3,3]}$ [MeV]
1.20	2.00	17.92	−27.73	7.522	−8.45	−0.93	−10.15	−9.97
1.30	1.90	21.03	−32.12	11.502	−13.19	−1.69	−11.61	−11.53
1.40	1.80	24.38	−36.20	16.907	−19.64	−2.73	−12.45	−12.73
1.50	1.75	27.99	−40.40	23.835	−27.35	−3.51	−12.77	−13.50
1.54	1.72	29.505	−41.86	27.157	−31.07	−3.91	−12.56	−13.61
1.56	1.72	30.277	−42.76	28.883	−32.80	−3.91	−12.52	−13.63
1.60	1.70	31.849	−44.26	32.624	−36.75	−4.13	−12.15	−13.56
1.70	1.655	35.955	−47.76	43.425	−47.71	**−4.29**	−10.50	−12.75
1.80	1.615	40.309	−50.84	56.405	−60.06	−3.65	−7.72	−10.87

Table 8. Nuclear Matter: C2 and PC with $g_R^{[3,3]}(\infty)=0.981$.

k_F [fm^{-1}]	μ	λ	$\varkappa, \xi$	ξ_3	$z_Q^{[2]}$	$z_Q^{[3]}$	$g_Q^{[3,3]}(\infty)$	$g_R^{[3,3]}(\infty)$	$g_Q^{[4,3]}(\infty)$
1.20	2.00	1.45	0.136	0.010	0.892	0.889	0.982	0.982	0.999
1.30	1.90	1.42	0.180	0.004	0.865	0.865	0.980	0.980	1.000
1.40	1.80	1.40	0.234	−0.013	0.836	0.839	0.981	0.981	1.001
1.50	1.75	1.39	0.295	−0.034	0.808	0.814	0.980	0.980	1.004
1.54	1.72	1.386	0.324	−0.049	0.795	0.803	0.982	0.982	1.005
1.56	1.72	1.386	0.338	−0.052	0.790	0.798	0.980	0.980	1.006
1.60	1.70	1.382	0.368	−0.067	0.777	0.788	0.981	0.981	1.007
1.70	1.655	1.374	0.453	−0.113	0.747	0.762	0.982	0.982	1.013
1.80	1.615	1.368	0.551	−0.173	0.717	0.736	0.981	0.981	1.020

Table 9. Nuclear Matter: C2 and $\mu=2.10$, $\lambda=1.45$ and $g_R^{[3,3]}(\infty)\approx 1.000$.

k_F [fm^{-1}]	$\varkappa$	ξ	ζ	ξ_3	$z_Q^{[2]}$	$z_Q^{[3]}$	$g_Q^{[3,3]}(\infty)$	$g_R^{[3,3]}(\infty)$	$g_Q^{[4,3]}(\infty)$
1.20	0.133	0.104	−0.0143	−0.008	0.913	0.916	0.999	0.999	1.001
1.30	0.169	0.136	−0.0167	−0.014	0.892	0.896	0.998	0.998	1.001
1.40	0.213	0.173	−0.0197	−0.024	0.869	0.875	0.998	0.998	1.002
1.50	0.263	0.216	−0.0235	−0.037	0.846	0.854	0.998	0.998	1.004
1.54	0.285	0.235	−0.0253	−0.044	0.836	0.846	0.999	0.999	1.004
1.60	0.321	0.264	−0.0283	−0.057	0.822	0.833	0.999	0.999	1.006
1.70	0.387	0.318	−0.0346	−0.084	0.798	0.812	1.001	1.001	1.009
1.80	0.462	0.377	−0.0425	−0.122	0.774	0.793	1.005	1.005	1.013

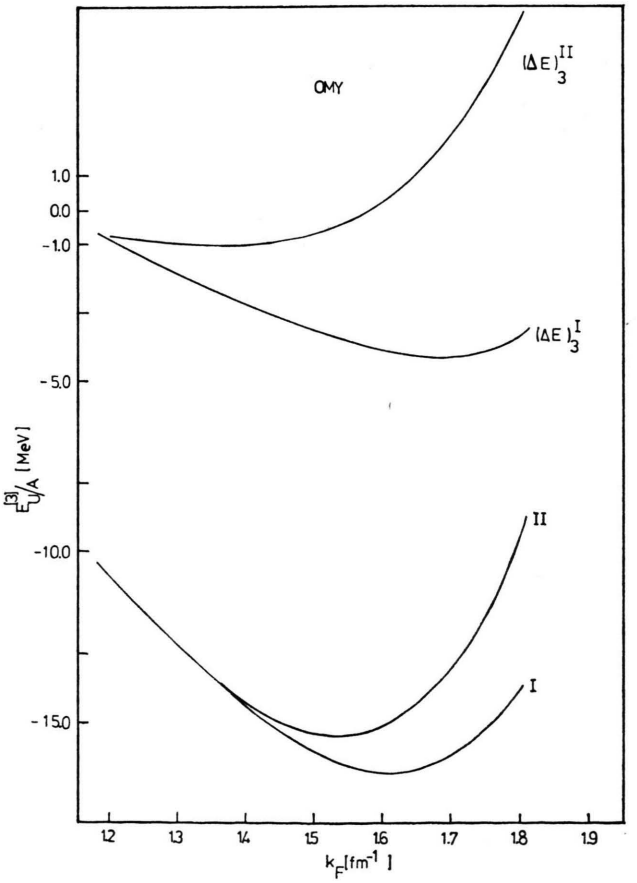

Fig. 3. Nuclear Matter. $E_U^{[3]}$ in dependence on k_F for two different procedures: I) $g_R^{[3,3]}(\infty)=0.981$ and the average Pauli condition is fulfilled; II) $g_R^{[3,3]}(\infty)\approx 1.000$ and $\mu=2.10$ and $\lambda=1.45$ for each density.

strongly repulsive above $k_F \approx 1.58\,\mathrm{fm}^{-1}$, because of the influence of the correlation function with shorter range. The absolute magnitude of $(\Delta E)_3{}^{(2)}$ and $(\Delta E)_3{}^{(3)}$ are very large (in special cases even larger than $|(\Delta E)_2|$). Because they have opposite signs they cancel to give a small contribution $(\Delta E)_3$ (in maximum, 10% of the two-body contribution). Therefore $(\Delta E)_2$ mainly contributes to the binding energy.

In the renormalized expansion of E the situation is drastically changed. The ratio $|(z_Q^{[3]})^2(\Delta E)_2/(z_Q^{[3]})^3(\Delta E)_3{}^{(3)}|$ turns out to be between 1/5 and 1 for both procedures, i. e., the renormalized three-hole-line contributions to the energy can be as large as the two-body terms in the most unfavourable case (this happens for high densities). The saturation property in such situations is obtained by the repulsion of the kinetic energy. Because of the bad numerical convergence of the renormalized approximation of the energy expectation value, we at least must take into account higher-order cluster contributions.

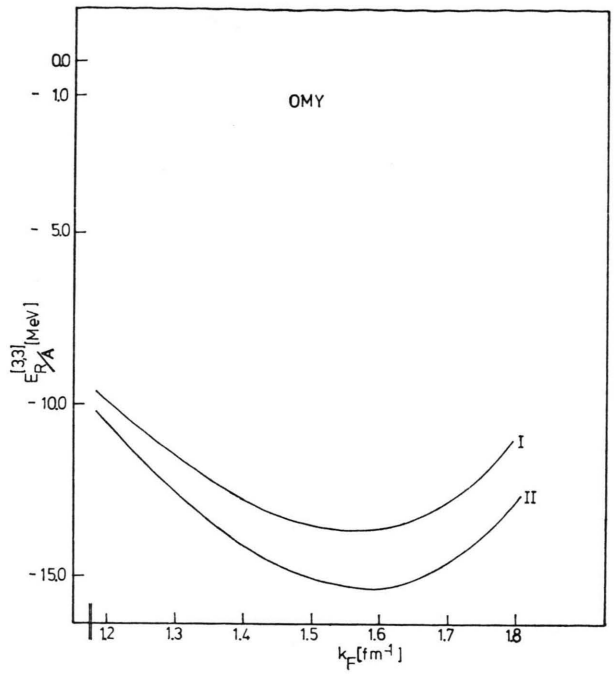

Fig. 4. Nuclear Matter. Density dependence of $E_R^{[3,3]}$. The denotation I) and II) is explained below Figure 3.

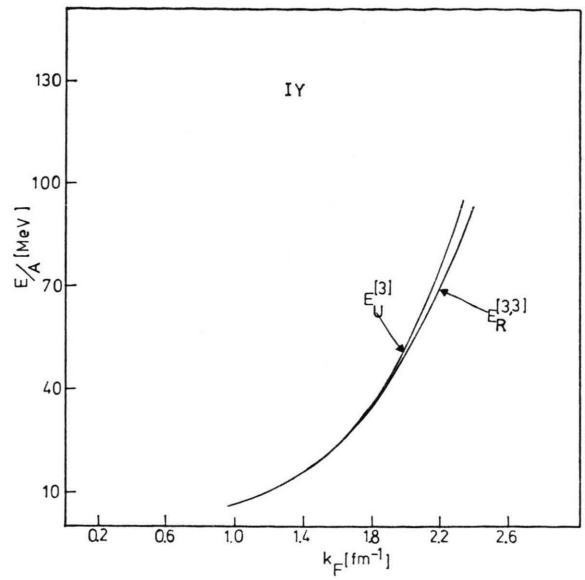

Fig. 5. Neutron Matter. $E_U^{[3]}$ and $E_R^{[3,3]}$ in dependence on k_F .

(b) Neutron Matter

The energy per particle of neutron matter ($1.00 \leqq k_F \leqq 2.60\,\mathrm{fm}^{-1}$) is presented in Figure 5. Table 10 shows the results for the "smallness-parameter" $\varkappa$, the "ordering-parameter" ξ, the averaged weight functions $z_Q^{[2]}$, $z_Q^{[3]}$, the asymptotic values of the radial distribution function and the contributions from the different terms of the energy expansions.

We note that in the lower density region ($k_F \leqq 1.8\,\mathrm{fm}^{-1}$) the approximated energies $E_R^{[3,3]}$ and $E_U^{[3]}$ are in very good agreement while they deviate from each other with increasing density. At $k_F = 2.60\,\mathrm{fm}^{-1}$ this deviation already amounts to 30 MeV. For densities below $k_F = 1.70\,\mathrm{fm}^{-1}$ the three-body effects are negligibly small compared with $(\Delta E)_2$. For higher densities they increase to be comparable to $(\Delta E)_2$. This tendency corresponds to the behavior of ξ and ξ_3. At $k_F = 1.50\,\mathrm{fm}^{-1}$ ξ reaches the value 0.1 but then grows up to a size of the ^{3}He "ordering-parameter" at $k_F = 2.40\,\mathrm{fm}^{-1}$. ξ_3 is negligibly small in the lower density region. Above $k_F \approx 1.5\,\mathrm{fm}^{-1}$ both approximations $E_R^{[3,3}$ and $E_U^{[3]}$ of the energy expectation value result in much higher energy values than one should expect for the "true" ground-state energy [14]. We recall the fact that the IY potential is of "Serber"-type. Therefore the IY potential is applicable to low energies where the even-states dominate. But, for higher energies at which the odd-states become important the IY potential is inadequate.

Table 10. Neutron Matter results.

k_F [fm^{-1}]	μ	λ	$\varkappa, \xi$	ξ_3	$z_Q^{[2]}$	$z_Q^{[3]}$	$g_Q^{[4,3]}$	E_0 [MeV]	$(\Delta E)_2$ [MeV]	$(\Delta E)_3^{(2)}$ [MeV]	$(\Delta E)_3^{(3)}$ [MeV]	$E_R^{[3,2]}$ [MeV]
1.00	2.10	1.413	0.027	−0.000	0.975	0.975	1.000	12.441	−4.933	0.260	−0.403	7.378
1.20	2.30	1.447	0.045	−0.001	0.959	0.959	1.000	17.915	−6.604	0.582	−0.803	11.126
1.40	2.30	1.440	0.073	−0.005	0.936	0.938	1.000	24.384	−7.763	1.116	−1.342	16.464
1.60	2.30	1.439	0.112	−0.012	0.907	0.911	1.001	31.849	−7.733	1.714	−1.420	24.397
1.80	2.28	1.437	0.166	−0.024	0.874	0.880	1.002	40.309	−6.030	2.001	0.044	35.740
2.00	2.20	1.427	0.239	−0.047	0.834	0.844	1.005	49.764	−2.679	1.411	4.674	50.718
2.20	2.07	1.411	0.341	−0.092	0.788	0.804	1.012	60.215	2.279	−1.094	15.118	69.377
2.40	1.96	1.399	0.474	−0.155	0.741	0.763	1.026	71.661	9.734	−8.168	36.404	92.470
2.60	1.85	1.388	0.648	−0.255	0.692	0.721	1.052	84.102	19.553	−23.355	74.985	119.318

5. Conclusions

In the last two sections we have investigated the renormalized and unrenormalized Iwamoto-Yamada expansions of the energy expectation value for ^{3}He, nuclear matter and neutron matter. Comparing the results of these systems, we stress the following points:

(1) The values of the parameters $\varkappa$ and ξ are small (cf. Table 10) for neutron matter in the "lower" density region: $k_F \leqq 1.80\,\mathrm{fm}^{-1}$. They become larger in nuclear matter and reach a considerable size (~ 0.63) in ^{3}He.

(2) The three-body (and higher) correlations ξ_3 have to be taken into account in ^{3}He and for high densities also in neutron matter.

(3) Depending on the magnitudes of ξ and ξ_3 the weight functions z_Q take values between 0.975 in neutron matter and 0.679 in ^{3}He.

(4) Imposing of the auxiliary condition on $g_R^{[3,3]}(\infty)$ to be equal to 1.000 [the "true" value of $g(\infty)$] gives a considerable increase of the binding energy in the nuclear matter system whereas this condition leads to no binding in ^{3}He.

Above all, we can say that for dense systems such as ^{3}He, nuclear matter and neutron matter at high densities the clustre effects of higher order ($n \geqq 3$; for the energy expectation value as well as for the particle-correlations) become very important. In addition, it must be emphasized that in ^{3}He the long-range correlations due to the longer range character of the potential play a more important role than in nuclear matter and neutron matter. One should use state-dependent particle-correlations, especially for systems with state-dependent potentials. In order to improve the asymptotic behavior of the approximated radial distribution function, we suppose that it is also necessary to generalize the BDJ-Ansatz in a "natural" way

$$F(1,2,3,\ldots,A) = \prod_{i<j} f_2(i\,j) \prod_{i<j<k} f_3(i\,j\,k) \cdot \prod_{i<j<k<l} f_4(i\,j\,k\,l) \ldots \qquad (57)$$

and to include, at least, three-body correlations $f_3(i\,j\,k)$.

Despite the fact that our numerical result of the renormalized and unrenormalized energy expansions are encouraging, we are not able to draw any quantitative and definite conclusions. Further numerical as well as "formal" studies of the convergence problem might help to proceed a step further.

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