Renormalized and Unrenormalized Jastrow Expansions of the Liquid Structure Function for Dense Fermi Liquids

Jürgen Nitsch

Institut für Theoretische Physik der Universität zu Köln, Germany

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We present approximate representations of the liquid structure function S(k) for Fermi systems in the framework of the renormalized and unrenormalized Jastrow theory. Using short range correlations we study the behavior of S(k) in the range of low momenta and compare our numerical results with the experimental data of the liquid structure function of liquid ³He. We conclude that the usual Jastrow ansatz $\Psi = \prod_{i=1}^{n} f(r_{ij})\Phi$ for the trial wave function of a dense Fermi system,

together with an application of the cluster expansion method developed by Clark and Westhaus, does not sufficiently describe these systems. Improvements are discussed.

1. Introduction

The liquid structure function plays an important role in describing classical as well as quantum liquids. Several experiments 1, 2, 3 have been made to determine the structure function of liquid helium. For liquid ³He, neutron-scattering experiments are not feasible, because of the efficiency with which neutrons are absorbed by 3He nuclei. X-ray scattering experiments, however, have been carried out by Achter and Meyer² and by Hallock³ who determined the liquid structure function of ³He at low temperatures over a wide range of momenta. Therefore, both types of liquid helium, Fermi 3He and Bose 4He, form a suitable testing ground for manybody techniques used in dense neutron star matter, and hence it is of special interest to compare the results of a calculation of the liquid structure function with experimental data. Also, for the purpose of a variational description of the ground state 4 and of the transport properties 5 of neutron - and of neutron star - matter, one needs to know the structure function of the corresponding system. Unfortunately, in this case there is no direct experimental proof for the liquid structure function.

We present in this paper an approximate representation of the radial distribution function and, thereby, of the static liquid structure function in the framework of the renormalized and unrenormalized extended Jastrow theory. In doing so, we rely heavily on the definitions and on the notations we presented in a previous work ⁶ on the application of the CBF-method on Fermi systems.

Reprint requests to Dr. J. Nitsch, Institut für Theoretische Physik der Universität zu Köln, *D-5000 Köln 41*, Zülpicher Str. 77.

Since spatial correlations are supposed to be the most important correlations in dense Fermi fluids, the common Jastrow ansatz

$$\Psi = F \Phi$$
, $F = \prod_{i < j} f(r_{ij})$, $\eta(r) := f^2(r) - 1$ (1)

has turned out to be suitably adapted for calculating the expectation value of the Hamiltonian H = T + V with respect to the correlated state (1)

$$E := \langle H \rangle = \langle \Psi \mid H \mid \Psi \rangle / \langle \Psi \mid \Psi \rangle . \tag{2}$$

Here Φ is a model wave function which embodies statistical correlations and represents the ground state wave function of a gas of A independent fermions, whereas the correlation operator F usually is assumed to be of short range, due to the repulsive part of the potential. The expectation value (2) can be evaluated in a cluster expansion employing the well-established Iwamoto-Yamada procedure 7 or its factorized version 6 (FIY-expansion). Such expansions have been truncated at the two- or three-body level and yielded reliable results for the ground state energy 4, 6-8 of nuclear matter and of neutron matter up to the range of normal nuclear densities. In the region of higher densities in neutron matter and for ³He this procedure seems to be insufficient and a more accurate many-body method has to be applied, with emphasis on admitting long range and at least three-body correlations. In recent papers 9, 10 Krotscheck developed further the conventional Jastrow theory in a very promising way, adopting diagrammatic techniques which initially have been used by Gaudin et al. 11. This new description of equilibrium (and hopefully also transport-) properties of dense Fermi as well as Bose systems allows the occurence of even long range correlations in a rearranged



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cluster expansion of the expectation value of a certain physical operator (e.g. the Hamiltonian H) according to the number of correlation lines (see also Ref. ¹²). The long range part of the correlations is closely related to the behavior of the static structure function in the range of low momenta ⁹.

In Section 2 we study the approximants of the radial distribution function and thereby those of the related liquid structure function derived from a truncated FIY-expansion of the energy expectation value. We only take into account short range correlation (i.e. $f(r) \sim r^{-n}$ if $r \to \infty$; $n \ge 4$) so that the slope of the structure function for small momenta behaves like the structure function of a free Fermi gas. Furthermore, we discuss the renormalized and unrenormalized FIY-representations of the structure function at zero momentum.

The final section, Section 3, is devoted to a discussion of our results.

2. Radial Distribution Function and Static Structure Function

A general starting-point for defining the radial distribution function g(r) and the structure function S(k) as well as for learning their properties is the set of n-particle distribution functions ¹³

$$= \frac{\frac{p^{[n]}(1,2,\ldots,n):}{A(A-1)\ldots(A-n+1)\sum\limits_{\{\sigma,\tau\}}\int |\Psi|^2 d^3r_{n+1}\ldots d^3r_{\rm A}}}{\sum\limits_{\{\sigma,\tau\}}\int |\Psi|^2 d^3r_{1}\ldots d^3r_{\rm A}},$$

where the sum $\sum_{\{\sigma,\tau\}}$ is extended over all spin and isospin coordinates. From this definition the "normalization condition" for $p^{[2]}(1,2)$ reads:

$$(A-1)^{-1}\int \mathrm{d}^3r_2\,p^{[2]}(1,2)=A\,\Omega^{-1}=\varrho=p^{[1]}$$

or, equivalently,

$$\varrho^{-1} \int (p^{[2]}(1,2) - \varrho^2) d^3r_2 = -1.$$
 (4)

The quantity ϱ is the particle density which is related to the Fermi wave number $k_{\rm F}$ by the expression $\varrho = \nu \, (6 \, \pi^2)^{-1} \, k_{\rm F}^3$ where the factor ν gives the degeneracy of the single particle states ($\nu = 2$ for neutron matter or ³He, $\nu = 4$ for nuclear matter). In a homogeneous system $p^{[2]}(\pmb{r}_{12})$ does not depend on the direction of the space-vector \pmb{r}_{12} . In this case, one usually defines the radial distribution function as

$$g(r) := \varrho^{-2} p^{[2]}(r)$$
. (5)

Using this definition in Eq. (4) we obtain

$$\varrho \int d^3r \left(g(r) - g(\infty) \right) + A \left(g(\infty) - 1 \right) = -1 \qquad (6)$$

The static structure function is closely related to g(r) by

$$S(k) := \begin{cases} 1 + \varrho \int d^3 r \, g(r) \, e^{i \, k \, r} & (k \neq 0), \\ S(0+) & (k=0). \end{cases}$$
 (7)

Together with the "normalization condition" (4) we thus find the following relation

$$S(0) = A \left(1 - g(\infty) \right). \tag{8}$$

For the true ground state it is well known that according to the "structure-factor sum rule" the equation

$$S(0) = 0 \tag{9}$$

holds. In a previous paper ⁶ it was shown that Eq. (9) is fulfilled for each test wave function of type (1), admitting a FIY-expansion of the energy expectation value. However, a truncated FIY-cluster expansion for the energy expectation value does not lead to a corresponding approximation of the liquid structure function which automatically fulfills Equation (9). It is nonetheless possible to restrict the class of the correlation operators such that the sum rule (9) holds in each order of the truncated cluster expansion ¹⁴.

We get the FIY-expansion of the radial distribution function, extracting the term

$$\frac{1}{2} \varrho \int \mathrm{d}^3 r \, g(r) \, v'(r) \tag{10}$$

from the FIY-expansion of the energy expectation value. Here v'(r) is the state-independent (JLST-independent), local, central component of the two-body potential v (12). We employ this procedure to construct the renormalized approximants $g_{\rm R}^{\rm [2]}$ and $g_{\rm R}^{\rm [3]}$ of

$$g_{\mathbf{R}}(r) := A^{-2} \sum_{ij} z_i^{0} z_j^{0} (\Delta g)_{ij}$$

$$+ A^{-3} \sum_{iik} z_i^{0} z_j^{0} z_k^{0} (\Delta g)_{ijk} + \dots \quad (11)$$

and obtain the results:

$$g_{\mathbf{R}}^{[2]}(r) := A^{-2} \sum_{ij} z_i^0 z_j^0 (\Delta g)_{ij}$$
 (12)

with

$$(\Delta g)_{ij} = f^2(r) \left\{ 1 - \nu^{-1} \, j_0(k_i \, r) \, j_0(k_j \, r) \right\}$$

and

$$g_{\mathbf{R}}^{[3]}(r) := g_{\mathbf{R}}^{[2]}(r) + A^{-3} \sum_{ijk} z_i^0 z_j^0 z_k^0 (\Delta g)_{ijk}$$
 (13)

with

The function j_0 is the spherical Bessel function

$$j_0(x) = x^{-1}\sin(x)$$
. (14)

The unrenormalized approximants $g_{\overline{U}}^{[2]}(r)$ and $g_{\overline{U}}^{[3]}(r)$ of the radial distribution function are derived from the renormalized ones by inserting the unrenormalized expansion of the weight functions z_i^0, z_j^0, \ldots (cf. Ref. 6) in Eq. (11) and taking into consideration all the contributions up to the required number of hole-lines n (i.e. n=2 for $g_{\overline{U}}^{[2]}(r)$ and n=3 for $g_{\overline{U}}^{[3]}(r)$). Thus we find for the simplest unrenormalized approximation of g(r)

$$g_{\rm U}^{[2]}(r) = f^2(r)g_{\rm F}(r)$$
. (15)

The function $g_{\rm F}(r)$ is the familiar distribution function of a gas of independent fermions:

$$g_{\rm F}(r) = 1 - \nu^{-1} l^2(r k_{\rm F}),$$

 $l(x) = 3 x^{-3} (\sin(x) - x \cos(x)).$ (16)

The asymptotic behavior of the renormalized radial distribution functions $g_{\mathbf{R}}^{[n]}(r)$ is quite different from that of their unrenormalized pendants $g_{\mathbf{U}}^{[n]}(r)$. In each order n (n refers to the maximal number of hole-lines involved in the cluster expansion considered) of the cluster expansion we observe:

$$\lim_{r \to \infty} g_{\mathrm{U}}^{[n]}(r) = 1. \tag{17}$$

Investigating the renormalized approximants $g_{\mathbf{R}}^{[n]}$ (r) we arrive at the result *

$$g_{\mathbf{R}}^{[n]}(\infty)|_{O(A^{\mathbf{o}})} = \left(A^{-1} \sum_{k} z_{k} \frac{\delta(\Omega \chi)}{\delta z_{k}}\right)^{2} \Big|_{\substack{z_{k}=z_{k} \\ \beta=0}}^{[n]} . \tag{18}$$

Here, the superscript n of the right hand side of this equation refers to the maximal number of holelines which have to be involved after squaring the functional in brackets, i.e. contributions with (n+1),

(n+2), ... hole-lines have to be omitted. We then deduce the following expressions choosing n=2 and n=3:

$$g_{\mathbb{R}}^{[2]}(\infty) = (A^{-1} \sum_{i} z_{i}^{0})^{2} = : z_{\mathbb{Q}}^{2}$$
 (19)

and

$$g_{\rm R}^{[3]}(\infty) = z_{\rm Q}^2 + 2 \, z_{\rm Q} \, A^{-1} \, \sum_{ik} z_j{}^0 \, z_k{}^0 \, \eta_{jk}(0) \; . \eqno(20)$$

The results could have also been gathered from Eqs. (12) and (13).

It is now easy to define the approximants $S^{[n]}(k)$ of the liquid structure function by:

$$S_{\mathrm{R,U}}^{[n]}(k) := 1 + \varrho \int \mathrm{d}^3 r \left(g_{\mathrm{R,U}}^{[n]}(r) - g_{\mathrm{R,U}}^{[n]}(\infty) \right) e^{i \, kr}.$$
 (21)

In the lowest cluster order of the unrenormalized version this equation can be written for zero wave number

$$S_{\rm T}^{[2]}(0) = o \int d^3 r (f^2(r) - 1) q_{\rm E}(r) = : \xi.$$
 (22)

For n = 3 we obtain

$$S_{\mathbf{U}}^{[3]}(0) = -\xi - 2A^{-1} \sum_{ijk} \eta_{ij} \eta_{jk} + A^{-1} \sum_{ijk} \eta_{ijk},$$
(23)

using the relations

$$\int l^{2}(r' k_{F}) d^{3}r' = \varrho^{-1} \nu,
\int d^{3}r' l(r' k_{F}) l(k_{F} | \mathbf{r} - \mathbf{r}' |) = \varrho^{-1} \nu l(r k_{F}).$$
(24)

We notice that $S_{\rm U}^{[3]}(0)$ still embodies a term of the order $O(\xi)$. In the corresponding expansion of the structure function with respect to *independent* holelines ⁷ [Iwamoto-Yamada (IY)-expansion] all contributions of the order $O(\xi)$ cancel each other. In our FIY-scheme, however, only $S_{\rm U}^{[4]}(0)$ is of the order $O(\xi^2)$.

 $S_{\rm R}^{[3]}(0)$ can be approximated in a simple analytical form by the "quasi-classical" expression $S_{\rm Q}^{[3]}(0)$ which we obtain by inserting $z_{\rm Q}$ in $S_{\rm R}^{[3]}(0)$. Integration of Eq. (21) leads to the result ¹⁶:

^{*} It is possible to rearrange the cluster expansion for the renormalized radial distribution function to achieve the asymptotic values $\tilde{g}_{R}^{(n)}(\infty)$ of the "new" expansion to become unity ¹⁵.

$$S_{\rm Q}^{[3]}\left(0\right)=\left(1-z_{\rm Q}^{2}\right)\,+z_{\rm Q}^{2}\,\xi+z_{\rm Q}^{3}\left(-4\,\xi+\xi_{3}\right)\,. \tag{25}$$

The averaged quantity ξ_3 is related to the three-body correlation matrix element by

$$\xi_3 := A^{-1} \sum_{ijk} \eta_{ijk}(0) . \tag{26}$$

For the application of the FIY-expansion method, the unrestricted minimalization of the truncated energy expectation values $E_{\mathrm{U,R}}^{[2]}$ and $E_{\mathrm{U,R}}^{[3]}$ with respect to f(r) leads to a non-converging cluster series. This difficulty can be avoided by imposing subsidiary conditions on the correlation functions. In our study of the Fermi liquids ³He, nuclear matter and neutron matter we have imposed two subsidiary conditions on the parametrized correlation function which are described in Reference 6. In the ³He calculations it turned out (by comparison of the numerical results) that the restrictions on f(r) which were used could have been replaced by the following two requirements:

(1)
$$\zeta := A^{-1} \sum \langle ij | (f(12) - 1) | ij \rangle_a = 0,$$
 (27)

(2)
$$S_{\Omega}^{[3,3]}(0) = 0$$
. (28)

Now, since we know that the sum rule S(0) = 0 is valid ^{6, 9} for each trial wave function (1), we may be led to impose Eq. (28) on $S_{\mathbf{Q}}^{[3,3]}(k)$ as a possible constraint.

3. Results and Discussion

The results for the liquid structure functions $S_{\mathbf{U}}^{[3]}(k)$ and $S_{\mathbf{R}}^{[3,3]}(k)$ of the Fermi system ³He are displayed in Figures 1 and 2. In Figures 3 and 4 we show the radial distribution functions $g_{\mathbf{U}}^{[3]}(r)$ and $g_{\mathbf{R}}^{[3,3]}(r)$ of liquid ³He. Since we are able to compare our ³He results with the experimental data of ³He-X-ray experiments ² we confine ourselves to show exclusively our results for ³He in Figures 1 to 4. We have also calculated the approximate structure functions $S_{\mathbf{U}}^{[3]}(k)$ and $S_{\mathbf{R}}^{[3,3]}(k)$ for nuclear matter. These results are presented in Reference 16. In our discussion, however, we want to include the nuclear matter system.

From Fig. 1 we expect that the value of $S_{\mathrm{U}}^{[3]}(0)$ differs strongly (the numerical result is $S_{\mathrm{U}}^{[3]}(0)\approx -1.3$) from the exact result, contrary to the value of $S_{\mathrm{R}}^{[3,3]}(0)$ which equals almost zero. The latter result is not too surprising since the parameter set of the two-body correlation function is restricted

to fulfill Equation (28). The reason for the deviation of $S_{\mathbb{U}}^{[3]}(0)$ from the value zero is to be seen on account of omitting $(\Delta E)_4^{(2)\mathbb{R}}$ and possibly higher order cluster contributions in the approximate evaluation of the energy expectation value. In the region of low momenta k, however, the static structure function $S_{\mathbb{U}}^{[3]}(k)$ behaves almost like the structure function $S_{\mathbb{F}}(k)$ of an uncorrelated Fermi system

$$S_{\rm F}(k) = \alpha_{\rm F} \cdot k \,, \ \alpha_{\rm F} = 3 (4 k_{\rm F})^{-1} \,.$$
 (29)

The particle correlations occur in $S_{\rm U}^{[3]}(k)$ only for larger k-values ($k \gtrsim 0.5 \,\text{Å}^{-1}$) changing the linear increase. This may be one of the reasons that $S_{IJ}^{[3]}(k)$ shows a very marked "shoulder" in the range of 0.5 to 1.0 Å⁻¹ (in Ref. ¹⁷ we find arguments for similar features of the structure function S(k) of liquid ⁴He). Since we know ^{9, 16} that only long range particle correlations $(f(r) \sim r^{-2}; r \to \infty)$ can influence the slope of S(k) in the range of low momenta, it is necessary for getting a better agreement between calculations and experiment to allow long range correlations in the Jastrow ansatz (1). Also for momenta k between $1.0 \,\text{Å}^{-1}$ and $2.5 \,\text{Å}^{-1}$ the structure functions $S_{II}^{[3]}(k)$ and $S_{R}^{[3,3]}(k)$ show much less structure than that gained by experimental data. For comparison, see Figures 1 and 2. However, these structure functions are in good agreement with experiment for larger k-values ($k \gtrsim 2.5 \,\text{Å}^{-1}$).

In the nuclear matter system the liquid structure functions $S_{\rm U}^{[3]}(k)$ and $S_{\rm R}^{[3,3]}(k)$ show the same qualitative behavior as those of ³He. In the range of low momenta the slope of $S_{\rm U}^{[3]}(k)$ differs from $\alpha_{\rm F}$ by the expression (which we present in terms of the radial distribution function)

$$-9\pi \varrho (k_{\rm F} r)^{-4} \int dr' r'^2 \eta(r') \cdot \{1 - 4^{-1} l(r' k_{\rm F}) j_0(r' k_{\rm F})\}, (30)$$

where we have adopted the three-parameter correlation function $\eta(r')$ of Bäckman et al. ^{16, 18}. From our numerical results we conclude that the contribution of expression (30) to the structure function is of such a small order of magnitude that the linear increase of $S_0^{(3)}(k)$ is well approximated by α_F . We have to emphasize, however, that the appearance of the term (30) in the radial distribution function $g_0^{(3)}(r)$ is a special feature of the FIY-expansion. In Reference 16 we have proved that the contribution (30) to the radial distribution function is cancelled in the corresponding IY-expansion. Therefore one gets instead of (23)

$$S_{\mathrm{U}|_{\mathrm{IY}}}^{[3]}(0) = 0 + O(\xi^2)$$
. (31)

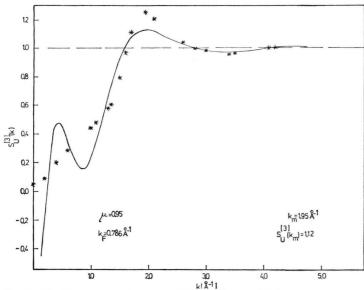
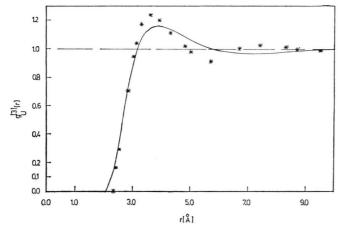


Fig. 1. Liquid structure function of liquid ${}^3\mathrm{He}$; solid line: unrenormalized Jastrow theory; stars: experimental data of Achter and Meyer. The structure function $S_{u}^{(3)}$ has its absolute maximum at $k\!=\!k_{\mathrm{m}}$. The pair-correlation-function f(r) used here is given in Reference 6.



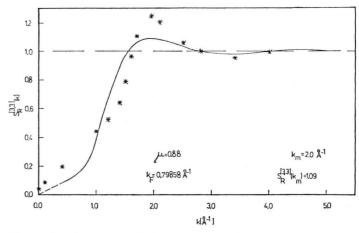


Fig. 2. The "renormalized" liquid structure function of liquid ³He versus momentum k. Dashed part: visual interpolation.

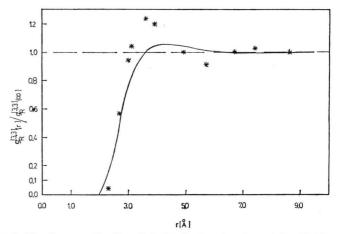


Fig. 4. The "renormalized" radial distribution function of liquid ³He at $k_{\rm F}$ =0.79858 Å⁻¹. The peak $(g_{\rm R}^{\rm [3,8]}\ (r_{\rm m})/g_{\rm R}^{\rm [3,3]}\ (\infty)$ =1.05) occurs at $r=r_{\rm m}$ =4.2 Å.

As far as the approximants $g_{U}^{[3]}(r)$ and $g_{R}^{[3,3]}(r)$ of the radial distribution function are concerned, we recognize from Figs. 3 and 4 a good agreement with the "experimental distribution function $g_{\text{exp.}}(r)$ " in the region up to ≈ 3.0 Å. Nevertheless, their maxima are too low, and their long range behavior strongly fails $g_{\text{exp.}}(r)$. The disagreement of $g_{\text{U}}^{[3]}(r)$ and $g_{\rm R}^{[3,3]}(r)$ with $g_{\rm exp.}(r)$ in the long range regime mainly results from the omission of long range particle correlations, while the discrepancies between the calculated and experimental values of the maxima of the radial distribution functions may particularly arise from the severe subsidiary conditions imposed on the Jastrow function f(r). In order to overcome the defects of the "FIY-radial distribution functions" mentioned above a more accurate many-body

¹ R. A. Cowley and A. D. B. Woods, Can. J. Phys. 49, 177 [1971].

E. K. Achter and L. Meyer, Phys. Rev. 188, 291 [1969].

³ R. B. Hallock, Phys. Rev. A 5, 320 [1972].

 M. Miller, C. W. Woo, J. W. Clark and W. J. Ter Louw, Nucl. Phys. A 184, 1 [1972].

⁵ E. Flowers, N. Itoh, preprint [1975].

⁶ J. Nitsch, Z. Naturforsch. 30 a, 923 [1975].

J. W. Clark and P. Westhaus, Phys. Rev. 141, 833 [1966]; D. A. Chakkalakal, Ph. D. Thesis, Washington University, 1968 (unpublished).

⁸ V. R. Pandharipanda, Nucl. Phys. A 174, 641 [1971];

A 178, 123 [1971].

⁹ E. Krotscheck, Phys. Lett. 54 A, 123 [1975].

method is called for. In a recent work ¹⁰ Krotscheck developed a method which enables us to deal with short — and long — range correlations in a quantum fluid, and the optimization procedure for the expectation value of the ground state energy (2) with respect to a correlated wave function (1) can be performed without the commonly used restrictions ^{7, 14} on the Jastrow two-body correlation function.

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10 E. Krotscheck, preprint [1975].

M. Gaudin, J. Gillespie and G. Ripka, Nucl. Phys. A 176, 237 [1971].

¹² E. Krotscheck, Dissertation, Köln 1974.

18 E. Feenberg, Theory of Quantum Fluids, Academic Press, New York 1969.

¹⁴ G. P. Mueller, Nucl. Phys. A 210, 544 [1973].

¹⁵ T. L. Hill, Statistical Mechanics, McGraw-Hill, New York 1956.

¹⁶ J. Nitsch, Dissertation, Köln 1974.

¹⁷ W. E. Massey, Phys. Rev. **151**, 153 [1966].

¹⁸ S.-O. Bäckman, D. A. Chakkalakal and J. W. Clark, Nucl. Phys. A 130, 635 [1969].