THE JACKSON–FEENBERG FORM OF THE KINETIC ENERGY OF FERMIONS IN THE CHAIN, HYPERNETTED CHAIN, AND PERCUS–YEVICK APPROXIMATIONS

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Expressions for the Jackson–Feenberg form of the kinetic energy of fermion systems in the chain, hypernetted chain and Percus–Yevick approximations are derived, and critically compared with earlier expressions of this type.

1. Introduction

In the present paper, we consider an infinite, homogeneous system of N identical fermions of mass M, and spin-isospin degeneracy ν. All the particles of the system are contained in a periodicity box of volume Ω.

In the Jastrow theory [1, 2], for the ground state wave function we assume the form:

$$\Psi(1, \ldots, N) = F\Phi(1, \ldots, \mathrm{N}), \tag{1.1}$$

where the arguments of the functions indicated by numbers denote full sets of space and spin-isospin coordinates of the respective particles. The Slater determinant function Φ is an antisymmetrized product of single particle wave functions (products of spin-isospin functions and plane wave functions, normalized in the periodicity box).

For the correlation operator, we assume the simplest form,

$$F = \prod_{i<j} f_{ij}, \tag{1.2}$$

with state independent correlation functions $f_{ij} = f(r_{ij})$, where r_{ij} is the distance between the i-th and j-th particles.

The essential problem of the Jastrow theory is the calculation of the expectation value of the hamiltonian $\hat{H} = \hat{T} + \hat{V}$, where the kinetic energy operator

$$\hat{T} = -\frac{\hbar^2}{2M} \sum_i \Delta_i, \tag{1.3}$$

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and $\hat{V}$ is the total inter-particle interaction. We have $E = T + V$, where

$$T = \langle \Psi | \hat{T} | \Psi \rangle / \langle \Psi | \Psi \rangle, \tag{1.4}$$

$$V = \langle \Psi | \hat{V} | \Psi \rangle / \langle \Psi | \Psi \rangle. \tag{1.5}$$

In the usual case when there are only two-body forces acting in the system, V may be expressed by two-body distribution function. In the simplest case when $\hat{V} = \frac{1}{2}\sum_{ij} v(r_{ij})$, we have

$$V = \tfrac{1}{2}\varrho^2 \int dr_1 dr_2 g_2(r_1 r_2) v(r_{12}), \tag{1.6}$$

where $\varrho = N/\Omega$, and g_2 is the two-body radial distribution function,

$$\varrho^2 g_2(xy) = \langle \Psi | \sum_{i \neq j} \delta(r_i - x)\delta(r_j - y) | \Psi \rangle / \langle \Psi | \Psi \rangle. \tag{1.7}$$

The kinetic energy T may be expressed with the help of the mixed one-body radial distribution function $g_1(r_1 r_1')$ (expression for $g_1(r_1, r_1')$ and its low order cluster approximation is given, e.g., in [3]). With the Jastrow form of Ψ, Eqs. (1.1–2), we are able to avoid the necessity of calculating $g_1(r_1, r_1')$. By applying directly the definition of $\hat{T}$, Eq. (1.3), one obtains the basic prescription (BP) for the kinetic energy, T^{BP}, used by Iwamoto and Yamada [4, 5], and in other early papers on the Jastrow theory, as well as in recent papers by Pandharipande and Bethe (see, e.g. [6]). By partial integration, one may transform T into two other forms used in the literature: the Clark–Westhaus [7] form T^{CW}, and the Jackson–Feenberg [8] form T^{JF}. In the present paper, we use the JF form:

$$T^{\mathrm{JF}}/(\hbar^2/2M) = \tfrac{3}{5} k_{\mathrm{F}}^2 N + T_f + \tfrac{1}{4}\tau, \tag{1.8}$$

where k_{F} is the Fermi momentum (in units of $\hbar$),

$$T_f = \langle \Phi | \sum_i [\tfrac{1}{2}(\nabla_i F)^2 - \tfrac{1}{2} F(\Delta_i F)] | \Phi \rangle / \langle \Psi | \Psi \rangle$$

$$= \varrho^2 \int dr_1 dr_2 \{\tfrac{1}{2}[(\nabla_1 f_{12})/f_{12}]^2 - \tfrac{1}{2}(\Delta_1 f_{12})/f_{12}\} g_2(r_1, r_2), \tag{1.9}$$

$$\tau = \int d\tau F^2 \sum_i \Delta_i |\Phi|^2 / \langle \Psi | \Psi \rangle = \varrho \int dr_1 \Delta_1^{\Phi} g_1(r_1). \tag{1.10}$$

By $\Delta_1^{\Phi} = (\nabla_1^{\Phi})^2$, we denote the Laplace operator acting on r_1 which appears in $|\Phi|^2$ (i.e., only statistical correlations contribute to Δ_1^{Φ}). The one-body radial distribution function is defined by

$$\varrho g_1(r_1) = \langle \Psi | \sum_i \delta(r_i - x) | \Psi \rangle / \langle \Psi | \Psi \rangle. \tag{1.11}$$

To calculate T^{JF}, we have to determine (except for g_2 needed anyhow in calculating V, Eq. (1.6)) only g_1, or strictly speaking ,only that part of g_1 which contributes to τ. This is the great advantage of the JF form of T over the other two forms. In case of T^{CW}, we have to determine, in addition to g_2, the more complicated three-body radial distribution function g_3. Least convenient is the BP form, T^{BP}, which requires both the knowledge of g_3, and the determination of an additional term similar to τ.

In calculating radial distribution functions, one usually assumes that $f(r)$ deviates from unity for relatively small values of r only, and applies cluster expansion methods, originally introduced by Ursell in the statistical mechanics (see, e.g., [9]). Recently, an important progress in the cluster expansion method was made by Fantoni and Rosati [10] who adopted to the case of the ground state of fermion systems the powerful methods of selective summation of cluster diagrams, known since a long time in classical statistical mechanics [11]. Summation of single chain diagrams built of the simplest links leads to the chain (CH) approximation. The (Fermi) hypernetted chain (HNC) approximation is obtained by parallel connection of chain diagrams, built of links which in turn are constructed by parallel connection of chains and simplest links. If in the HNC approximation the parallel connection of chains is disregarded one obtains the (Fermi) PY approximation [12] originally introduced by Percus and Yevick [13] in classical statistical mechanics.

In the present paper, we derive expressions for τ in the CH, HNC, and PY approximations. We assume that we know, from the work of Fantoni and Rosati [10] (and [12]), how to calculate g_2 (and, consequently, T_f, Eq. (1.9)) in the three approximations. Hence, our present results for τ enable us to calculate the total kinetic energy in the CH, HNC, and PY approximations.

Eq. (1.10) was used by Fantoni and Rosati to calculate τ in the CH approximation in [10], and in the HNC approximation in [14]. Our results differ from the results of [10], and [14]. For this reason, we present some details of our derivation, and test our results in first few orders in the expansion in powers of h factors, where

$$h_{ij} = f_{ij}^2 - 1. \tag{1.12}$$

In Section 2, we apply the power series (PS) expansion method in calculating τ, and present the results up to the third order in h. In Section 3, τ is calculated in the CH approximation. In Section 4, we calculate τ in the HNC approximation. The PY approximation of τ is presented in Section 4. A critical comparison of our expressions for τ with earlier expressions of this type is given in Section 5.

Our CH and HNC results for τ have been reported in [21].

2. *PS expansion of* τ

The PS expansion (Fantoni, Rosati [15, 16, 10]) appears to us to be the most natural method of the cluster expansion. In this expansion, various terms are classified according to the number of h factors contained.

The PS expansion of τ is described by Fantoni and Rosati in [10]. Their result may be best expressed by means of diagrams. Here, we use their diagrams, in which h factors are represented by solid lines, λ factors by dashed lines, and $-l^2/\nu$ factors by helical lines. We use the notation

$$\lambda_{ij} = -l_{ij}/\nu = -[3j_1(k_F r_{ij})/k_F r_{ij}]/\nu. \tag{2.1}$$

Open circles depict external points. Closed circles (solid dots) depict internal points, and imply integration accompanied by a factor ϱ.

We write Eq. (1.10) in the form

$$\tau = \varrho \int d\boldsymbol{r}_1 \Delta_1^{\Phi} \gamma, \tag{2.2}$$

where $\gamma = \gamma(\boldsymbol{r}_1)$ is that part of $g_1(\boldsymbol{r}_1)$ which gives a non vanishing contribution to τ. If the external point 1 is connected with the rest of a $g_1(\boldsymbol{r}_1)$ diagram by solid lines only, then obviously such a diagram does not contribute to τ. Also, if point 1 is connected with the rest of the diagram only by a helical line or by dashed lines, the contribution of such a diagram to τ vanishes. Namely, we may then replace Δ_1^{Φ} in Eq. (2.2) by Δ_1, and apply the Gauss

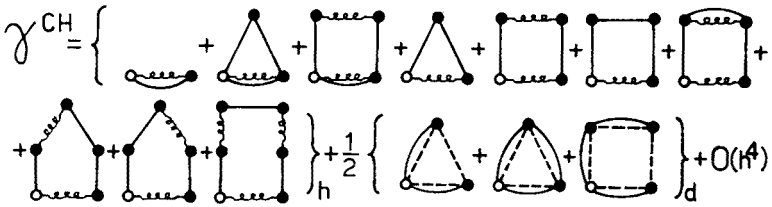


Fig. 1. The γ^{CH} diagrams

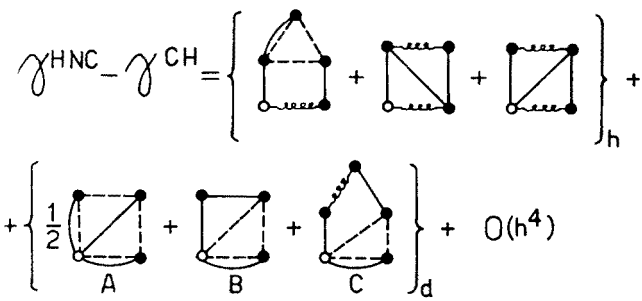


Fig. 2. The $\gamma^{HNC}-\gamma^{CH}$ diagrams

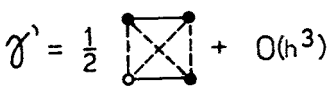


Fig. 3. The γ'diagrams

theorem. In conclusion, γ is depicted by the sum of all $g_1(\boldsymbol{r}_1)$ diagrams in which point 1 is connected with the rest of the diagram by at least one solid line *and* by a helical line or by two dashed lines.

By applying the rules of drawing diagrams [10] we get:

$$\gamma = \gamma^{CH} + (\gamma^{HNC} - \gamma^{CH}) + \gamma', \tag{2.3}$$

where γ^{CH}, γ^{HNC}, and γ' are depicted diagramatically in Figs 1, 2, and 3. By γ^{CH} and γ^{HCN}, we denote those parts of γ which are taken into account in the CH and HNC approximations, respectively. The elementary diagram in Fig. 3 is neglected in the CH and HNC

approximations. The part of γ, consisting of such diagrams neglected in the CH and HNC approximations, is denoted by γ'. Notice that the HNC approximation differs from the CH approximation only in the third and higher orders in h.

The last diagram in Fig. 1 is accompanied by a factor $\frac{1}{2}$, whereas the symmetry number of this diagram is 1. The explanation is that this diagram originates from the sum of two diagrams, shown in Fig. 4a. Furthermore, there are two diagrams missing in Fig. 1, which

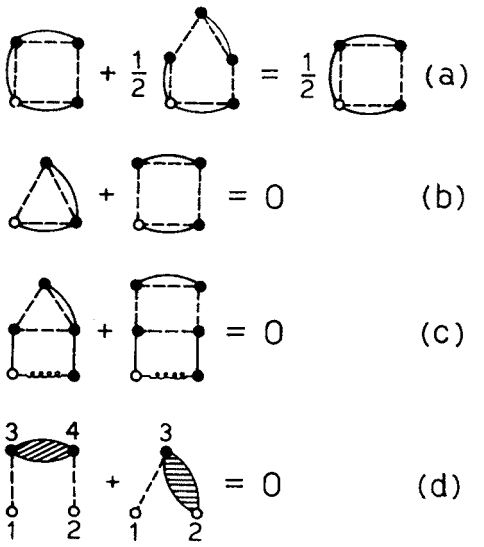


Fig. 4. Diagramatical relations

however cancel each other, as shown in Fig. 4b. Also in Fig. 2, there are diagrams missing which cancel each other, e.g., the two diagrams shown in Fig. 4c.

The diagramatic relations depicted in Figs 4a–c follow from the general relation shown in Fig. 4d, in which the blobs between two points represent any function of the distance between these points. The proof of this general relation is simple: one introduces $\boldsymbol{r}_4, \boldsymbol{r}_{43}$ as integration variables, and in perfoming the $\boldsymbol{r}_4$ integration, one uses the convolution identity of the λ functions:

$$\varrho \int d\boldsymbol{r}_j \lambda_{ij} \lambda_{jk} = -\lambda_{ik}. \tag{2.4}$$

In calculating γ, it is very important to realize that the relation depicted in Fig. 4d holds also in the presence of a differential operator acting on point 1 (but not on point 2!).

By inserting γ^{CH} and γ', shown in Figs 1 and 3, into Eq. (2.8), we get:

$$\tau^{\mathrm{CH}} = \varrho \int d\boldsymbol{r}_1 \Delta_1^{\mathrm{p}} \gamma^{\mathrm{CH}} = \varrho^2 \int d\boldsymbol{r}_1 d\boldsymbol{r}_2 h_{12} \Delta_1(-l_{12}^2/v) + \varrho^3 \int d\boldsymbol{r}_1 d\boldsymbol{r}_2 d\boldsymbol{r}_3 [h_{13} h_{23} \Delta_1(-l_{12}^2/v)$$

$$+ \tfrac{1}{2}(-2v) h_{12} h_{13} \lambda_{23} \Delta_1(\lambda_{12}\lambda_{13})] + \varrho^4 \int d\boldsymbol{r}_1 d\boldsymbol{r}_2 d\boldsymbol{r}_3 d\boldsymbol{r}_4 h_{13} h_{24} (l_{34}^2/v) \Delta_1(l_{12}^2/v) + O(h^3), \tag{2.5}$$

$$\tau' = \varrho \int d\boldsymbol{r}_1 \Delta_1^{\Phi} \gamma' = \tfrac{1}{2}(-2v) \varrho^4 \int d\boldsymbol{r}_1 d\boldsymbol{r}_2 d\boldsymbol{r}_3 d\boldsymbol{r}_4 h_{12} h_{34} \lambda_{32} \lambda_{24} \Delta_1(\lambda_{14}\lambda_{13}) + O(h^3). \tag{2.6}$$

In this quadratic (h^2-) approximation $\tau^{HNC} = \tau^{CH}$, and $\tau = \tau^{CH}+\tau'$. Let us mention that Eqs. (2.5), (2.6) may also be obtained (by partial integration) from the expressions for the kinetic energy, given by Iwamoto and Yamada [5].

3. *CH approximation of* τ

In the CH approximation, we approximate γ by

$$\gamma^{CH} = \gamma_h^{CH}+\gamma_d^{CH}, \tag{3.1}$$

where γ_h^{CH} and γ_d^{CH} contain all chain diagrams in which the external point 1 is connected with the rest of a diagram by helical and dashed lines, respectively.

In the h^3-approximation, all the γ_h^{CH} diagrams are contained within the $\{\ \}_h$ brakets in Fig. 1. By extending the sum of these diagrams to all possible chains, we obtain the

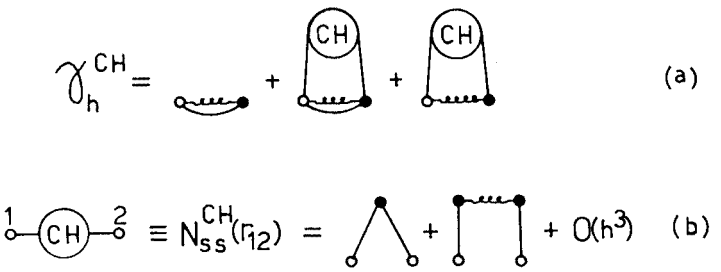


Fig. 5. Result for γ_h^{CH}

result shown in Fig. 5 in which $N_{ss}^{CH}(r_{12})$ represents the sum of all CH nodal diagrams, i.e., the sum of all chains built of the links: h, $-l^2/v$, and $-l^2h/v$, which start and end with an h link (solid line). (In [10], N_{ss}^{CH} is denoted by $\mathscr{G}_{ss}^{(ch)}$).

All the γ_d^{CH} diagrams with two and three h factors are contained in the $\{\ \}_d$ brackets in Fig. 1. By extending the sum of these diagrams to all possible chains, we obtain the

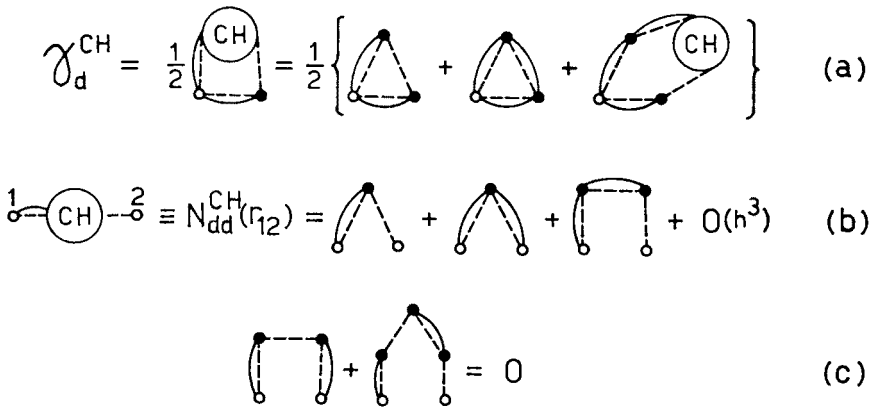


Fig. 6. Results for γ_d^{CH}

result shown in Fig. 6 where $N_{dd}^{CH}(r_{12})$ represents the sum of all CH nodal diagrams, i.e., the sum of all chains of the links: λ and λh. In general, both the λ and the λh links may start and end the N_{dd}^{CH} chains. However, all the $N_{dd}^{CH}(r_{12})$ chains which start at 1 with the λ link, and end at 2 with either a λ or a λh link, cancel, as may easily be shown with the help of the relation depicted in Fig. 4d. Consequently, only chains which start at point 1 with the λh link (dashed line superimposed on a solid line), contribute to $N_{dd}^{CH}(r_{12})$. For this reason, in Fig. 6, for $N_{dd}^{CH}(r_{12})$ we use the picture in which the dashed line starting in 1 is superimposed on a solid line, and in which it is understood that the dashed line ending in 2 may be superimposed or not on a solid line. (Notice that there are two possible diagrams missing in Fig. 6b. These are the two diagrams in Fig. 6c which cancel each other.)

The chain equation for N_{dd}^{CH} (denoted in [10] by $\mathscr{G}_{dd}^{(ch)}$) is:

$$N_{dd}^{CH}(r_{12}) = \varrho \int dr_3 h_{13}\lambda_{13}[f_{32}^2\lambda_{32} + N_{dd}^{CH}(r_{32})]. \tag{3.2}$$

This equation is responsible for the last part of the equation shown in Fig. 6a.

With the help of the expressions for γ_h^{CH} and γ_d^{CH}, shown in Figs 5a and 5b, we get

$$\tau^{CH} = \varrho^2 \int dr_1 dr_2 [h_{12} + f_{12}^2 N_{ss}^{CH}(r_{12})]\Delta_1(-l_{12}^2/v)$$
$$+\tfrac{1}{2}(-2v)\varrho^3 \int dr_1 dr_2 dr_3 [f_{23}^2\lambda_{23} + N_{dd}^{CH}(r_{23})]h_{12}h_{13}\Delta_1(\lambda_{12}\lambda_{13}). \tag{3.3}$$

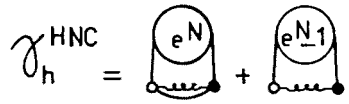
With the help of Eq. (3.2), we may write τ^{CH} also in the form:

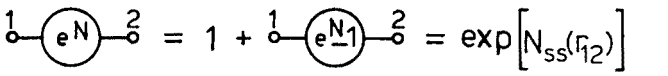
$$\tau^{CH} = \varrho^2 \int dr_1 dr_2 \{[h_{12} + f_{12}^2 N_{ss}^{CH}(r_{12})]\Delta_1(-l_{12}^2/v) - 2v h_{12} N_{dd}^{CH}(r_{12})\Delta_1\lambda_{12}\}$$
$$+(-2v)\varrho^3 \int dr_1 dr_2 dr_3 h_{12}h_{13}[f_{23}^2\lambda_{23} + N_{dd}^{CH}(r_{23})]\,(\nabla_1\lambda_{12})\,(\nabla_1\lambda_{13}). \tag{3.4}$$

4. HNC approximation of τ

In the HNC approximation, we approximate γ by

$$\gamma^{HNC} = \gamma_h^{HNC} + \gamma_d^{HNC}, \tag{4.1}$$





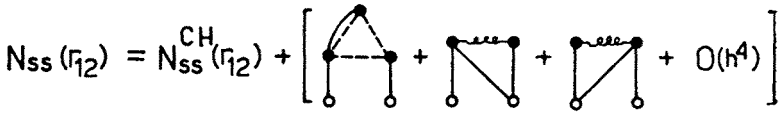


Fig. 7. Result for γ_h^{HNC}

where γ_h^{HNC} and γ_d^{HNC} contain all hypernetted chain diagrams in which the external point 1 is connected with the rest of a diagram by helical or dashed lines, respectively.

The γ_h^{HNC} diagrams with one, two, and three h factors are those contained within the $\{\ \}_h$ brackets in Fig. 1 plus those within the $\{\ \}_h$ brackets in Fig. 2. By extending the sum of these diagrams to all possible hypernetted chains, we obtain the result shown in Fig. 7 (similarly as before, diagrams which cancel each other are omitted here, and also in all other figures) in which $N_{ss}(r_{12})$ represents the sum of all HNC modal diagrams, i.e., the sum of all chains which start at 1 and end at 2 with solid lines only. (In [10], N_{ss} is denoted by $\mathscr{G}_{ss}$ (with $E_{mn} = 0$).)

For the h-part of τ^{HNC}, we get

$$\tau_h^{HNC} = \varrho \int d\boldsymbol{r}_1 \Delta_1^{\Phi} \gamma_h^{HNC} = \varrho^2 \int d\boldsymbol{r}_1 d\boldsymbol{r}_2 \{f_{12}^2 \exp[N_{ss}(r_{12})] - 1\} \Delta_1(-l_{12}^2/v). \tag{4.2}$$

In the h^3-approximation, all the γ_d^{HNC} diagrams are those contained within the $\{\ \}_d$ brackets in Fig. 1 plus those within $\{\ \}_h$ brackets in Fig. 2. By extending the sum of these diagrams to all possible hypernetted chains, we obtain the result shown in Fig. 8 where $N_{dd}(r_{12})$ represents the sum of all HNC nodal diagrams, i.e., the sum of all chains, which in general may start at 1 and end at 2 with a dashed line superimposed or not on solid lines. However, all the $N_{dd}(r_{12})$ chains which start at 1 with only a dashed line cancel

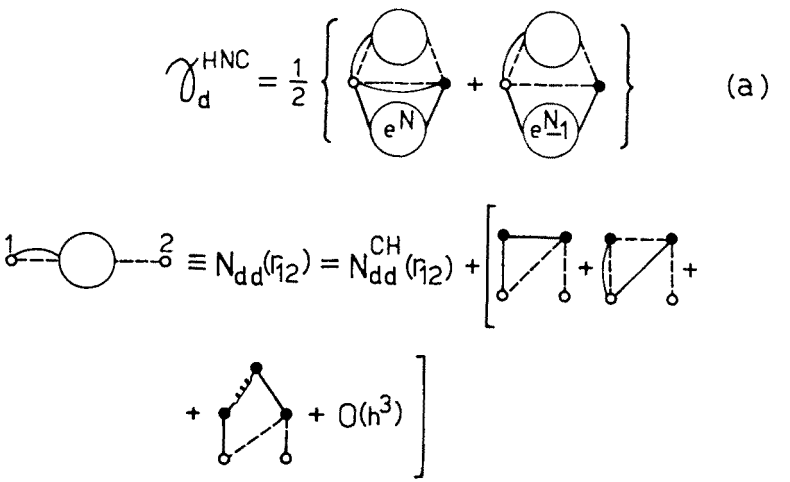


Fig. 8. Result for γ_d^{HNC}

(similarly as in the case of N_{dd}^{CH}). Consequently, only chains which start at point 1 with a dashed line superimposed on solid lines contribute to $N_{dd}(r_{12})$. This is reflected in the way $N_{dd}(r_{12})$ is depicted in Fig. 8. Notice that this property of $N_{dd}(r_{12})$ is preserved when we differentiate $N_{dd}(r_{12})$ with respect to the coordinates of point 1. In [10], N_{dd} is denoted by $\mathscr{G}_{dd}$ (with $E_{mn} = 0$).

To understand the source of the factor $\frac{1}{2}$ in the expression for γ_d^{HNC} in Fig. 8, we write the sum of the diagrams in the $\{\ \}_d$ brackets in Fig. 2 in the way shown in Fig. 9. We see that the diagram A, with symmetry number 2, is contained only in the first term in Fig. 8a,

and the diagrams B and C, each with symmetry number 1, are contained both in the first *and* second terms in Fig. 8a. This occurs with all diagrams of γ_d^{HNC}: diagrams with symmetry number 2 are contained only in one of the two terms in Fig. 8a, and diagrams with symmetry number 1 are always contained in the first *and* second terms of the expression for γ_d^{HNC}

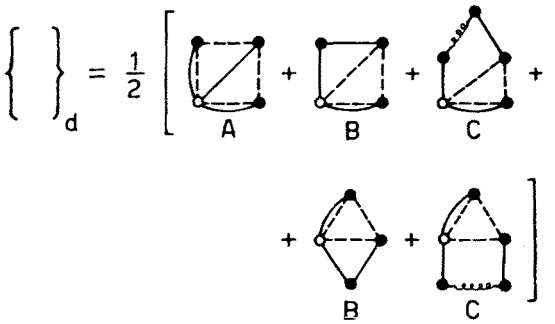


Fig. 9. The $\gamma_d^{HNC}-\gamma_d^{CH}$ diagrams

shown in Fig. 8a. Consequently, the factor $\frac{1}{2}$ is necessary to prevent double counting of identical diagrams.

Notice that in our expression for γ_d^{HNC}, Fig. 8a, we do not have the diagram D, shown in Fig. 10. If $N_{dd}(r_{12})$ ends in point 2 with a dashed line only, than this part of the diagram D

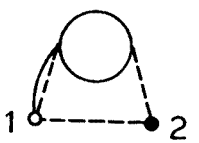


Fig. 10. Diagram which does not contribute to γ_d^{HNC}

is illegal. With the help of the chain equations satisfied by the remaining part of $N_{dd}(r_{12})$ (which ends in point 2 with a dashed line superimposed on solid lines), one may easily show that the corresponding remaining part of diagram D vanishes.

The chain equation for N_{dd} is:

$$N_{dd}(r_{12}) = \varrho \int dr_3 Y_{13}[\lambda_{32}+Y_{32}+N_{dd}(r_{32})], \tag{4.3}$$

where we use the notation

$$Y_{12} = [\lambda_{12}+N_{dd}(r_{12})]\{f_{12}^2 \exp[N_{ss}(r_{12})]-1\} \tag{4.4}$$

for the HNC non-nodal diagram, i.e., for the link of the chain, in which the two ends, 1 and 2, are connected with the rest of the link with dashed lines superimposed on solid lines. (There is only one other possible link in a N_{dd} chain, namely λ_{12}. In [10]. $Y_{12} = X_{dd}(r_{12})-\lambda_{12}$ is denoted by δ_{12} (with $E_{mn} = 0$).)

The sum of the expression for γ_h^{HNC} and γ_d^{HNC}, shown in Figs 7 and 8a, may be written in the form:

$$\gamma^{HNC} = \tfrac{1}{2}(-2v)\varrho \int dr_2 Y_{12}\lambda_{12}, \tag{4.5}$$

and for τ^{HNC}, we get

$$\tau^{HNC} = -v\varrho^2 \int dr_1 dr_2 \{Y_{12}\Delta_1\lambda_{12} + (\Delta_1^{\Phi}Y_{12})\lambda_{12} + 2(\nabla_1^{\Phi}Y_{12})\nabla_1\lambda_{12}\}. \tag{4.6}$$

We may replace the second term of the right hand side of Eq. (4.6) by the first term. Namely, acting on both sides of Eqs (4.3) and (4.4) with the operator Δ_1^{Φ} (notice that Δ_1^{Φ} does not affect the factor $\{f^2 \exp N_{ss} - 1\}$ in (4.4), we get

$$\Delta_1^{\Phi}Y_{12} = \{f_{12}^2 \exp [N_{ss}(r_{12})] - 1\}\{\Delta_1\lambda_{12} + \varrho \int dr_3 (\Delta_1^{\Phi}Y_{13})[\lambda_{32} + Y_{32} + N_{dd}(r_{32})]\}. \tag{4.7}$$

From Eq. (4.7), we obtain[1]:

$$\begin{aligned}
&\int dr_1 dr_2 (\Delta_1^{\Phi}Y_{12})[\lambda_{12} + N_{dd}(r_{12})] = \int dr_1 dr_2 \{f_{12}^2 \exp [N_{ss}(r_{12})] - 1\} \\
&\times (\Delta_1\lambda_{12})[\lambda_{12} + N_{dd}(r_{12})] + \varrho \int dr_1 dr_2 dr_3 \{f_{12}^2 \exp [N_{ss}(r_{12})] - 1\} \\
&\times (\Delta_1^{\Phi}Y_{13})[\lambda_{32} + Y_{32} + N_{dd}(r_{32})][\lambda_{12} + N_{dd}(r_{12})] = \int dr_1 dr_2 Y_{12}\Delta_1\lambda_{12} \\
&+ \varrho \int dr_1 dr_2 dr_3 (\Delta_1^{\Phi}Y_{13}) Y_{12}[\lambda_{32} + Y_{32} + N_{dd}(r_{32})] = \int dr_1 dr_2 Y_{12}\Delta_1\lambda_{12} \\
&+ \int dr_1 dr_3 (\Delta_1^{\Phi}Y_{13}) N_{dd}(r_{13}),
\end{aligned} \tag{4.8}$$

and conclude that

$$\int dr_1 dr_2 (\Delta_1^{\Phi}Y_{12})\lambda_{12} = \int dr_1 dr_2 Y_{12}\Delta_1\lambda_{12}. \tag{4.9}$$

Consequently, we may write (4.6):

$$\tau^{HNC} = -2v\varrho^2 \int dr_1 dr_2 \{Y_{12}\Delta_1\lambda_{12} + \chi_{12} d\lambda_{12}/dr_{12}\}, \tag{4.10}$$

where the function χ is defined by

$$\nabla_1^{\Phi}Y_{12} = \chi_{12}\hat{r}_{21}, \tag{4.11}$$

where $\hat{r}_{21} = (r_1 - r_2)/r_{12}$.

The equation for χ, obtained analogically as Eq. (4.7), is

$$\chi_{12} = \chi^{(0)} + \{f_{12}^2 \exp [N_{ss}(r_{12})] - 1\}\varrho \int dr_3 (\hat{r}_{21}\hat{r}_{31})\chi_{13}[\lambda_{32} + Y_{32} + N_{dd}(r_{32})], \tag{4.12}$$

where

$$\chi^{(0)} = \{f_{12}^2 \exp [N_{ss}(r_{12})] - 1\} d\lambda_{12}/dr_{12}. \tag{4.13}$$

If for Y we use expression (4.4), we may write Eq. (4.10) in the form:

$$\begin{aligned}
\tau^{HNC} = \varrho^2 \int dr_1 dr_2 \{&[f_{12}^2 \exp [N_{ss}(r_{12})] - 1][\Delta_1(-l_{12}^2/v) + (-2v)N_{dd}(r_{12})\Delta_1\lambda_{12}] \\
&+ (-2v)[\chi_{12} - \chi_{12}^{(0)}] d\lambda_{12}/dr_{12}\}.
\end{aligned} \tag{4.14}$$

[1] Here, we follow Ref. [22].

For the sake of comparison with the results of Fantoni and Rosati, we write Eq. (4.14) as

$$\tau^{\mathrm{HNC}} = \tau_2^{\mathrm{HNC}} + \tau_3^{\mathrm{HNC}}, \tag{4.15}$$

$$\tau_2^{\mathrm{HNC}} = \varrho^2 \int d\boldsymbol{r}_1 d\boldsymbol{r}_2 [f_{12}^2 \exp[N_{\mathrm{ss}}(r_{12})] - 1][\Delta_1(-l_{12}^2/v) + (-2v) N_{\mathrm{dd}}(r_{12}) \Delta_1 \lambda_{12}], \tag{4.16}$$

$$\tau_3^{\mathrm{HNC}} = 2v\varrho^3 \int d\boldsymbol{r}_1 d\boldsymbol{r}_2 d\boldsymbol{r}_3 (\hat{r}_{21}\hat{r}_{31}) \chi_{12}^{(0)} \chi_{13} [\lambda_{32} + Y_{32} + N_{\mathrm{dd}}(r_{32})]. \tag{4.17}$$

In writing expression (4.17), we have used Eq. (4.12).

5. *PY approximation of* τ

The PY approximation was originally introduced by Percus and Yevick [13] in classical statistical mechanics. It is well known (see, e.g., [17]) that in the study of hard sphere gases, the PY approximation yields better results than the HNC approximation. The original PY approximation has been generalized to fermion systems by Campani, Rosati,

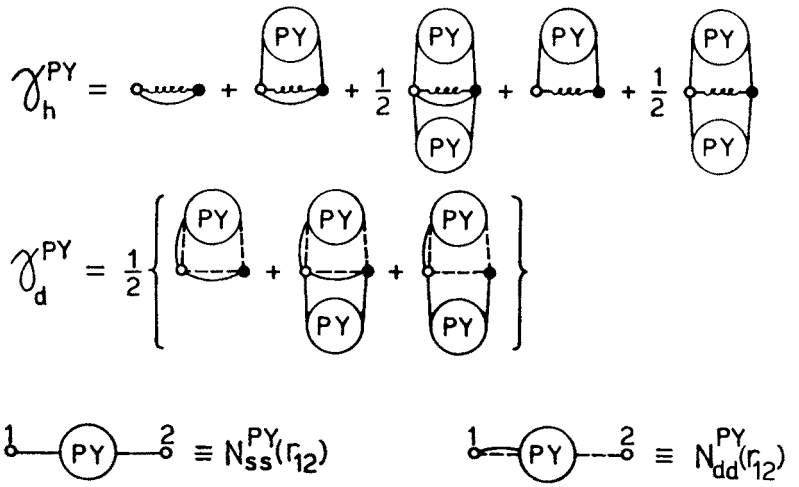


Fig. 11. Result for γ^{PY}

and Fantoni [12], whose results imply that also in fermion systems the PY approximation might be better than the HNC approximation (at least for certain types of two-body interaction).

The PY approximation may be obtained from the HNC approximation, by disregarding the parallel connection of chains. In this way, from $\gamma_{\mathrm{h}}^{\mathrm{HNC}}$ and $\gamma_{\mathrm{d}}^{\mathrm{HNC}}$, we obtain for $\gamma_{\mathrm{h}}^{\mathrm{PY}}$ and $\gamma_{\mathrm{d}}^{\mathrm{PY}}$ the expressions shown in Fig. 11. Hence, we have:

$$\gamma^{\mathrm{PY}} = \gamma_h^{\mathrm{PY}} + \gamma_{\mathrm{d}}^{\mathrm{PY}} = \varrho \int d\boldsymbol{r}_2 \{[h_{12} + f_{12}^2 N_{\mathrm{ss}}^{\mathrm{PY}}(r_{12})$$

$$+ \tfrac{1}{2} f_{12}^2 N_{\mathrm{ss}}^{\mathrm{PY}}(r_{12})^2] (-l_{12}^2/v) + \tfrac{1}{2}(-2v)[h_{12} + f_{12}^2 N_{\mathrm{ss}}^{\mathrm{PY}}(r_{12})] N_{\mathrm{dd}}^{\mathrm{PY}}(r_{12}) \lambda_{12}\}. \tag{5.1}$$

The functions N_{ss}^{PY} and N_{dd}^{PY} represent the PY chains. They differ from the corresponding HNC functions in the way in which the links of the chains are constructed. Namely, the PY links are defined by equations linearized in the chain functions. In particular, in place of Eqs (4.3), (4.4), we have:

$$N_{dd}^{PY}(r_{12}) = \varrho \int dr_3 Y_{13}^{PY}[\lambda_{32} + Y_{32} + N_{dd}^{PY}(r_{32})], \tag{5.2}$$

$$Y_{12}^{PY} = [h_{12} + f_{12}^2 N_{ss}^{PY}(r_{12})]\lambda_{12} + h_{12} N_{dd}^{PY}(r_{12}). \tag{5.3}$$

With expression (5.1), we get

$$\tau^{PY} = \varrho \int dr_1 \Delta_1^{\Phi} \gamma^{PY} = \tfrac{1}{2}(-2v)\varrho^2 \int dr_1 dr_2 \{\lambda_{12} \Delta_1^{\Phi}[Y_{12}^{PY} + f_{12}^2 N_{ss}^{PY}(r_{12}) N_{dd}^{PY}(r_{12})]$$
$$+ [Y_{12}^{PY} + f_{12}^2 N_{ss}^{PY}(r_{12}) N_{dd}^{PY}(r_{12})] \Delta_1 \lambda_{12} + 2(\nabla_1 \lambda_{12}) \nabla_1^{\Phi}[Y_{12}^{PY} + f_{12}^2 N_{ss}^{PY}(r_{12}) N_{dd}^{PY}(r_{12})]$$
$$+ \tfrac{1}{2} f_{12}^2 N_{ss}^{PY}(r_{12})^2 \Delta_1 \lambda_{12}^2\}. \tag{5.4}$$

To simplify this expression, we need the equation

$$\Delta_1^{\Phi} Y_{12}^{PY} = [h_{12} + f_{12}^2 N_{ss}(r_{12})] \Delta_1 \lambda_{12} + h_{12} \varrho \int dr_3 (\Delta_1^{\Phi} Y_{13}^{PY}) [\lambda_{32} + Y_{32}^{PY} + N_{dd}^{PY}(r_{32})], \tag{5.5}$$

which follows from Eqs (5.2) and (5.3). With the help of Eq. (5.5) we may calculate the left hand side of Eq. (4.8) with the functions Y^{PY}, and N_{dd}^{PY}. Proceeding similarly as in Eq. (4.8) we conclude that

$$\int dr_1 dr_2 \lambda_{12} \Delta_1^{\Phi}[Y_{12}^{PY} + f_{12}^2 N_{ss}^{PY}(r_{12}) N_{dd}^{PY}(r_{12})]$$
$$= \int dr_1 dr_2 [Y_{12}^{PY} + f_{12}^2 N_{ss}^{PY}(r_{12}) N_{dd}^{PY}(r_{12})] \Delta_1 \lambda_{12}. \tag{5.6}$$

Consequently, we have

$$\tau^{PY} = -2v\varrho^2 \int dr_1 dr_2 \{[Y_{12}^{PY} + f_{12}^2 N_{ss}^{PY}(r_{12}) N_{dd}^{PY}(r_{12})] \Delta_1 \lambda_{12}$$
$$+ (\nabla_1 \lambda_{12}) \nabla_1^{\Phi}[Y_{12}^{PY} + f_{12}^2 N_{ss}^{PY}(r_{12}) N_{dd}^{PY}(r_{12})] + \tfrac{1}{4} f_{12}^2 N_{ss}^{PY}(r_{12})^2 \Delta_1 \lambda_{12}^2\}. \tag{5.7}$$

With the help of (5.3), we may write expression (5.7) in the form:

$$\tau^{PY} = \varrho^2 \int dr_1 dr_2 \{[h_{12} + f_{12}^2 N_{ss}(r_{12})]\, [\Delta_1(-l_{12}^2/v) + (-2v) N_{dd}(r_{12}) \Delta_1 \lambda_{12}$$
$$+ (-2v) \eta_{12}^{PY} d\lambda_{12}/dr_{12}] + \tfrac{1}{2} f_{12}^2 N_{ss}^{PY}(r_{12})^2 \Delta_1(-l_{12}^2/v)\}, \tag{5.8}$$

where the function η is defined by

$$\nabla_1^{\Phi} N_{dd}^{PY}(r_{12}) = \eta_{12}^{PY} \hat{r}_{21}, \tag{5.9}$$

and satifies the equation

$$\eta_{12}^{PY} = \varrho \int dr_3 (\hat{r}_{21} \hat{r}_{31}) \{[h_{13} + f_{13}^2 N_{ss}^{PY}(r_{13})] d\lambda_{13}/dr_{13} + h_{13} \eta_{13}^{PY}\} \{\lambda_{32} + Y_{32}^{PY} + N_{dd}^{PY}(r_{32})\}, \tag{5.10}$$

which one may obtain by acting on both sides of Eqs (5.2) and (5.3) with the operator ∇_1^{Φ}.

With the help of (5.3), we may also write τ^{PY} in an alternative form:

$$\tau^{PY} = \varrho^2 \int d\boldsymbol{r}_1 d\boldsymbol{r}_2 \{[h_{12}+f_{12}^2 N_{ss}^{PY}(r_{12})]\,[\Delta_1(-l_{12}^2/v)+(-2v)N_{dd}^{PY}(r_{12})\Delta_1\lambda_{12}$$
$$+(-2v)h_{12}^{-1}(\chi_{12}^{PY}-\chi_{12}^{(0)PY})d\lambda_{12}/dr_{12}]+\tfrac{1}{2}f_{12}^2 N_{ss}^{PY}(r_{12})^2\Delta_1(-l_{12}^2/v)\}, \tag{5.11}$$

where the function χ^{PY} is defined by

$$\nabla_1^{\Phi} Y_{12}^{\Phi} = \chi_{12}^{PY}\hat{r}_{21}, \tag{5.12}$$

and stisfies the equation (which follows from (5.2) and (5.3)):

$$\chi_{12}^{PY} = \chi_{12}^{(0)PY}+h_{12}\varrho \int d\boldsymbol{r}_3(\hat{r}_{21}\hat{r}_{31})\chi_{13}^{PY}[\lambda_{32}+Y_{32}^{PY}+N_{dd}^{PY}(r_{32})], \tag{5.13}$$

where

$$\chi_{12}^{(0)PY} = [h_{12}+f_{12}^2 N_{ss}(r_{12})]d\lambda_{12}/dr_{12}. \tag{5.14}$$

Eq. (5.11) may be written as:

$$\tau^{PY} = \tau_2^{PY}+\tau_3^{PY}, \tag{5.15}$$

$$\tau_2^{PY} = \varrho^2 \int d\boldsymbol{r}_1 d\boldsymbol{r}_2 \{[h_{12}+f_{12}^2 N_{ss}^{PY}(r_{12})]\,[\Delta_1(-l_{12}^2/v)+(-2v)N_{dd}^{PY}(r_{12})\Delta_1\lambda_{12}]$$
$$+\tfrac{1}{2}f_{12}^2 N_{ss}^{PY}(r_{12})^2\Delta_1(-l_{12}^2/v)\}, \tag{5.16}$$

$$\tau_3^{PY} = -2v\varrho^3 \int d\boldsymbol{r}_1 d\boldsymbol{r}_2 d\boldsymbol{r}_3(\hat{r}_{21}\hat{r}_{31})\chi_{12}^{(0)PY}\chi_{13}^{PY}[\lambda_{32}+Y_{32}^{PY}+N_{dd}^{PY}(r_{32})]. \tag{5.17}$$

6. *Discussion*

Our result for τ^{CH}, Eq. (3.3), differs from the expression for τ^{CH} given by Fantoni and Rosati in [10]. Namely, in place of the factor $h_{12}h_{13}$ in our expression (3.3), a factor $f_{12}^2 f_{13}^2$ is printed in Eq. (A.4) of [10]. As a consequence, the expression for τ^{CH} of [10] gives the term linear in h with the wrong sign.

Our result for τ^{HNC} differs from the expression for τ^{HNC} of Fantoni and Rosati (Eqs (4), (5), and (6) of [14]), whose expression for τ_3^{HNC} differs from our expression (4.17) by the presence of the function χ_{12} in place of $\chi_{12}^{(0)}$. This incorrect form of τ_3^{HNC} of [14] leads to erroneous terms of third and higher orders in h in the PS expansion of τ^{HNC}.

Recently, Fantoni and Rosati [22] have corrected their expression for τ^{HNC}, and have shown its equivalence to the expression for τ^{HNC} given by us in [21]. Consequently, the whole problem of τ^{HNC} is now completely clarified (as well as that of τ^{CH}; the expression for τ^{HNC}, when properly simplified to the case of the CH approximation, leads to our Eq. (3.3)).

The expression for τ^{HNC}, given in [21], contains two functions χ_{12} and $\mu_{12} = \Delta_1^{\Phi} Y_{12}$. As shown in Section 4, we may eliminate μ with the help of identity (4.9). By doing it, we have obtained expressions for τ^{HNC} which are simpler that the otherwise correct expression given in [21].

The simplest expressions for τ^{HNC} are given in (4.10) and (4.14). Effectively, they involve only one-dimensional integration (over r_{12}). Of course, first one has to solve the integral equation (4.12) for χ.

The expression for τ^{HNC}, given in Eqs (4.15–17), appears much more complicated because τ_3^{HNC} effectively involves three-dimensional integration (over r_{12}, r_{13}, and r_{23}). Of course, if we replace χ_{13} in (4.17) by $\chi_{13}^{(0)}$, the resulting approximate expression for τ_3^{HNC} (which is exact up to terms $\sim h^2$) becomes useful because it does not require solving the integral equation for χ.

Obviously, the easiest procedure is to neglect τ_3^{HNC} altogether, i.e., to use the approximation $\chi \simeq \chi^{(0)}$ in (4.14). In this approximation, only the part of τ^{HNC} linear in h is exactly reproduced. In this approximation, used by Lantto and Siemens [18] in determining the optimal correlation function, the expression for τ^{HNC} of [14] is correct.

These approximations, in which some terms in τ^{HNC} of order in h higher than linear or quadratic are neglected, are certainly justified at not too high densities. Then, however, one might simply use one or two first terms of the PS expansion. On the other hand, one should be careful with these approximations at higher densities.

Our expressions for τ in the PY approximation are slightly more complicated than in the HNC approximation. Eq. (5.8) appears to be the simplest expression for τ^{PY}. So far, no explicit expressions for τ^{PY} have been published in the literature.

The results of this paper are presently applied in studying the spin-isospin stability of dense nuclear matter. The results obtained so far with the Iwamoto–Yamada [4–5] cluster expansion method indicate a possible spin-isospin instability of nuclear matter with pure hard core interaction. However, this occurs at very high density where the convergence of the cluster expansion is doubtful [19–20]. We expect to settle the problem of the possible spin-isospin instability with the help of the HNC method. Now, in case of pure hard core interaction, the total energy is the kinetic energy. Furthermore, to settle the problem of spin-isospin instability, we need comparatively high calculational accuracy. This is the reason for our careful examination of the expression for τ which in itself forms only a small fraction of the total kinetic energy.

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