Journal of Theoretical and Applied Physics, **5**-2, 77-81 (2011)

Spin-dependent correlations of fermi liquids at nonzero temperatures within correlated density-matrix approach

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Received: 11 July 2011/Accepted: 10 September 2011/ Published: 20 September 2011

Abstract

Correlated density matrix theory is generalized to investigate equilibrium properties of normal Fermi Liquids such as ^{3}He and nuclear matter at nonzero temperatures. The results also generalize the Fermi-hypernetted-chain technique that is familiar from studies of the ground state of correlated fermions. By employing the concept of renormalized bosons and fermions the formal results are cast in a form that permits the direct evaluation of the statistical properties of the correlated liquid such as the entropy and the specific heat at constant volume among other quantities.

PACs: 61.20.-p; 61.25.EM.
Keywords: *Fermi liquids; density-matrix theory; spin correlations.*

1. Introduction

Correlations in normal liquid helium and in nuclear matter are of long standing interest. Numerous studies have been performed to analyze the ground and excited states of normal liquid ^{3}He, nuclear and neutron matter with various quantum many-body approaches such as lowest order constrained techniques, cluster expansion methods, hypernetted-chain summation etc. Two very recent examples are provided in Refs [1, 2] that also present an exhaustive list of references to earlier work.

In this paper we concentrate on the generalization and further development of Correlated Density Matrix (CDM) theory adapting it to pursue a sophisticated analysis and enumeration of the equilibrium properties and correlation functions of such Fermi liquids.

Correlated Density Matrix theory [3] of interacting Bose fluids or liquids is a profound tool to analyze strong spatial correlations and thermal gross properties of boson systems. The algorithm has been applied successfully for a quantitative enumeration of physical quantities of liquid para-hydrogen [4] and for normal liquid ^{4}He [5] at nonzero temperatures. It has been demonstrated theoretically and experimentally [6] that the hydrogen liquid can be described (quantitatively) as a quantum Boltzmann liquid at temperatures even very close to its triple point [7]. The CDM algorithm has been also applied to the normal ^{4}He fluid at supercritical temperatures and close to the Bose-Einstein transition temperature T_{BE} = 2.17 K [8-10]. The CDM formalism has been also developed for condensed and/or superfluid boson systems [11, 12]. Recent advances [13,14] now permit numerical calculations which may be quantitatively comparable with experimental data.

The temperature dependent CDM formalism for spinless fermions has been also outlined in Ref. [3]. We generalize now this formalism to analyze such systems like normal liquid ^{3}He with spin-dependent correlations or nuclear matter where the correlations depend also on isospin. The development follows, in spirit, the outline presented in Ref. [3] to derive the associated temperature dependent hypernetted-chain (HNC) equations for the spin (and isospin) dependent radial distribution function. These equations relate the direct (dd) components with direct-exchange (de) pieces and exchange-exchange (ee) portions. A particular role plays the statistical or exchange (cc) function that describes the correlations between like spin (isospin) components. The algorithm requires a restriction on the general spin (isospin) dependence. In general, the correlations depend on the spin (isospin) vector. However, we assume that the correlations depend only on one spin component, say σ^z (τ^z). To deal with correlations that also depend on σ^x, σ^y one may employ, in a further step, the formidable technique of operator FHNC.

Thereupon we turn our attention to investigate the evaluation of the statistical quantities entropy and the specific heat at constant volume that is related to the temperature derivative of the entropy. This task can be achieved within the concept of renormalized bosons and fermions outlined recently [14, 13]. These entities form a non-interacting gas of bosons or fermions with appropriately renormalized single particle energies

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and serve as a background system for a strongly correlated quantum liquid. The concept is, in the present paper, generalized for fermion systems with spin degeneracy ν (ν = 1, 2, 4).

Sections 2 and 3 report on the decomposition of the spin (and isospin) dependent radial distribution functions at nonzero temperatures and the relationships between them for degeneracy ν. At zero temperature and with a particular choice of statistical input function the set of HNC equations specializes to the familiar FHNC equations developed by S. Fantoni and S. Rosati for correlated ground states [15, 16].

Section 3 that deals with the projection of the correlation functions onto coordinate space is followed by describing the concept of renormalized fermions (Sec. 4). It enables us to view the physics of the correlated fermions from a different aspect. This formulation also offers a profound new tool for numerical calculations of correlations and equilibrium quantities. Section 5 presents our conclusion.

2. Decomposition of Correlation functions

This Section focuses on the structure of the diagonal elements of the two-body reduced matrix elements of the correlated *N*-body density matrix. They characterize thermal equilibrium properties of Fermi liquids such as normal liquid ^{3}He and nuclear matter within CDM theory.

Completely polarized liquid ^{3}He provides the simplest case. The correlations depend only on the radial distance r between two helium atoms since there is no spin-degeneracy (ν = 1). The corresponding CDM analysis has been reported in Ref [3]. There, the radial distribution function is decomposed,

$$g(r) = 1 + G_{dd}(r) + 2T_{de}(r) + G_{ee}(r) \qquad (1)$$

with the direct-direct (*dd*) component $G_{ee}(r)$, the exchange-direct portion $G_{de}(r)$, and the exchange-exchange (*ee*) part $G_{ee}(r)$.The statistical properties of the fluid are characterized by the exchange (or cyclic) correlation function $G_{cc}(r)$ at given density and temperature. The further analysis of the functions $G_{\alpha\beta}(r)$ has been performed by employing the HNC technique ($\alpha\beta$ represents the indices *dd*, *de*, *ee,* or *cc*). The algorithm then permits numerical calculations of the components $G_{\alpha\beta}(r)$ and the associated structure functions $S_{\alpha\beta}(k)$, the dimensionless Fourier transform of $G_{\alpha\beta}(r)$.

In symmetric liquid ^{3}He and nuclear matter the correlation functions depend not only on the relative distance r between two constituents but also on their spin (or/and isospin). In the following we limit our study and assume that the correlation functions depend only on one spin component σ^z and, in the case of nuclear matter, also on $\tau^z = \pm 1$. For convenience we henceforth drop the superscript z and abbreviate $G_{\alpha\beta}(r_{12}, \sigma_1, \sigma_2)$ or $G_{\alpha\beta}(r_{12}, \sigma_1, \sigma_2; \tau_1, \tau_2)$ by $G_{\alpha\beta}$ (12). We indicate the spin and isospin degeneracy by ν = 2 and ν = 4. Spin-polarized ^{3}He is characterized by ν = 1. Thus in the general case with ν-fold degeneracy we replace Eq. (1) by the decomposition

$$g(12) = 1 + G_{dd}(12) + 2\,G_{de}(12) + G_{ee}(12). \qquad (2)$$

We are now permitted to follow the CDM procedure of Ref. [3]. The decomposition of functions $G_{\alpha\beta}(12)$ into nodal ($N_{\alpha\beta}$) and non-nodal ($X_{\alpha\beta}$) components reads

$$G_{\alpha\beta}(12) = X_{\alpha\beta}(12) + N_{\alpha\beta}(12) \qquad (3)$$

except for the statistical correlation function that contains in addition the statistical generator Γ_{cc} (12),

$$\mathrm{G}_{cc}(12) = \mathrm{X}_{cc}(12) + \mathrm{N}_{cc}(12) - \Gamma_{cc}(12). \qquad (4)$$

The hypernet equations corresponding to quantities (3) are,

$$1 + G_{dd}(12) = \exp\{u(12) + N_{dd}(12) + E_{dd}(12)\},$$

$$G_{de}(12) = [1 + G_{dd}(12)]\{N_{de}(12) + E_{de}(12)\},$$

$$\begin{aligned} G_{ee}(12) = [1 + G_{dd}(12)]\{&N_{ee}(12) + E_{ee}(12) \\ &+ [N_{de}(12) + E_{de}(12)]^2 \\ &- [N_{cc}(12) + E_{cc}(12) - \Gamma_{cc}(12)]^2\} \end{aligned}$$

$$G_{cc}(12) = [1 + G_{dd}(12)]\{N_{cc}(12) + E_{cc}(12) - \Gamma_{cc}(12)\}. \qquad (5)$$

The set (5) contains the so-called elementary portions $E_{\alpha\beta}$ (12) and holds for any ν. The first hypernet equation contains the dynamic generator (or pseudopotential) *u*(12) that is a functional of the bare particle-particle potential ν(12). The generalization of the chain equations for ν = 1 reported in Ref. [3] is easily generalized for the case ν = 2

$$\begin{aligned} N_{dd}(12) &= \frac{\rho}{\nu}\sum_{\sigma_3}\int d\vec{r}_3\,\{X_{dd}(13)G_{de}(23) \\ &\quad + [X_{dd}(13) + X_{de}(13)]G_{dd}(32)\} \\ N_{de}(12) &= \frac{\rho}{\nu}\sum_{\sigma_3}\int d\vec{r}_3\,\{X_{de}(13)G_{de}(32) \\ &\quad + [X_{de}(13) + X_{ee}(13)]G_{dd}(32)\} \\ N_{ee}(12) &= \frac{\rho}{\nu}\sum_{\sigma_3}\int d\vec{r}_3\,\{X_{de}(13)G_{ee}(32) \\ &\quad + [X_{de}(13) + X_{ee}(13)]G_{de}(32)\}. \end{aligned} \qquad (6)$$

The cyclic chain equation reads

$$N_{cc}(12) = \frac{\rho}{\nu}\sum_{\sigma_3}\int d\vec{r}_3\,[X_{cc}(13) - \Gamma_{cc}(13)]G_{cc}(32). \qquad (7)$$

For nuclear matter (ν = 4) the summations over the spin coordinate σ_3 have to be complemented by the isospin summations over the isospin component $\tau_3 = \pm 1$.

By suitably choosing the statistical generator $\Gamma_{cc}(13)$ we recover the hypernet equations reported in Ref. [17] for the fermionic ground state at $T = 0$.

3. Representation in coordinate space

For convenience we perform the projection onto the *r*-space for symmetric normal ^{3}He (ν = 2). The final results represent also the correct *r*-space reduction for ν = 4 and an additional set of equations for the isospin components. The projection of the HNC equations of Section 2 for ν = 2 may be achieved by splitting any function L (12) into a spin-parallel component (superscript p) and a spin-antiparallel (superscript a) component

$$L(12) = L^p(r)\delta_{\sigma_1\sigma_2} + L^a(r)\big[1 - \delta_{\sigma_1\sigma_2}\big]. \tag{9}$$

The relations between $L^p(r)$, $L^a(r)$ and $L(r)$, $L^\sigma(r)$ are determined by the identity $\delta_{\sigma_1\sigma_2} = (1/2)\big(1 + \delta_{\sigma_1\sigma_2}\big)$ that leads to

$$\begin{aligned} 2L(r) &= L^p(r) + L^a(r), \\ 2L^\sigma(r) &= L^p(r) - L^a(r). \end{aligned} \tag{10}$$

The input functions $\Gamma_{cc}(12)$ and $u(12)$ in these representations are given by

$$\Gamma_{cc}(12) = \Gamma_{cc}(r)\delta_{\sigma_1\sigma_2} = \frac{1}{2}\Gamma_{cc}(r)[1 + \sigma_1\sigma_2] \tag{11}$$

and

$$\begin{aligned} u(12) &= u^p(r)\sigma_1\sigma_2 + (1 - \sigma_1\sigma_2)u^a(r) \\ &= u(r) + u^\sigma(r)\sigma_1\sigma_2. \end{aligned} \tag{12}$$

The functions $G_{\alpha\beta}(12)$, $X_{\alpha\beta}(12)$, $N_{\alpha\beta}(12)$, $E_{\alpha\beta}(12)$ maybe also decomposed into spin-parallel parts and spin anti-parallel portions,

$$G_{\alpha\beta}(12) = G^p_{\alpha\beta}(r)\delta_{\sigma_1\sigma_2} + G^a_{\alpha\beta}(r)\big(1 - \delta_{\sigma_1\sigma_2}\big) \tag{13}$$

and analogously for $X_{\alpha\beta}(12)$, etc. In this representation the set of hypernet equations decouples into two sets of the same form as Eqs.(5) but one set for the spin-parallel components and a second set for the spin-antiparallel components (for ν = 4 the decomposition must be also done in isospin space).

In contrast, the chain equations separate in the representation (9) of functions $G_{\alpha\beta}(12)$, etc.

$$G_{\alpha\beta}(12) = G_{\alpha\beta}(r) + G^\sigma_{\alpha\beta}(r)\sigma_1\sigma_2, \tag{14}$$

and similar for $X_{\alpha\beta}(12)$ and $N_{\alpha\beta}(12)$. This is due to the relationship

$$\begin{aligned} \frac{1}{\nu}\sum_{\sigma_3} L(13)\,K(32) &= L(r_{13})K(r_{32}) \\ &\quad + L^\sigma(r_{13})K^\sigma(r_{32})\sigma_1\sigma_2. \end{aligned} \tag{15}$$

(and a similar relation for the isospin for ν = 4). The convolutions of $L(r_{13})K(r_{32})$ and $L(r_{13})K(r_{32})\sigma_1\sigma_2$ appearing in the two sets of chain equations (for the spin-independent and the spin-dependent portions are most conveniently expressed as products in momentum space. Employing the Fourier transforms

$$S_{\alpha\beta}(k) = \rho\int d\vec{r}\, e^{i\vec{k}\cdot\vec{r}}G_{\alpha\beta}(r) \tag{16}$$

and

$$S^\sigma_{\alpha\beta}(k) = \rho\int d\vec{r}\, e^{i\vec{k}\cdot\vec{r}}G^\sigma_{\alpha\beta}(r) \tag{17}$$

as well as the Fourier transforms $X_{\alpha\beta}(k)$ and $N_{\alpha\beta}(k)$ for $X_{\alpha\beta}(r)$ and $N_{\alpha\beta}(r)$ (analogously for the spin-dependent functions) the chain equations (6) assume the form familiar from the case ν = 1 given in Ref. [3], but hold for any ν . The set of chain equations for the spin-independent components reads

$$\begin{aligned} N_{dd}(k) &= X_{dd}(k)S_{de}(k) + [X_{dd}(k) + X_{de}(k)]S_{dd}(k) \\ N_{de}(k) &= X_{de}(k)S_{de}(k) + [X_{de}(k) + X_{ee}(k)]S_{dd}(k) \\ N_{ee}(k) &= X_{de}(k)S_{ee}(k) + [X_{de}(k) + X_{ee}(k)]S_{de}(k). \end{aligned} \tag{18}$$

An analogous set of equations holds for the spin-dependent portions (the quantities with superscript sigma). The exchange component (7) reads in k-space

$$N_{cc}(k) = [X_{cc}(k) - \Gamma_{cc}(k)]S_{cc}(k). \tag{19}$$

Note, that the spin-independent component is identically zero.

The CDM results reported in this section represent a generalization of the familiar FHNC theory [16] of the correlated ground state of strongly correlated Fermi liquids to nonzero temperatures. The temperature dependence is generated by appropriate choices of the generator $\Gamma_{cc}(12)$ and $u(12)$ as functions of temperature T. By specializing the statistical function $\Gamma_{cc}(r)$ to the Slater exchange function $\ell(rk_F)$ with $\ell(x) = (3/x^3)$ (sin x – $x$cos x) we recover the FHNC equations at zero temperature.

4. Renormalized fermions

We may exploit the statistical (*cc*) chain equations to introduce a background system of non-interacting fermions with a renormalized excitation spectrum. This can be done in close analogy to the recent studies performed for strongly correlated bosons [14, 13].

Starting from equations (4) and (7), or from the corresponding expression in Fourier space,

$$S_{cc}(k) = X_{cc}(k) + N_{cc}(k) - \Gamma_{cc}(k) \tag{20}$$

and eq. (19) we may eliminate the nodal contribution $N_{cc}(k)$ and express the exchange structure function $S_{cc}(k)$ by the statistical factor $\Gamma_{cc}(k)$ and the correlation quantity $X_{cc}(k)$. The result reads

$$S_{cc}(k) = [X_{cc}(k) - \Gamma_{cc}(k)]\{1 - [X_{cc}(k) - \Gamma_{cc}(k)]\}^{-1}. \tag{21}$$

DM theory has shown (in the case ν = 1) that a momentum distribution $n_{qp}(k)$ can be defined that determines the entropy of the correlated Fermi fluid by the expression

$$S(T) = \sum_k \{-[1 - n_{qp}(k)] \ln[1 - n_{qp}(k)] + n_{qp}(k) \ln n_{qp}(k)\} \tag{22}$$

Expression (22) is of the familiar form valid for non-interacting free Fermi gases. However, in the present case the fermions are not moving with the single particle kinetic energy $\epsilon_0(k) = \hbar^2 k^2/2m$, where *m* is the bare mass of a particle but have a renormalized energy $\epsilon_{qp}(k)$. In CDM theory the associated renormalized momentum distribution is determined by the statistical generator $\Gamma_{cc}(k)$ and the exchange structure function S_{cc} (*k*).

For spinless fermions (completely polarized liquid 3He) the relation is [3]

$$n_{qp}(k) = \Gamma_{cc}(k)[1 - X_{cc}(k) + \Gamma_{cc}(k)]^{-1} = \Gamma_{cc}(k)[1 + S_{cc}(k)]. \tag{23}$$

Its generalization for symmetric normal liquid ^{3}He yields the same form

$$n_{qp}(k) = \Gamma_{cc}(k)[1 - X_{cc} + \Gamma_{cc}]^{-1} \tag{24}$$

We may insert Eq. (21) in relation (24) and get the expression

$$n_{qp}(k) = \Gamma_{cc}(k)\{1 + S_{cc}(k)\} \tag{25}$$

Next, we may renormalize the bare statistical generator by defining the renormalized statistical factor

$$\Gamma_{qp}(k) = \Gamma_{cc}(k)[1 - X_{cc}(k)]^{-1}. \tag{26}$$

Replacing $\Gamma_{cc}(k)$ in Eq. (25) by $\Gamma_{qp}(k)$ via Eq. (26), we find then

$$n_{qp}(k) = \Gamma_{qp}(k)[1 + \Gamma_{qp}(k)]^{-1}. \tag{27}$$

Result (27) expresses the momentum distribution $n_{qp}(k)$ by a Fermi distribution for free renormalized fermions with a kinetic single-particle energy $\epsilon_{qp}(k)$, i.e., the renormalized statistical factor is given by $\Gamma_{qp}(k) = \exp\beta\,[\mu_{qp} - \epsilon_{qp}(k)]$ with inverse temperature $\beta = T^{-1}$.

For a perfect Fermi gas the correlation function $X_{cc}(k)$ vanishes identically and consequently $\Gamma_{qp}(k) = \Gamma_{cc}(k)$ and $\epsilon_{qp}(k) = \epsilon_0(k)$ and $\mu_{qp} = \epsilon_0(k_F)$. If we choose $\epsilon_{qp}(k) = \epsilon_0(k)$ in the case of interacting fermions and take the limit $T \to 0$ the formalism reduces to the FHNC algorithm designed for the correlated ground state of a system of fermions with degeneracy ν.

The optimal choice of renormalized factor $\Gamma_{qp}(k)$ at a temperature *T* should be determined by an appropriate minimum principle.

Ignoring all dynamic correlation functions generated by the particle-particle interaction the results collapse to the familiar expressions for a non-interacting Fermi gas of degeneracy ν at density ρ and temperature $T \geq 0$.

4. Conclusion

We have generalized CDM theory to analyze the spin (isospin)-dependent correlations in Fermi liquids at non-zero temperatures such as unpolarized liquid ^{3}He (ν = 2) and symmetric nuclear matter (ν = 4). The generalization is based on the algorithm reported in Ref. [3] that only applies to completely polarized liquid helium. It also exploits recent developments in CDM theory for correlated Bose systems, where the equilibrium properties are described with respect to a non-interacting background system of renormalized bosons in the normal phase [13, 14]. Here this concept is carried over to deal with spin-dependent correlated fermions. We note that this formulation permits a direct study of statistical entanglement properties of interacting Fermi systems at $T > 0$ [18].

The study focuses foremost on the diagonal two-body reduced matrix elements of the correlated N-body density matrix and the analysis of the statistical properties generated by the exchange of fermions embodied in the exchange structure function $S_{cc}(k)$. This quantity entirely suffices to determine the entropy $S(T)$ of the correlated quantum fluid and therewith also to evaluate the specific heat of the system at constant volume (density) $C_y(T)$.

The CDM formalism provides a profound tool for numerical calculations of thermal equilibrium properties. To perform such calculations one needs the input functions $\Gamma_{cc}(r)$ or, preferably, $\Gamma_{qp}(r)$ and the pseudopotential $u(12)$. They may be determined in principle by the CDM functional for the Helmholtz free energy $F(T)$ employing an associated minimum principle. Taking the functional derivatives of $F(T)$ with respect to the statistical distribution $n_{qp}(k)$ and with

respect to the dynamic potential $u(12)$ one arrives at Euler-Lagrange equations for these input functions. At present one is satisfied employing suitable ansätze for the statistical functions $\Gamma_{cc}(r)$ or $\Gamma_{qp}(k)$. For example, one might adopt the one-body reduced density matrix of non-interacting fermions as a suitable ansatz for $\Gamma_{cc}(r)$. This natural choice would lead in the limit $T \to 0$ to the FHNC algorithm for the correlated ground state of interacting fermions. The pseudopotential $u(12)$ can be optimized by solving an effective Schrödinger equation [5] appropriately generalized to include the spin (isospin) dependence.

Acknowledgment

I am indebted to the late Prof. M.L. Ristig for many discussions and helpful suggestions during this work. I also acknowledge a DAAD scholarship during this work.

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