Method of correlated basis functions and FHNC theory

1982 J. Phys. A: Math. Gen. 15 1715

(http://iopscience.iop.org/0305-4470/15/5/032)

J. Phys. A: Math. Gen. **15** (1982) 1715–1731. Printed in Great Britain

Method of correlated basis functions and FHNC theory

P Hatzikonstantinou and J M Irvine

Department of Theoretical Physics, The University, Manchester M13 9PL, UK

Received 7 September 1981

Abstract. A method for the accurate evaluation of the diagonal and off-diagonal matrix elements of the Hamiltonian operator within the correlated basis function scheme is presented. Considering a basis consisting of Slater determinants correlated with a Jastrow correlation factor, the expectation value of the kinetic energy operator has been expressed in the Jackson–Feenberg form. A diagrammatic analysis is presented for the construction and evaluation of the cluster expansions of the required quantities incorporating the Fermi hypernetted chain theory.

1. Introduction

The correlated basis functions (CBF) seem to provide a particularly powerful means of studying a strongly interacting system, where special long-range correlations are present. The method has been applied by Clark and coworkers (Clark *et al* 1979, Clark and Westhaus 1966 (CW)) to describe weak state-dependent correlations, which are entirely due to the antisymmetry of the wavefunctions of the system and not to the short-range (state-independent) correlation operators. More recently Krotscheck and Clark (KC 1979) have formulated a scheme to evaluate certain quantities incorporating the Fermi hypernetted chain (FHNC) approximation which permits an extensive collection and resummation of cluster diagrams. They have considered a state-independent correlation function and their analysis is based on the Clark–Westhaus (CW, Clark 1979) form for the ground-state energy expectation value.

The present work is devoted to the derivation and analysis of a graphical scheme, incorporating the FHNC approximation, for the evaluation of certain quantities which are expressed in terms of diagonal and non-diagonal matrix elements of the Hamiltonian operator within the CBF method. Using normalised but non-orthogonal wavefunctions employing a Jastrow correlation factor, we express the expectation value of the kinetic energy in the Jackson–Feenberg (JF) (Clark 1979) form. Our scheme compared with that of KC does not include terms depending on a three-body effective interaction, so that the main contribution to the energy comes from terms depending on a two-body effective interaction, and consequently we can evaluate the required quantities more easily than KC within a FHNC approximation which maintains the Fermi cancellation, keeping terms which incorporate non-local effective potentials.

Let us consider an infinitely extended Fermion system with a finite density $\rho = \nu k_F^3/6\pi^2$, ν being the spin–isospin degeneracy factor. Then a set of non-orthogonal trial wavefunctions is constructed in the form

$$|\psi_m\rangle = F|\phi_m\rangle\langle\phi_m|F^+F|\phi_m\rangle^{-1/2} \tag{1.1}$$

0305-4470/82/051715+17$02.00

where the Jastrow correlation operator F and the complete set ϕ_m of Slater determinants are defined as follows:

$$F = \prod_{i<j} f(ij) \tag{1.2}$$

$$\phi_m = (N!)^{-1/2} |m_1, m_2, \ldots, m_A\rangle_\alpha, \qquad m = \{m_1, m_2, \ldots, m_A\}. \tag{1.3}$$

The α means 'antisymmetrised'. Each m_i signifies a distinct collection of single-particle quantum numbers. The uncorrelated ground state is defined as $\phi_0 = \phi_F$ where $0 = \{0_1, 0_2, \ldots, 0_A\}$ corresponds to the Fermi sea. The system is described by a Hamiltonian with the configuration space form

$$H = \sum_{i=1} t(i) + \sum_{i<j} V(ij) \tag{1.4}$$

where $t(i) = -(\hbar^2/2m)\nabla_i^2$ with

$$\varepsilon_{m_i}^{(1)} = \langle m_i | t(i) | m_i \rangle = \hbar^2 k_{m_i}^2 / 2m \tag{1.5}$$

and $V(ij)$ is a two-body state-independent potential.

The expectation values of the Hamiltonian and unit operators with respect to the normalised wavefunctions (1.1) are given by

$$H_{mn} = h_{mn} / [I_{mm} I_{nn}]^{1/2}, \tag{1.6}$$

$$N_{mn}^{(1)} = I_{mn} / [I_{mm} I_{nn}]^{1/2}, \tag{1.7}$$

where

$$h_{mn} = \langle \phi_m | F^+ H F | \phi_n \rangle, \qquad I_{mn} = \langle \phi_m | F^+ F | \phi_n \rangle. \tag{1.8}$$

Since momentum conservation implies that H_{mn} and $N_{mn}^{(1)}$ vanish unless $\Sigma_i \boldsymbol{k}_{m_i} = \Sigma_i \boldsymbol{k}_{n_i}$ it is evident that matrix elements using sets m and n which differ only in one single-particle state are zero. Hence in the case of a state-independent potential our simplest choice is to assume configurations which differ only in two states. The sequence of states can be arranged such that $m_1 \neq n_1, n_2$; $m_2 \neq n_1, n_2$ and $m_i = n_i$ for $i > 2$. Either of the sets m, n may coincide with the set 0. The matrix elements H_{mn} and $N_{mn}^{(1)}$ have certain symmetries that are Hermitian and are invariant under a unitary transformation of the model functions ϕ_m, ϕ_n.

Quantities which are going to be evaluated in full analogy with the evaluation of the ground-state energy are:

(i) the diagonal expressions

$$G^{mm} - G^{nn} = \ln I_{mm} - \ln I_{nn}, \tag{1.9}$$

$$H_{mm} - H_{nn} = T_F^m - T_F^n + \frac{\partial}{\partial \beta} [G^{mm}(\beta) - G^{nn}(\beta)]|_{\beta=0}, \tag{1.10}$$

with $T_F^m = \Sigma_i \varepsilon_{m_i}^{(1)}$ and $G^{mm}(\beta) = \ln I_{mm}(\beta)$;

(ii) the off-diagonal matrix elements

$$W_{mn} = H_{mn} - \tfrac{1}{2}(H_{mm} + H_{nn}) N_{mn}^{(1)}. \tag{1.11}$$

The generalised normalisation integral $I_{mn}(\beta)$ is given by

$$I_{mn}(\beta) = (N!)^{1/2} \langle \phi_m | F^+ \exp[\beta(H - T_F^m)] F \prod_i \left(1 + \alpha_i \frac{|n_i\rangle}{|m_i\rangle}\right) \prod_i |m_i\rangle|_{\alpha_1 = \ldots = \alpha_N = 0}. \tag{1.12}$$

2. General formalism

The kinetic energy contribution to the expectation value of h_{mn}/I_{mn} is given by

$$\frac{(h_{mn})_T}{I_{mn}} = \frac{\hbar^2}{2m} I_{mn}^{-1} \sum_i \langle -\nabla_i^2 \rangle, \tag{2.1}$$

$$\langle -\nabla_i^2 \rangle = \langle \phi_m | F(-\nabla_i^2) F | \phi_n \rangle. \tag{2.2}$$

Equation (2.2) can be written in two alternative forms

$$\langle -\nabla_i^2 \rangle_{\mathrm{CW}} = -\tfrac{1}{2} \int F^2 \phi_m^* \nabla_i^2 \phi_n \, \mathrm{d}\tau + \mathrm{HC} + \int \phi_m^* \phi_n (\nabla_i F)^2 \, \mathrm{d}\tau \tag{2.3}$$

and

$$\langle -\nabla_i^2 \rangle = \int \nabla_i (F\phi_m^*) \nabla_i (F\phi_n) \, \mathrm{d}\tau = \int (F^2 \nabla_i \phi_m^* \nabla \phi_n - \phi_m^* \phi_n F \nabla_i^2 F) \, \mathrm{d}\tau \tag{2.4}$$

or alternatively

$$\langle -\nabla_i^2 \rangle_{\mathrm{CF}} = -\tfrac{1}{2} \int F^2 \phi_m^* \nabla_i^2 \phi_n \, \mathrm{d}\tau + \mathrm{HC} + \int [\tfrac{1}{2} F^2 \nabla_i^2 (\phi_m^* \phi_n) - \phi_m^* \phi_n F \nabla_i^2 F] \, \mathrm{d}\tau \tag{2.5}$$

where $\mathrm{d}\tau$ represents the $3N$-dimensional volume element $\mathrm{d}\boldsymbol{r}_1 \, \mathrm{d}\boldsymbol{r}_2 \ldots \mathrm{d}\boldsymbol{r}_N$. Equations (2.3) and (2.5) correspond to the CW and CF (Clark–Feenberg) forms for the kinetic energy respectively. Taking the average of (2.3) and (2.5), we arrive at the JF form for the kinetic energy

$$\langle -\nabla_i^2 \rangle_{\mathrm{JF}} = \tfrac{1}{2} \left(\int \phi_m^* F^2 \nabla_i^2 \phi_n \, \mathrm{d}\tau + \mathrm{HC} \right) - \tfrac{1}{4} \int \phi_m^* \phi_n F^2 \nabla_i^2 \ln F^2 \, \mathrm{d}\tau + \tfrac{1}{4} \int F^2 \nabla_i^2 (\phi_m^* \phi_n) \, \mathrm{d}\tau. \tag{2.6}$$

Using equations (1.8) and (2.6) we finally arrive at the expression

$$h_{mn}/I_{mn} = \tfrac{1}{2}(T_{\mathrm{F}}^m + T_{\mathrm{F}}^n) + I_{mn}^{-1} \langle \phi_m | F V^* F | \phi_m \rangle + W_{mn}^{(1)} \tag{2.7}$$

with

$$V^* = \tfrac{1}{2} \sum_{i \neq j} W_2(ij), \qquad W_2(ij) = -\frac{\hbar^2}{4m} \nabla_i^2 \ln f^2(ij) + V(ij),$$

$$W_{mn}^{(1)} = \frac{\hbar^2 \rho}{8m} \int \nabla_i^2 g_{mn}(\boldsymbol{r}_1) \, \mathrm{d}\boldsymbol{r}_1. \tag{2.8}$$

The operator ∇_1^2 acts only upon the functions ϕ_m and ϕ_m^*. The non-diagonal matrix elements of the single-particle distribution function $g_{mn}(\boldsymbol{r}_1)$ are defined by

$$\rho g_{mn}(\boldsymbol{r}_1) = N I_{mn}^{-1} \int \phi_m^* \phi_n F^2 \, \mathrm{d}\boldsymbol{r}_2 \, \mathrm{d}\boldsymbol{r}_3 \ldots \mathrm{d}\boldsymbol{r}_N. \tag{2.9}$$

Equation (2.7) can be re-expressed as

$$\frac{h_{mn}}{I_{mn}} = \tfrac{1}{2}(T_{\mathrm{F}}^m + T_{\mathrm{F}}^n) + \frac{\partial}{\partial \beta} \ln I_{mn}(\beta)|_{\beta=0} \tag{2.10}$$

where the generalised normalisation integral $I_{mn}(\beta)$ is defined by

$$I_{mn}(\beta) = n_{mn}(\beta) \exp(\beta W_{mn}^{(1)}), \qquad n_{mn}(\beta) = \langle \phi_m | F \exp(\beta V^*) F | \phi_n \rangle. \tag{2.11}$$

Using the definition (1.7) we can write

$$N^{(1)}_{mn}(\beta) = N_{mn}(\beta)\exp\{\beta[W^{(1)}_{mn} - \tfrac{1}{2}(W^{(1)}_{mm} + W^{(1)}_{nn})]\}, \tag{2.12}$$

$$N_{mn}(\beta) = n_{mn}(\beta)[n_{mm}(\beta)n_{nn}(\beta)]^{-1/2}, \tag{2.13}$$

with $N^{(1)}_{mn} = N^{(1)}_{mn}(0) = N_{mn}(0)$.

Using the above definitions for $I_{mn}(\beta)$ we can evaluate all the required quantities in terms of cluster expansions of $I_{mn}(\beta)$ and $N^{(1)}_{mn}(\beta)$.

3. FHNC theory and matrix elements of the unit operator

The matrix elements which are involved in the CBF method are expressed in a series of cluster terms represented by diagrams which can be resummed within the FHNC approximation. In the FHNC procedure a set of quantities is constructed, each one of which represents an infinite partial summation of cluster terms, and their evaluation is performed by means of integral equations.

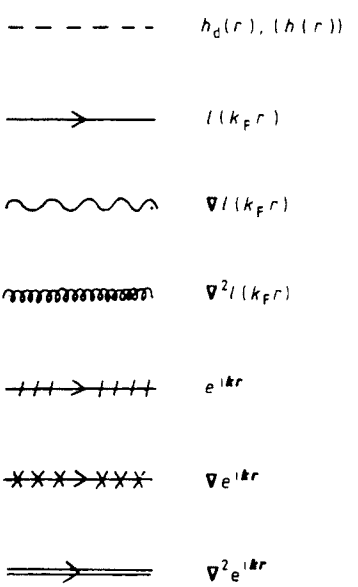

Figure 1. The simplest elements used in the construction of the diagrammatic representation of the cluster terms. The function in parentheses indicates the bare correlation line $h(r)$.

In this section we review the main definitions and the diagrammatic notation which are compatible with those developed in the articles of KC and Clark (1979).

A diagram is constructed using a number of dynamical (broken) and exchange (full) lines which represent factors

$$h(r_{ij}) = f^2(r_{ij}) - 1 \qquad \text{and} \qquad \nu^{-1} l(k_F r_{ij}) = j_1(k_F r_{ij})/\nu k_F r_{ij} \tag{3.1}$$

respectively. The lines end in open and full dots which are called external and internal points respectively. The exchange lines form closed loops each one of which introduces

a factor $-\nu$. An open dot indicates a dependence on the particle coordinates represented and a full dot represents an integration over the dummy coordinates of a particle accompanied by a density factor ρ.

Important quantities involved in our analysis are constructed by series connection of diagrams which contribute to the two-body distribution function $g(r_{12})$ evaluated with the 'ground-state' wavefunction of the form $\psi_0 = F\phi_0$. Accordingly we consider the sum of diagrams Γ_{ab} with $ab = dd$, de and ee signifying whether none, one or two exchange lines are attached to its external points. The sum Γ_{ab} is decomposed into the sum N_{ab} of nodal and the sum X_{ab} of non-nodal diagrams. The function $h_d(r_{12}) = \Gamma_{dd}(r_{12})$ is determined by the set of coupled equations

$$\begin{aligned} h_d(r) &= f^2(r)\exp[N_{dd}(r) + E_{dd}(r)] - 1, \\ \tilde{N}_{dd}(k) &= \tilde{h}_d(k)\{1 - [1 - \tilde{X}_{de}(k)]^2/[1 + (1 + \tilde{X}_{ee}(k))\tilde{h}_d(k)]\}, \end{aligned} \tag{3.2}$$

where E_{dd} is the sum of the elementary diagrams (representing non-nodal diagrams which do not decompose into two or more independent factors). The tilde denotes the Fourier transform following the notation

$$\tilde{A}(k) = \rho \int A(r)\, e^{ikr}\, dr, \qquad A(r) = \frac{1}{(2\pi)^3 \rho} \int \tilde{A}(k)\, e^{-ikr}\, dk. \tag{3.3}$$

The set of FHNC equations (3.2) may be solved following a sequence of successive approximations beginning with $E_{dd} = 0$. The sets X_{de} and X_{ee} are evaluated either by successive truncation of their cluster series within the KR-FHNC scheme (Krotscheck and Ristig 1975, Krotscheck 1977) or by means of the additional set of four coupled nonlinear integral equations within the FR-FHNC scheme (Fantoni and Rosati 1975). An alternative method to obtain the sets h_d and N_{dd} is to solve the equations (3.2) in conjunction with a variationally obtained Euler–Lagrange equation or system of equations within an optimisation scheme which minimises the ground-state energy (Owen 1979b, Lantto and Siemens 1977). Of course the function $h_d(r)$ may be evaluated by truncating its cluster expansion or by means of the Percus–Yevick integral.

In figure 2(a) the leading graphs of $h_d(r)$ are shown. The process of the systematic resummation of diagrams is further extended by replacing each bare correlation line $h(r)$ by the dressed correlation line $h_d(r)$. Before proceeding to our analysis we review the evaluation of certain quantities within the CBF scheme, following the technique developed by KC.

An observation shows that the diagrammatic contributions to the diagonal matrix elements

$$G^{mm}(0) = \ln\langle\phi_m|FF|\phi_m\rangle \tag{3.4}$$

are generated from the diagrams of the generating function $G^{00}(0)$ by substituting for the Slater function $l(k_F r_{ij})$ its generalised form

$$l_m(r_{ij}) = N^{-1} \sum_{l=1}^{N} \exp(i\boldsymbol{k}_{m_l} \cdot \boldsymbol{r}_{ij}) \tag{3.5}$$

where $\boldsymbol{k}_{m_l}$ are the associated wavevectors with the set of orbitals m. Hence, neglecting terms of order N^{-1}, the difference $G^{mm}(0) - G^{nn}(0)$ is expanded in cluster terms containing at most one of the single-particle states m_1, m_2, n_1 and n_2 so that

$$G^{mm}(0) - G^{nn}(0) = \delta G(m_1) + \delta G(m_2) - \delta G(n_1) - \delta G(n_2) \tag{3.6}$$

with

$$\delta G(m_l) = N^{-1} \int \frac{\delta G^{00}(0)}{\delta l(k_F r_{ij})} \exp(\mathrm{i}\boldsymbol{k}_{m_l} \cdot \boldsymbol{r}_{ij})\, \mathrm{d}\boldsymbol{r}_1\, d\boldsymbol{r}_2. \tag{3.7}$$

The diagrammatic expansion of $\delta G(m_l)$ is obtained from the graphical expansion of $G^{00}(0)$ by removing, in turn, each exchange line $l(k_F r_{ij})$ and converting the pair of

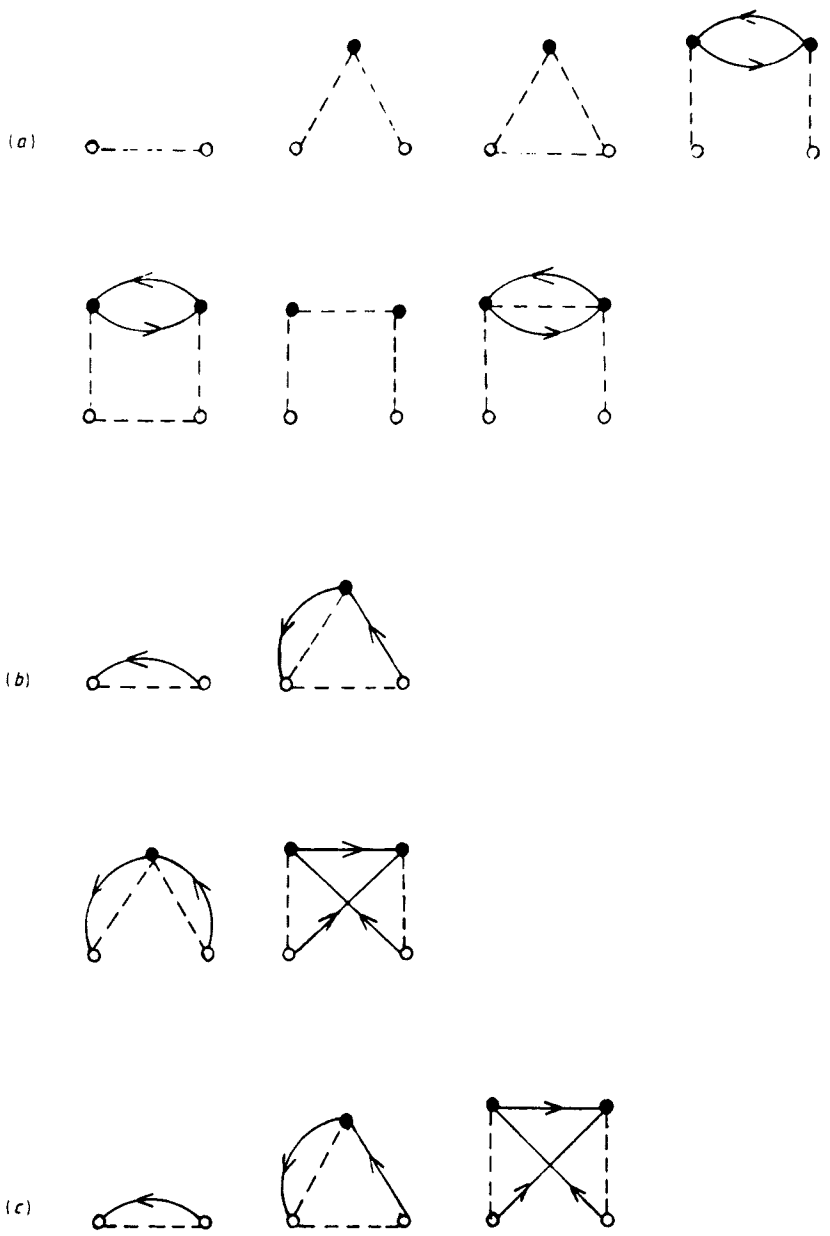

Figure 2. (*a*) All contributions to $h_d(r_{12}) \equiv \Gamma_{dd}(r_{12})$ with no more than three correlation lines and four points. (*b*) and (*c*) represent all contributions to $\delta G(r_{12})$ and $X_{cc}(r_{12})$ respectively with no more than two dressed correlation lines and four points.

points i, j to external points. Before starting the construction of $\delta G(m_l)$ the function $G^{00}(0)$ is expanded using the IY method or the PS method (Clark 1979) after the collection of all 'equivalent' diagrams, in order to avoid complications arising from the sums over the single-particle states.

The process of series connection of diagrams yields the expression

$$\delta G(m_l) = -\ln[1 - \tilde{X}_{cc}(k_{m_l})] \tag{3.8}$$

where $\tilde{X}_{cc}(k_{m_l})$ is the Fourier transform of the function $X_{cc}(r)$ which is constructed from the function $\nu^{-1}l(k_F r_{12})$, by adding the sum of the non-nodal contributions to $g(r)$, with a single exchange line joining its external points. The sum $X_{cc}(r)$ is defined by the set of coupled FHNC equations

$$\begin{aligned} X_{cc}(r) &= h_d(r)[N_{cc}(r) + E_{cc}(r) - \nu^{-1}l(k_F r)] + E_{cc}(r) \\ \tilde{N}_{cc}(k) &= [\tilde{X}_{cc}(k) - \nu^{-1}\tilde{l}(k)]\tilde{X}_{cc}(k)/(1 - \tilde{X}_{cc}(k)), \end{aligned} \tag{3.9}$$

where $\nu^{-1}\tilde{l}(k) = \theta(k_F - k)$ is the Heaviside unit step function. Again an approximate solution of the equations (3.9) is obtained by setting $E_{cc}(r) = 0$. The first few diagrams of $G^{00}(0)$, $\delta G(r)$ and $X_{cc}(r)$ with no more than two correlation lines are shown in figures 3, 2(b), and 2(c) respectively.

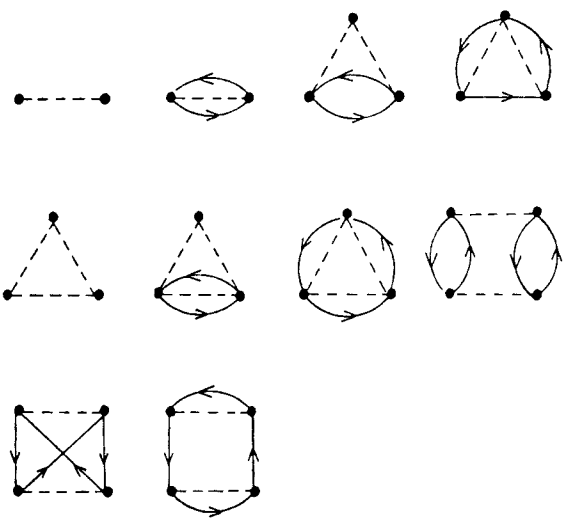

Figure 3. Diagrams which contribute to $G^{00}(0)$ with no more than three dressed correlation lines and four points.

The off-diagonal matrix elements of the unit operator N_{mn} may be written

$$N_{mn} \equiv N_{mn}(0) = \sum_{s,t} (\Delta N_{mn})_s^{(t)}, \tag{3.10}$$

$$(\Delta N_{mn})_s^{(t)} = \sum_{j(1)\ldots j(p)} \langle m_1 m_2 j(1)\ldots j(p-2)|D(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_p)|A(n_1 n_2 j(1)\ldots j(p-2)\rangle. \tag{3.11}$$

The indices $s = p+2$ and t stand for the number of particles (points) and the number of dynamical lines h_d with $1 \leqslant i, j \leqslant p$ respectively. The function $D(\boldsymbol{r}_i \ldots \boldsymbol{r}_p)$ is a product of the functions h_d.

Following the KC analysis for the shifting of the orbitals n_1, n_2 out of the permutation operator A, equation (3.10) can be expressed in the 'dressed form'

$$N_{mn} = \langle m_1 m_2 | N(12; 1'2') | n_1 n_2 \rangle_\alpha \tag{3.12}$$

where a factorisation of the non-local operator $N(12; 1'2')$ leads to the relation

$$N_{mn} = \frac{\langle m_1 m_2 | N^{\mathrm{D}}(12; 1'2') | n_1 n_2 \rangle_\alpha}{[(1-\hat{X}_{cc}(m_1))(1-\hat{X}_{cc}(m_2))(1-\hat{X}_{cc}(n_1))(1-\hat{X}_{cc}(n_2))]^{1/2}} \tag{3.13}$$

where

$$\begin{aligned}
N^{\mathrm{D}}(12; 1'2') &= N^{\mathrm{D}}_{dd}(12; 1'2') + N^{\mathrm{D}}_{dcc}(12; 1'2') + N^{\mathrm{D}}_{dcc}(21; 2'1') + N^{\mathrm{D}}_{cc,cc}(12; 1'2') \\
&\quad + N^{\mathrm{D}}_{cc,cc}(21; 1'2'), \\
N^{\mathrm{D}}_{dd}(12; 1'2') &= N^{\mathrm{D}}_{dd}(1, 2)\delta(\boldsymbol{r}_1 - \boldsymbol{r}_{1'})\delta(\boldsymbol{r}_2 - \boldsymbol{r}_{2'})\delta_{\sigma_1\sigma_{1'}}\delta_{\sigma_2\sigma_{2'}}, \\
N^{\mathrm{D}}_{dcc}(12; 1'2') &= N^{\mathrm{D}}_{dcc}(\boldsymbol{r}_1, \boldsymbol{r}_2; \boldsymbol{r}'_1, \boldsymbol{r}'_2)\delta(\boldsymbol{r}_2 - \boldsymbol{r}_{2'})\delta_{\sigma_1\sigma_{1'}}\delta_{\sigma_2\sigma_{2'}}, \\
N^{\mathrm{D}}_{cc,cc}(12; 1'2') &= N^{\mathrm{D}}_{cc,cc}(\boldsymbol{r}_1, \boldsymbol{r}_2; \boldsymbol{r}'_1, \boldsymbol{r}'_2)\delta_{\sigma_1\sigma_{1'}}\delta_{\sigma_2\sigma_{2'}}.
\end{aligned} \tag{3.14}$$

The local portion of $N^{\mathrm{D}}(12; 1'2')$ is determined to be $N^{\mathrm{D}}_{dd}(r_{12}) = h_{\mathrm{d}}(r_{12})$.

Within the above representation of N_{mn} the reducibility and irreducibility are defined as follows.

A diagrammatic contribution to N_{mn} is defined as reducible if it may be factorised (non-trivially) in such a way that at least one of the factors depends on only one of the state labels m_1, m_2, n_1, n_2.

A diagram is defined as basic if it is irreducible and does contain proper i–j subdiagrams with exchange lines attached to i or j or both, except the single correlation line.

The leading diagrams of the non-local parts $(\nu/\rho)N^{\mathrm{D}}_{dcc}(12; 1'2')$ and $(\nu/\rho)^2 N^{\mathrm{D}}_{cc,cc}(12; 1'2')$ are shown in figure 4 by the sets (a) and (b) respectively. More precisely, considering that the broken line represents the 'dressed' correlation factor $h_{\mathrm{d}}(r_{ij})$, the former function above sums all the basic diagrams with three external points 1, 1', 2 and an exchange line connecting the points 1 and 1'. There is no exchange line which ends on the point 2. The latter function sums all the basic diagrams having four external points 1, 1', 2, 2' with exchange lines connecting the pairs of points 1, 1' and 2, 2'. If the broken line represents a simple correlation function instead of the dressed bond function $h_{\mathrm{d}}(r_{ij})$, the word 'basic' must be replaced by the word 'irreducible' in the definitions of the non-local portions of $N^{\mathrm{D}}(12; 1'2')$. In the case where $m_1 \to n_1$ or $m_1 \to n_2$ a number of diagrams cancel out (figure 4(c)).

In the thermodynamic limit with fixed density the 'diagonal' G functions are proportional to N and the quantity N_{mn} behaves like N^{-1}.

4. Matrix elements of the Hamiltonian

In this section we will study the evaluation of the diagonal and non-diagonal matrix elements of the Hamiltonian within a Fermi hypernetted chain approximation scheme, which consistently preserves the Fermi cancellation effects. As we have mentioned in §1, our diagrammatical analysis is based on the Jackson–Feenberg form for the kinetic energy. In the graphical representation of the terms which contribute to the

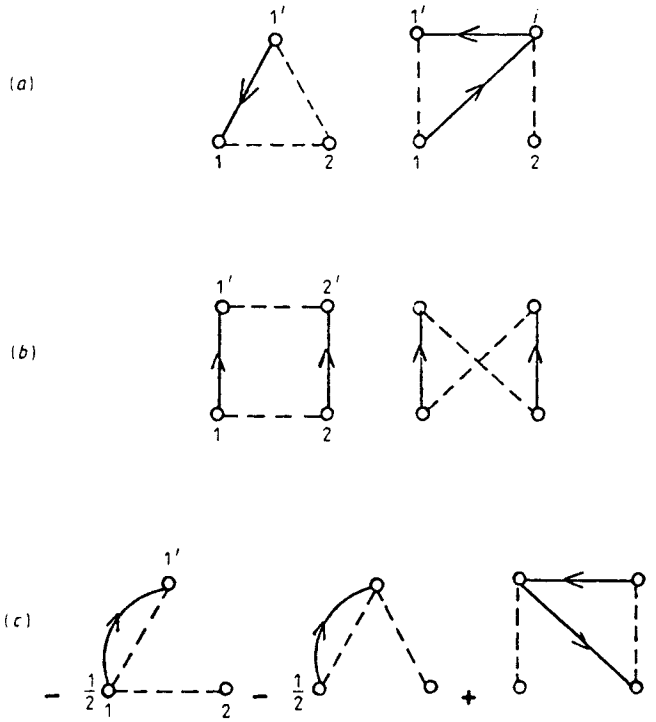

Figure 4. (*a*) and (*b*) 'asymmetrical' diagrammatic contributions to $(\nu/\rho)N^{D}_{dcc}(12;1'2)$ and $(\nu/\rho)^2 N^{D}_{cc,cc}(12;1'2')$ respectively with no more than two dressed correlation lines. The full function $(\nu/\rho)N^{D}_{dcc}(12;1'2)$ is obtained by averaging over the diagrams shown in the figure plus those obtained from the latter by exchanging the coordinates 1 and 1'. The full function $(\nu/\rho)^2 N^{D}_{cc,cc}(12;1'2')$ is obtained as above by exchanging the coordinate pairs (1, 1') and (2, 2'), (1, 2) and (1'2'), and both. (*c*) Example of diagrams which cancel for $m_1 \to n_1$ or $m_1 \to n_2$.

matrix elements the broken line represents the dressed correlation function $h_d(r)$ rather than the bare correlation $h(r)$.

We begin the study of the diagonal matrix elements of the Hamiltonian, expressing the generating functions G, in terms which represent compound diagrammatic sums.

From (1.9) and (2.11) we obtain

$$G^{mm}(\beta) = G_2^{mm}(\beta) + \beta W^{(1)}_{mm} \tag{4.1}$$

defining

$$G_2^{mm}(\beta) = \ln n_{mm}(\beta), \qquad G^{mm}(0) = G_2^{mm}(0). \tag{4.2}$$

Considering the relations (3.6) and (3.7), equation (1.10) takes the form

$$H_{mm} - H_{nn} = T^m_F - T^n_F + u(m_1) + u(m_2) - u(n_1) - u(n_2) + W^{(1)}_{mm} - W^{(1)}_{nn} \tag{4.3}$$

where

$$u(m) = \tilde{X}'_{cc}(m)/(1 - \tilde{X}_{cc}(m)). \tag{4.4}$$

The diagonal quantities $W^{(1)}$ are defined by (2.8) with $m = n$. The prime denotes a derivative with respect to β.

In order to evaluate the difference $W^{(1)}_{mm} - W^{(1)}_{nn}$ we write (in the thermodynamic limit)

$$W^{(1)}_{mm} - W^{(1)}_{nn} = \frac{\hbar^2\rho^2}{8m}\int \nabla_1^2[g_2^{mm}(r_{12}) - g_2^{nn}(r_{12})]\,\mathrm{d}\boldsymbol{r}_2\,\mathrm{d}\boldsymbol{r}_1 \tag{4.5}$$

where the diagonal '$g_2(r_{12})$' functions represent the two-body distribution function. The difference under the integration can be written

$$\begin{aligned}\rho^2[g_2^{mm}(r) - g_2^{nn}(r)] &= \frac{\partial}{\partial\beta}[G_2^{mm}(\beta) - G_2^{nn}(\beta)]|_{\beta=0} \\ &= [\delta G'(m_1,\beta) + \delta G'(m_2,\beta) - \delta G'(n_1,\beta) - \delta G'(n_2,\beta)]|_{\beta=0}.\end{aligned} \tag{4.6}$$

Here $f(r)$ is redefined as $f(r,\beta) = f(r)\exp[\frac{1}{2}\beta\bar{w}_2(r)]$ and $\bar{w}_2(ij) = \delta(\boldsymbol{r}_1 - \boldsymbol{r}_i')\delta(\boldsymbol{r}_2 - \boldsymbol{r}_j') + \delta(\boldsymbol{r}_1 - \boldsymbol{r}_j')\delta(\boldsymbol{r}_2 - \boldsymbol{r}_i')$. The graphical contributions to the distribution functions $g_2^{mm}(r)$ and $g_2^{nn}(r)$ are obtained from the diagrammatic expansion of the quantities $\delta G'(m,\beta)$ by means of equation (3.7).

Some of the leading contributions to $\delta G'(m,\beta)|_{\beta=0}$ can be obtained from the diagrams of $\delta G(r_{12})$, which have been shown in figure 2(*b*), adding a line which represents the plane wave factor $l(\boldsymbol{k}_m \cdot \boldsymbol{r}_{12}) = \exp(\mathrm{i}\boldsymbol{k}_m \cdot \boldsymbol{r}_{12})$.

Substituting (4.6) into (4.5), we may write

$$W^{(1)}_{mm} - W^{(1)}_{nn} = W^{(1)}(m_1) + W^{(1)}(m_2) - W^{(1)}(n_1) - W^{(1)}(n_2) \tag{4.7}$$

where $W^{(1)}(m)$ is defined by the right-hand side of equation (4.5) after the replacement of the quantity within the brackets by $\delta G'(m)$.

We return now to the evaluation of (4.5). The diagrammatic decomposition of the quantities $W^{(1)}(m)$ may be obtained as follows. We take all diagrams contributing to $\delta G'(m)$ and replace, in turn, each exchange line $l(k_F r_{1j})$ and wavefactor $l(\boldsymbol{k}_m \cdot \boldsymbol{r}_{12})$ by $\nabla_1^2 l(k_F r_{1j})$ and $\nabla_1^2 l(\boldsymbol{k}_m \cdot \boldsymbol{r}_{12})$ respectively. In addition we replace, in turn, each connected pair of lines $l(k_F r_{1j})l(\boldsymbol{k}_m \cdot \boldsymbol{r}_{12})$ by $2\nabla_1 l(k_F r_{1j}) \cdot \nabla_1 l(\boldsymbol{k}_m \cdot \boldsymbol{r}_{12})$. The least complicated diagrams are shown in figure 5. We have included all the diagrams with no more than two dressed correlation lines. In figure 1 we present the basic elements which are used in the construction of diagrams.

The contributions to $\tilde{X}'_{cc}(m)$ are obtained by replacing in turn each correlation line in the diagrammatic representation of $\tilde{X}_{cc}(m)$ by an effective interaction $w_2(ij)$ line.

For the evaluation of the primed quantities it is more convenient to use the dressed effective potential $h'_d(r)$ rather than the bare $w_2(r)$ in conjunction with the term $h_d(r)$ instead of $h(r)$. The physical concept of the dressed functions, which are used in our expressions, is that they incorporate the effects which appear in the presence of the medium.

Constructing the function $h_d(r,\beta)$ from $h_d(r)$, redefining $f^2(r)$ as $f^2(r,\beta) = f(r)\exp[\frac{1}{2}\beta w_2(r)]$ and obtaining the β derivative of (3.2), we arrive at the set of coupled equations

$$\begin{aligned} h'_d(r) &= [h_d(r)+1][w_2(r) + N'_{dd}(r) + E'_{dd}(r)], \\ \tilde{N}'_{dd}(k) &= \tilde{h}'_d(k)\left[1 - \left(\frac{1-\tilde{P}(k)}{1-\tilde{X}_{de}(k)}\right)^2\right] + \frac{\tilde{X}_{dd}(k)}{1-\tilde{X}'_{de}(k)}\left(2\tilde{X}'_{de}(k) + \frac{\tilde{X}_{dd}(k)\tilde{X}'_{ee}(k)}{1-\tilde{X}_{de}(k)}\right), \end{aligned} \tag{4.8}$$

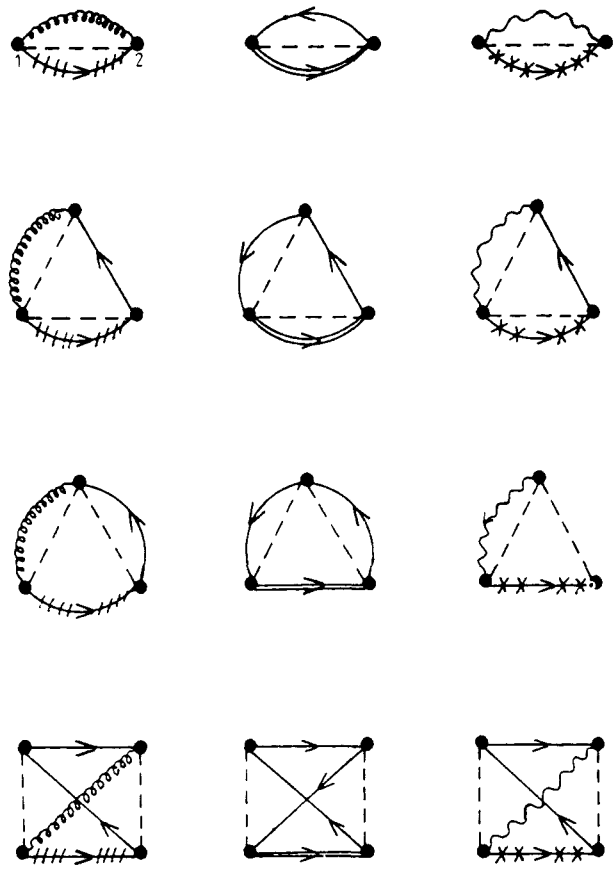

Figure 5. All the diagrams which contribute to $W^{(1)}(k)$ ($k = k_{m_1}$) with no more than two dressed correlation lines.

where

$$h_d(r) = X_{dd}(r) + N_{dd}(r), \tag{4.9}$$

$$\tilde{P}(k) = \tilde{X}_{dd}(k)(1 + \tilde{X}_{ee}(k)) + 2\tilde{X}_{de}(k) - \tilde{X}^2_{de}(k). \tag{4.10}$$

The sums $h_d(r)$ and $\tilde{N}_{dd}(k)$ are defined by the equations (3.2). The quantities $\tilde{X}_{de}$, $\tilde{X}'_{de}$, $\tilde{X}_{ee}$ and $E'_{dd}(r)$ are determined either by keeping the leading terms in suitable diagrammatic expansions or by means of additional integral equations within a FR-FHNC or a variational scheme (Owen 1979b). In a first approximation a simple solution of the set of coupled equations (4.8) is obtained neglecting the sum of the elementary diagrams $E_{dd}(r)$ because of their complexity and setting $E_{dd}(r) = 0$.

Finally the β derivatives of the equations (3.9) lead to the set of coupled linear equations

$$\begin{aligned} X'_{cc}(r) &= h'_d(r)[N_{cc}(r) + E_{cc}(r) - v^{-1}l(k_F r)] + h_d(r)[N'_{cc}(r) + E'_{cc}(r)] + E'_{cc}(r), \\ \tilde{N}'_{cc} &= \tilde{X}'_{cc}\left(\frac{1 - \tilde{l}(k_F r)/v}{(1 - \tilde{X}_{cc})^2}\right) - 1. \end{aligned} \tag{4.11}$$

Again for a simple solution of these equations we set E_{cc} and E'_{cc} zero.

The off-diagonal matrix elements of the Hamiltonian H_{mn} contribute in the evaluation of the quantity W_{mn} which is defined by the equation (1.11).

Introducing the normalising denominators into equation (2.10), we obtain

$$H_{mn} = \tfrac{1}{2}(T_F^m + T_F^n)N_{mn}^{(1)} + \tfrac{1}{2}[I_{mm}(0)I_{nn}(0)]^{-1/2}\frac{\partial}{\partial\beta}(I_{mn}(\beta) + I_{nm}^*(\beta)). \tag{4.12}$$

Using the definitions of the diagonal matrix elements of the Hamiltonian and substituting the equations (2.11) and (4.12) into (1.11) yields

$$W_{mn} = \frac{\partial}{\partial\beta}N_{mn}^{(1)}(\beta)|_{\beta=0} = \frac{\partial}{\partial\beta}N_{mn}(\beta)|_{\beta=0} + N_{mn}(0)[W_{mn}^{(1)} - \tfrac{1}{2}(W_{mm}^{(1)} + W_{nn}^{(1)})] \tag{4.13}$$

where

$$W_{mn}^{(1)} = \frac{\hbar^2\rho^2}{8m}\int \nabla_1^2 g_2^{mm}(r_{12})\,\mathrm{d}\boldsymbol{r}_2\mathrm{d}\boldsymbol{r}_1 = \frac{\hbar^2}{8m}\int \nabla_1^2\left(\frac{\partial}{\partial\beta}\right)\ln(n_{mm}(\beta))\,\mathrm{d}\boldsymbol{r}_2\,\mathrm{d}\boldsymbol{r}_1 \tag{4.14}$$

and β indicates that each factor $f(r)$ has been replaced by $f(r,\beta) = f(r)\exp[\frac{1}{2}\beta\bar{w}_2(r)]$. We obtain by virtue of equation (2.13)

$$W_{mn}^{(1)} = \frac{\hbar^2}{8m}N_{mn}^{-1}(0)\int \nabla_1^2 N'_{mn}(\beta)|_{\beta=0}\,\mathrm{d}\boldsymbol{r}_2\mathrm{d}\boldsymbol{r}_1 + \tfrac{1}{2}(W_{mm}^{(1)} + W_{nn}^{(1)}), \tag{4.15}$$

hence equation (4.13) may be rewritten

$$W_{mn} = \frac{\partial}{\partial\beta}N_{mn}(\beta)|_{\beta=0} + \frac{\hbar^2}{8m}\int \nabla_1^2\left(\frac{\partial}{\partial\beta}N_{mn}(\beta)\right)_{\beta=0}\mathrm{d}\boldsymbol{r}_2\,\mathrm{d}\boldsymbol{r}_1. \tag{4.16}$$

The above equation indicates that the graphical representation of W_{mn} can be derived in a similar way to that for $N_{mn}(\beta)$, when the diagrammatic expansion of $N_{mn}(0)$ is given.

The diagrams which contribute to the quantity W_{mn} are obtained from $N_{mn}(0)$ in the following way. The contributions to W_{mn} from the first term of (4.16) are obtained by taking all the diagrams which contribute to $N_{mn}(0)$ and replacing in turn each correlation line $h(r)$ in a diagram by the effective interaction line $w_2(r)$. The graphical representation of the β derivative of $N_{mn}(\beta)$ under the integration has the same structure as that of the first term of equation (4.16), with the only exception that each $w_2(r)$ line is replaced by the line $\bar{w}_2(r)$. Hence the diagrammatic contributions to W_{mn} from the second term of (4.16) are obtained in the following way. We take all diagrams of the graphical representation of the quantity within the brackets and replace in turn each exchange line $l(k_F r_{1j})$ and wavefactor $l(n_1 - m_1, \boldsymbol{r}_{12})$ or $l(n_2 - m_1, \boldsymbol{r}_{12})$ by $\nabla_1^2 l(k_F r_{1j})$ and $\nabla_1^2 l(n_1 - m_1, \boldsymbol{r}_{12})$ or $\nabla_1^2 l(n_2 - m_1, \boldsymbol{r}_{12})$ respectively. We also replace, in turn, each connected pair of lines $l(n_1 - m_1, \boldsymbol{r}_{12})l(k_F r_{1j})$ and $l(n_2 - m_1, \boldsymbol{r}_{12})l(k_F r_{1j})$ by $2\nabla_1(n_1 - m_1, \boldsymbol{r}_{12})\cdot\nabla_1 l(k_F r_{1j})$ and $2\nabla_1 l(n_2 - m_1, \boldsymbol{r}_{12})\cdot\nabla_1 l(k_F r_{1j})$ respectively. Finally we use the dressed lines $h_d'(r)$ and $h_d(r)$ rather than the bare functions $w_2(r)$ and $h(r)$.

A more elaborate expression for W_{mn} can be obtained using the relation (3.12) for N_{mn}.

By substitution of (2.12) and (2.13) into (4.12) the expectation value of H_{mn} may be written

$$H_{mn} = N'_{mn} + N_{mn}[W_{mn}^{(1)} - \tfrac{1}{2}(W_{mm}^{(1)} + W_{nn}^{(1)})] + \tfrac{1}{2}[H_{mm} + H_{nn}]N_{mn}. \tag{4.17}$$

Neglecting terms $O(N^{-1})$ and considering only terms which do not include more than one of the single-orbital states m_1, m_2, n_1 and n_2, the diagonal quantities n may be approximated as

$$n_{mm} = \exp[G_2^{mm}(\beta)] = \exp[\delta G(m_1, \beta) + \delta G(m_2, \beta)]. \tag{4.18}$$

Hence the first term of (4.17) which is determined as the β derivative of (3.12) takes the form

$$\begin{aligned} N'_{mn} = &\{\langle m_1 m_2 | N^{B'}(12; 1'2') | n_1 n_2 \rangle_\alpha + \tfrac{1}{2}[u(m_1) + u(m_2) + u(n_1) + u(n_2)] \\ &\times \langle m_1 m_2 | N^{B}(12; 1'2') | n_1 n_2 \rangle\} \\ &\times [(1 - \tilde{X}_{cc}(m_1))(1 - \tilde{X}_{cc}(m_2))(1 - \tilde{X}_{cc}(n_1))(1 - \tilde{X}_{cc}(n_2))]^{-1/2}. \end{aligned} \tag{4.19}$$

Similarly for the second term of (4.17) we have

$$\begin{aligned} N_{mn}[W^{(1)}_{mn} - \tfrac{1}{2}(W^{(1)}_{mm} + W^{(1)}_{nn})] &= \frac{\hbar^2}{8m} \int \nabla_1^2 N'_{mn} \, d\boldsymbol{r}_2 d\boldsymbol{r}_1 \\ &= \frac{J_{mn}}{[(1 - \tilde{X}_{cc}(m_1))(1 - \tilde{X}_{cc}(m_2))(1 - \tilde{X}_{cc}(n_1))(1 - \tilde{X}_{cc}(n_2))]^{1/2}} \\ &\quad + \tfrac{1}{2} N_{mn}[W^{(1)}_{mm} + W^{(1)}_{nn}] \end{aligned} \tag{4.20}$$

where

$$J_{mn} = \frac{\hbar^2}{8m} \int \nabla_1^2 \langle m_1 m_2 | N^{B'}(12; 1'2') | n_1 n_2 \rangle_\alpha \, d\boldsymbol{r}_2 \, d\boldsymbol{r}_1. \tag{4.21}$$

Finally the expectation value of (4.16) is given by the equation

$$\begin{aligned} W_{mn} = &\{\langle m_1 m_2 | W^{B}(12; 1'2') | n_1 n_2 \rangle_\alpha + J_{mn} + \tfrac{1}{2}\langle m_1 m_2 | N^{B}(12; 1'2') | n_1 n_2 \rangle_\alpha \\ &+ [u(m_1) + u(m_2) + u(n_1) + u(n_2) + W^{(1)}(m_1) + W^{(1)}(m_2) + W^{(1)}(n_1) + W^{(1)}(n_2)]\} \\ &\times [(1 - \tilde{X}_{cc}(m_1))(1 - \tilde{X}_{cc}(m_2))(1 - \tilde{X}_{cc}(n_1))(1 - \tilde{X}_{cc}(n_2))]^{-1/2} \end{aligned} \tag{4.22}$$

where the non-local dressed effective potential $W^{B}(12; 1'2')$ is defined by the relations

$$\begin{aligned} W^{B}(12; 1'2') &= W^{B}_{dd}(12; 1'2') + W^{B}_{dcc}(12; 1'2') \\ &\quad + W^{B}_{dcc}(21; 2'1') + W^{B}_{cc,cc}(12; 1'2') + W^{B}_{cc,cc}(21; 1'2'), \\ W^{B}_{dd}(12; 1'2') &= W^{B}_{dd}(1, 2)\delta(\boldsymbol{r}_1 - \boldsymbol{r}'_1)\delta(\boldsymbol{r}_2 - \boldsymbol{r}'_2), \\ W^{B}_{dcc}(12; 1'2') &= W^{B}_{dcc}(12; 1'2')\delta(\boldsymbol{r}_2 - \boldsymbol{r}'_2). \end{aligned} \tag{4.23}$$

Each diagram contribution to $W^{B}(12; 1'2')$ contains exactly one line $h'_d(r)$. The superscript 'B' signifies that the diagrams which contribute are basic. The leading diagrams which contribute to J_{mn} with no more than two dressed correlation lines are shown in figure 6. In figure 6 the first diagram is local, the diagrams of the second and third line are generated from the matrix elements of N^{B}_{dcc} in (4.22) and the diagrams of the last two lines are generated from the matrix elements of $N^{B}_{cc,cc}$.

The quantities $W^{B}(12; 1'2')$ may be defined as follows:

$$\begin{aligned} W^{B}_{dd}(1, 2) = N^{B'}_{dd}(1, 2) = h'_B(r_{12}), \qquad W^{B}_{dcc}(12; 1'2) = N^{B'}_{dcc}(12; 1'2), \\ W^{B}_{cc,cc}(12; 1'2') = N^{B'}_{cc,cc}(12; 1'2'). \end{aligned} \tag{4.24}$$

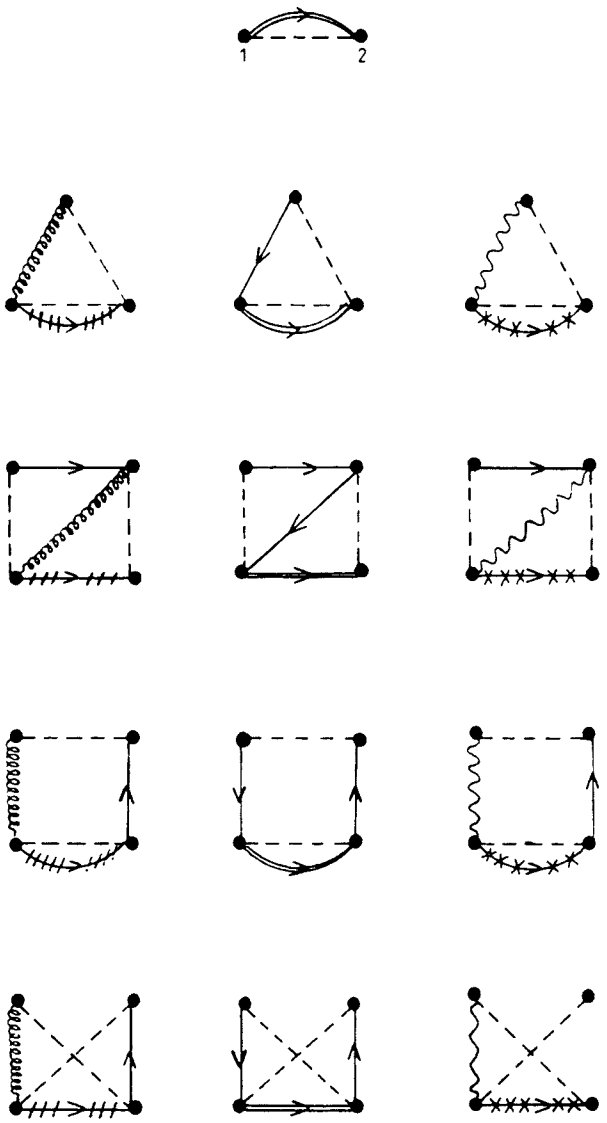

Figure 6. Graphical representation of J_{mn} which includes only the asymmetric non-local diagrams generated from the matrix elements of $N^{B'}(12;1'2')$ in equation (4.21) with no more than two dressed correlation lines.

It can be easily shown that in the thermodynamic limit, although the diagonal matrix elements of the Hamiltonian and unit operator behave like N and the last term of

The advantage of this formalism is that matrix elements of the three-body effective potential

The advantage of this formalism is that matrix elements of the three-body effective potential

$$W_3(i;j,k) = (\hbar^2/m)\nabla_i \ln f(ij)\nabla_i \ln f(ik) \tag{4.25}$$

are not involved in the evaluation of the CBF quantities above.

Analogous evaluations of the CBF quantities can be performed using alternative forms for the expectation value of the kinetic energy.

Strict expressions of the diagonal two-body distribution functions $g_2^{mm}(r_{12})$, in terms of the quantities $N^{\mathrm{B}}_{dd}(12)$, $N^{\mathrm{B}}_{dcc}(12;12')$ and $N^{\mathrm{B}}_{cc,cc}(12;1'2')$, may be obtained following the diagrammatic technique which has been developed by Krotscheck (1979).

For a state-dependent two-body potential

$$v(12)=\sum_{i=1} v^{(i)}(12)0^{(i)} \tag{4.26}$$

with

$$0^{(1)}=1, \qquad 0^{(2)}=\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2, \qquad 0^{(3)}=\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2, \qquad 0^{(4)}=(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2), \tag{4.27}$$

we can apply straightforwardly the KC formalism where

$$W^{\mathrm{B}}_{dd}(12)=W_{dd}(12)=\sum_{i=1}^{4} W^{(i)}_{dd}(12)0^{(i)} \tag{4.28}$$

and

$$W^{(1)}_{dd}(12)=h'_{\mathrm{d}}(12), \tag{4.29}$$

$$W^{(i)}_{dd}(12)=[h_{\mathrm{d}}(12)+1]V^{(i)}(12) \qquad \text{for } i=2,3,4. \tag{4.30}$$

The function $h'_{\mathrm{d}}(12)$ is determined by (4.8). The generalisation for potentials which describe tensor forces is straightforward.

4.1. Single-particle and hole energies

Other important quantities which have to be evaluated within the CBF approach are the single-particle and single-hole energies (Tan and Feenberg 1968) which are defined via

$$2\varepsilon(k)=H^{(A+2)}_{mm}-H^{(A)}_{00}, \qquad k>k_{\mathrm{F}}, \tag{4.31}$$

and

$$2\varepsilon(k)=H^{(A)}_{00}-H^{(A-2)}_{mm}, \qquad k\leqslant k_{\mathrm{F}}, \tag{4.32}$$

respectively. Here $N=A+2, A, A-2$ is the number of particles.

The chemical potential μ is defined by the relations

$$2\mu=H^{(A+2)}_{00}-H^{(A)}_{00}=H^{(A)}_{00}-H^{(A-2)}_{00}. \tag{4.33}$$

The difference (4.31) can be written

$$H^{(A+2)}_{mm}-H^{(A)}_{00}=\varepsilon^{(1)}_{m_1}+\varepsilon^{(1)}_{m_2}+\frac{\partial}{\partial\beta}[(G^{mm}_{A+2}(\beta)-G^{00}_{A+2}(\beta))+(G^{00}_{A+2}(\beta)-G^{00}_{A}(\beta))]|_{\beta=0}. \tag{4.34}$$

Substituting (3.6) and (4.1) into (4.34), we obtain

$$\frac{\partial}{\partial\beta}[G^{mm}_{A+2}(\beta)-G^{00}_{A+2}(\beta)]|_{\beta=0}=u(m_1)+u(m_2)-2u(k_{\mathrm{F}})+W^{(1)}_{mm}-W^{(1)}_{00}. \tag{4.35}$$

From (4.33) we have

$$\frac{\partial}{\partial\beta}[G^{00}_{A+2}(\beta)-G^{oo}_{A}(\beta)]]_{\beta=0}=2(\mu-\varepsilon^{(1)}(k_{\mathrm{F}})) \tag{4.36}$$

with $\mu=\varepsilon(k_{\mathrm{F}})=\mathrm{d}H_{00}/\mathrm{d}A$. In the thermodynamic limit the calculation of (4.35) for a system with A or $A\pm2$ particles does not make any difference, and consequently we may drop the N index.

The single-particle energy is then given by

$$\varepsilon(m_i)=\hbar^2k^2_{m_i}/2m+u(m_i)+W^{(1)}_{(m_i)}+\alpha_0, \qquad k_{m_i}>k_{\mathrm{F}}, \tag{4.37}$$

where

$$\alpha_0=-\hbar^2k^2_{\mathrm{F}}/2m-u(k_{\mathrm{F}})-W^{(1)}(k_{\mathrm{F}})+\mu. \tag{4.38}$$

Similarly the single-hole energy is given by

$$\varepsilon(m_i)=\hbar^2k^2_{m_i}/2m-u(m_i)-W^{(1)}(m_i)+\alpha_0, \qquad k_{m_i}\leqslant k_{\mathrm{F}}, \tag{4.39}$$

with

$$\alpha_0=-\hbar^2k^2_{\mathrm{F}}/2m+u(k_{\mathrm{F}})+W^{(1)}(k_{\mathrm{F}})+\mu. \tag{4.40}$$

Here $W^{(1)}(k_{\mathrm{F}})=W^{(1)}_{00}/2$.

Finally a combination of equations (4.31)–(4.33) yields the relation

$$H^{(A\pm2)}_{mm}-H^{(A\pm2)}_{00}=2|\varepsilon(k)-\mu|. \tag{4.41}$$

5. Discussion

In this work we have developed an elaborate formalism for the evaluation of such quantities as W_{mn}, $H_{mm}-H_{nn}$ and the single-particle/hole energies $\varepsilon(k_{m_i})$. These CBF quantities are the ingredients in terms of which certain perturbation corrections to the matrix elements of the Hamiltonians—based on the method of correlated basis functions—are expressed. Their accurate evaluation is achieved by incorporating the FHNC scheme for the massive resummation of their cluster contributions. Adopting the KR-FHNC scheme, the maintenance of the Fermi cancellations at every stage of the development may be achieved by keeping all diagrams with the same number of correlation lines and different number of particles.

The matrix elements N_{mn} and W_{mn} are evaluated in a first approximation within the FR-FHNC scheme, neglecting the non-local $N_{dcc}(12;1'2')$, $N_{cc,cc}(12;1'2')$, $W_{dcc}(12;1'2')$ and $W_{cc,cc}(12;1'2')$ contributions, or within the KR-FHNC scheme, keeping local and non-local contributions with no more than two dressed correlation lines.

Although we have concentrated on correlated states differing only in two single-particle states, our formalism can be generalised by considering states which differ in a higher number of single-particle states.

An extension of the CBF formalism, to allow a realistic treatment of systems like neutron and nuclear matter, requires a highly state-dependent correlation operator F. Calculations within the FHNC schemes which incorporate a highly state-dependent operator appears not to be an easy task. A first approach in this direction is achieved employing an appropriate state-dependent correlation operator which can be manipulated using simple functions, which will represent partial summations of an infinite

number of diagrams. In the case of liquid ^{3}He the situation is simpler because the two-body potential is state independent and a simple state-dependent correlation operator (Schmidt and Pandharipande 1979, Owen 1979a, Wiringa and Pandharipande 1978) can be applied without great difficulty. The formalism developed in this paper has been applied by us to the analysis of P-wave pairing in liquid ^{3}He (Hatzikonstantinou and Irvine 1981).

References

Clark J W 1979 *Progr. Part. Nucl. Phys.* **2** 89
Clark J W, Mead L R, Krotscheck E, Kürten K E and Ristig M L 1979 *Nucl. Phys.* A **328** 45
Clark J W and Westhaus P 1966 *Phys. Rev.* **141** 833
Fantoni S and Rosati S 1975 *Nuovo Cimento* **25A** 593
Hatzikonstantinou P and Irvine J M 1981 *Manchester Preprint M/C TH* 81/30 *J. Phys. A: Math. Gen.* **15** to be published (May)
Krotscheck E 1977 *J. Low. Temp. Phys.* **27** 199
—— 1979 *Z. Phys.* B **32** 395
Krotscheck E and Clark J W 1979 *Nucl. Phys.* A **328** 73
Krotscheck E and Ristig M L 1975 *Nucl. Phys.* A **242** 389
Lantto L J and Siemens P J 1977 *Phys. Lett.* B **68** 308
Owen J C 1979a *Ann. Phys.* **118** 373
—— 1979b *Phys. Lett.* B **89** 303
Schmidt K E and Pandharipande V R 1979 *Phys. Rev.* B **19** 2504
Tan H T and Feenberg E 1968 *Phys. Rev.* **176** 360
Wiringa R B and Pandharipande V R 1978 *Nucl. Phys.* **A 299** 1