$$\overline{\varphi}(x)=(R_{qI}|\varphi|)(x),\ \overline{\varphi}\in B,\ \overline{\varphi}(x)>0, \tag{A.4}$$

then it satisfies the conditions (14) and (15) for $\lambda = (q\|f\|)^{-1}$.

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MANY-PARTICLE CORRELATIONS OF FERMION CLUSTERS IN THE METHOD OF TRANSITION DENSITY OPERATORS

A. V. Luzanov

In the exact wave function of N fermions, we separate the s-particle clusters constructed from the single-particle states of the self-consistent single-determinant function. Transition density operators are introduced; they include all possible virtual transitions between s-particle and s-hole clusters. The transition operators are used to express the exact two-particle density matrix and the equations of motion (for the stationary case) that describe the correlation interaction of the clusters. In particular, the correlation of particles is estimated for an excited state in the Tamm–Dancoff approximation by means of the expression for the energy dispersion deduced from these equations.

1. Introduction

The exact wave function of a system of N identical fermions can be represented by an infinite series that is a superposition of configurations with different multiplicity of excitation with respect to some original single-determinant function $\Phi(1\ldots N)$ calculated, as a rule, in the self-consistent field approximation [1, 2]. The finding of the energy and other properties of such a multiconfiguration function $\tilde{\Phi}(1\ldots N)$ is a very complicated problem, which in each particular case of a bounded superposition must usually be solved from the start [2–5]. The investigation of exact N-particle states can however be based on the so-called cluster description, in which individual groups of the above infinite series are classified in such a way that the contributions of the corresponding configurations can be absorbed into a finite number of group functions or operators that act on Φ. Then, using them, one can make a further investigation in $\tilde{\Phi}$ of many-particle effects (correlations), which are in principle precluded by the single-determinant description of Φ. One of the first investigations in this region was Brenig's [6], and his work was developed further by Coester and Kümmel [7], who also particularized the two-particle density matrix $\tilde{\rho}_2$ when three-particle and higher correlations are ignored. The cluster expansion was subsequently used in new variants [8–10]. But because of difficulties of a combinatorial nature, an expression for the energy of the state $\tilde{\Phi}$ with allowance for all clusters was not obtained, and it was only in Brenig's approximation for the corresponding cluster functions that a complete system of equations was found; however, as regards particularization, this was only a slight advance on the classical Bogolyubov hierarchy [11].

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In this paper, we propose a cluster variant of the expansion of the exact wave function, which is formulated by means of some elementary transition operators T_k. These last carry all the necessary information about the k-particle excitations in $\tilde{\Phi}$, which are interpreted in terms of virtual transitions between clusters of particles and holes. Such an approach permits one to obtain a perspicuous algebraic expression (with respect to T_k) for the one- and two-particle density matrices $\tilde{\rho}_1$ and $\tilde{\rho}_2$ that correspond to $\tilde{\Phi}$ and are the most important for calculations, and then, from the variational principle, derive a system of coupled equations that directly describe many-particle correlations of the clusters. In the special case of the excited state Φ_* in the Tamm–Dancoff approximation [12], we use these equations to estimate the norm of the corresponding correlation potentials; this coincides with the dispersion of the energy of the state Φ_* (in the probability theory sense), whose finding by direct methods would entail the by no means trivial problem of calculating the mean value of the square of the Hamiltonian.

2. Wave Function and Transition Operators

We represent the wave function $\tilde{\Phi}$ of the complete configuration interaction in the form of an expansion of cluster type:

$$|\tilde{\Phi}(1\ldots N)\rangle=\Big(T_0+\sum_{1\leqslant i_1\leqslant N}T_1(i_1)+\ldots+\sum_{1\leqslant i_1<\ldots<i_k\leqslant N}T_k(i_1\ldots i_k)+\ldots+T_N(1\ldots N)\Big)|\Phi(1\ldots N)\rangle, \tag{1}$$

where the cluster operators $T_k(1\ \ldots\ k)$ realize a transition from the single-determinant state $\Phi(1\ \ldots\ N)$ to the superposition $\Phi_k(1\ \ldots\ N)$ of k-fold excited configurations constructed from Φ by replacing the filled one-particle states $|j\rangle$ by vacant states $|q\rangle$:

$$|\Phi_k|\rangle=\sum_{1\leqslant j_1<\ldots<j_k\leqslant N}\ \sum_{N+1\leqslant q_1<\ldots<q_k}t(q_1\ldots q_k|j_1\ldots j_k)\Big|\Phi_{\substack{j_1\to q_1\\ \vdots\\ j_k\to q_k}}\Big\rangle=\sum_{1\leqslant i_1<\ldots<i_k\leqslant N}T_k(i\ldots i_k)|\Phi\rangle, \tag{2}$$

where here and below the indices $i_1, \ldots, i_k$ label the numbers of the particles, in contrast to the symbols $j_1, \ldots, q_k, \ldots$, which label the single-particle states. The operators $T_k(1\ \ldots\ k)$, which are Hermitian and antisymmetric under permutations of the particles, are introduced by analogy with the one- and two-particle transition operators investigated in [4, 5]:

$$\begin{aligned}T_k(1\ldots k)=\sum_{1\leqslant j_1<\ldots<j_k\leqslant N}\ \sum_{N+1\leqslant q_1<\ldots<q_k}& t(q_1\ldots q_k|j_1\ldots j_k)\,|\varphi_{q_1\ldots q_k}(1\ldots k)\rangle\times\\ &\langle\varphi_{j_1\ldots j_k}(1\ldots k)|+t^*(q_1\ldots q_k|j_1\ldots j_k)\,|\varphi_{j_1\ldots j_k}(1\ldots k)\rangle\langle\varphi_{q_1\ldots q_k}(1\ldots k)|,\end{aligned} \tag{3}$$

where $|\varphi_{q_1\ldots q_k}(1\ldots k)\rangle$, $|\varphi_{j_1\ldots j_k}(1\ldots k)\rangle$ are normalized determinants formed from the single-particle vacant states and filled states, respectively. In our interpretation, these k-particle states describes free (before the interaction) clusters of particles and holes, so that T_k specify all possible particle–hole transitions of clusters with certain transition amplitudes $t(q_1\ldots q_k|j_1\ldots j_k)$.

It follows directly from the definition (3) that the operators T_k are characterized by the definite commutation properties

$$[T_k,\ \rho_k]_+=T_k \tag{4}$$

with k-particle density matrix of the single-determinant function

$$\rho_k=A_k\rho(1)\ldots\rho(k), \tag{5}$$

where A_k is the antisymmetrizer, $\rho=\sum_{j=1}^{N}|j\rangle\langle j|$ is the Fock–Dirac density matrix, and $[\,,]_\pm$ denotes the anticommutator or commutator. Indeed, the operator ρ as projector onto a filled shell annihilates the vacant states $|q\rangle$, which in (3) occur in the k-particle bra and ket states. A consequence of this is the vanishing of the operator projection

$$\rho_kT_k\rho_k=\rho(i)\,T_k\rho(i) \tag{6}$$

and the equivalence $T_k\rho(i) = T_k\rho(l)$ for $i, l \leq k$. This last identity enables us to write the product $T_k\rho(i)$ without specifying the particle index in the Fock–Dirac density matrix.

We now show that the operators T_k really do have the meaning of a k-particle transition density matrix (more precisely, its Hermitian component) between the single-determinant state Φ and the superposition Φ_k (2). For this, we calculate the s-particle transition matrix $\tau_s(|\Phi_k\rangle\langle\Phi|)$ for $s \geq k$ (for $s < k$, it automatically vanishes). With regard to the normalization of the density matrices and all the necessary terminology, we follow Löwdin's rules, which are described, for example, in [13]. From the definition of the reduced transition matrix

$$\tau_s(|\Phi_k\rangle\langle\Phi|) = \binom{N}{s}\langle|\Phi_k(1\ldots N)\rangle\langle\Phi(1\ldots N)|\rangle_{(s+1\ldots N)} \tag{7}$$

and the states Φ and Φ_k (2),

$$\tau_s(|\Phi_k\rangle\langle\Phi|) = \binom{N}{s}\left\langle \sum_{1\leq i_1<\ldots<i_k\leq N} T_k(i_1\ldots i_k)\rho_N(1\ldots N)\right\rangle_{(s+1\ldots N)}, \tag{7'}$$

where the construction of the operator $\rho_N(1\ldots N)=|\Phi\rangle\langle\Phi|$ follows in more detail from (4) after the identification $k = N$. As in [5], for the traces of the matrices we here use the abbreviated notation $\mathop{\mathrm{Sp}}\limits_{(k)} X(1\ldots k\ldots m)\equiv\langle X(1\ldots k\ldots m)\rangle_{(k)}$, and the particle indices are not specified only when the trace with respect to all particles is calculated. We decompose the sum into two:

$$\sum_{1\leq i_1<\ldots<i_k\leq N} = \sum_{1\leq i_1<\ldots<i_k\leq s} + \sum{}' , \tag{8}$$

where the second sum contains all the remaining terms in which at least one of the indices i_l ($l \leq k$) takes values equal to or greater than $s + 1$. As a result, we find that the formation of the contraction (7) for the second sum in (8) gives zero because of the condition $\rho^2 = \rho$, the invariance of the contraction under cyclic permutation needed to form $\rho T_k \rho$, and the requirement (6). At the same time, the first sum gives, by the definition of the type (7) of the reduced density matrix for Φ, a final result of the form

$$\tau_s(|\Phi_k\rangle\langle\Phi|) = \sum_{1\leq i_1<\ldots<i_k\leq s} T_k(i_1\ldots i_k)\rho_s(1\ldots s). \tag{9}$$

In the special case $s = k$, we have $\tau_k = T_k\rho_k$, and for the Hermitian component τ_k with allowance for (4) we obtain

$$\tau_k + \tau_k{}^+ = T_k, \tag{10}$$

which justifies our calling T_k an elementary transition density operator. This consequence does not exhaust the significance of Eq. (9). In fact, it is one of our points of departure in the further calculations of the density matrices $\tilde{\rho}_1$ and $\tilde{\rho}_2$ for the wave function (1).

3. Construction of Density Matrices

For an arbitrary N-particle operator $R_N(1\ldots N)$ and arbitrary k-particle $V_k(1\ldots k)$ with the usual conditions of permutational symmetry, we introduce constructions of the form of a contraction of their symmetrized product to a two-particle level:

$$\hat{r}_2[V_k, R_N] \equiv \frac{N(N-1)}{2}\left\langle \sum_{1\leq i_1<\ldots<i_k\leq N} V_k(i_1\ldots i_k)R_N(1\ldots N)\right\rangle_{(3\ldots N)} \tag{11}$$

Further, we split the sum in (11) into three parts:

$$\sum_{1\leq i_1<\ldots<i_k\leq N} V_k(i_1\ldots i_k) = \sum_{3\leq i_1\ldots<i_{k-2}<N} V_k(12i_1\ldots i_{k-2}) + \sum_{3\leq i_1<\ldots<i_{k-1}\leq N}\{V_k(1i_1\ldots i_{k-1}) + V_k(2i_1\ldots i_{k-1})\} +$$

$$\sum_{3\leq i_1<\ldots<i_k\leq N} V_k(i_1\ldots i_k). \tag{12}$$

Then for the construction (11) we find the more detailed form

$$\hat{r}_2[V_k, R_N] = \frac{k(k-1)}{2}\langle V_k(12\ldots k)R_k(12\ldots k)\rangle_{(3\ldots k)} + \frac{k(k+1)}{2}\langle\{V_k(13\ldots k+1) + V_k(23\ldots k+1)\}\times$$

$$R_{k+1}(12\ldots k+1)\rangle_{(3\ldots k+1)} + \frac{(k+1)(k+2)}{2}\langle V_k(3\ldots k+2)R_{k+2}(12\ldots k+2)\rangle_{(3\ldots k+2)}, \tag{13}$$

where $R_k(1\ldots k)$ is the k-particle reduced density operator generated by $R_N(1\ldots N)$ in accordance with the general definition of the type (7).

It is not difficult to show that the required two-particle density matrix $\tilde{\rho}_2(12)$ of the wave function (1) can be expressed as a sum of constructions similar to (11), namely

$$\tilde{\rho}_2(12)=\sum_{k,l=0}^{N}\hat{r}_2[T_k,\tau_N^{+}(|\Phi_l\rangle\langle\Phi|)]. \tag{14}$$

Since the reduced operators $\tau_s(|\Phi_l\rangle\langle\Phi|)$ needed to perform the contraction (13) have already been calculated in (9), the expression (14) for $\tilde{\rho}_2(12)$ reduces, after a number of transformations, to a purely algebraic form, that contains only the transition operators T_k and the Fock–Dirac density matrix ρ (or the involution operator $Y = 2\rho - I$). We note only that our reduction is based on twofold application of the obvious lowering formula for antisymmetrizers:

$$A_{k+1}(1\ldots k+1)=\frac{1}{k+1}\Big(I-\sum_{2\leqslant i\leqslant k+1}P_{1,i}\Big)A_k(2\ldots k+1) \tag{15}$$

and the simple rules of commutation of the operators of transposition $P_{i,k}$ with the operators of the form X(k), where it is assumed that X(k) also depends on the arguments of any other particle except for particle i:

$$P_{i,k}X(k)=X(i)P_{i,k}. \tag{15$'$}$$

The desired result for the two-particle density matrix can be represented finally as

$$\begin{aligned}\tilde{\rho}_2(12)=\rho_2(12)+A_2\Big\{&\rho(1)\Delta(2)+\Delta(1)\rho(2)+{}^1/_2(I-Y(1)Y(2))T_1(1)T_1(2)+\\ &\sum_{2\leqslant k\leqslant N}k^2\langle T_k(13\ldots k+1)T_k(23\ldots k+1)\rangle_{(3\ldots k+1)}\Big\}+T_2^2(12)+[T_2Y(12),T_1(1)+T_1(2)]_-+T_0T_2(12)+\\ &\sum_{3\leqslant k\leqslant N}\frac{k(k-1)}{2}\langle T_k^2(1\ldots k)+[T_kY(1\ldots k),T_{k-1}(13\ldots k)+T_{k-1}(23\ldots k)]_-+T_k(1\ldots k)T_{k-2}(3\ldots k)\rangle_{(3\ldots k)}.\end{aligned} \tag{16}$$

Here, the single-particle quantity Δ is determined by the expression

$$\Delta(1)=T_0T_1(1)-T_1^2Y(1)+\sum_{2\leqslant k\leqslant N}\{\langle T_k(12\ldots k)T_{k-1}(2\ldots k)\rangle_{(2\ldots k)}-\langle T_k^2(1\ldots k)\rangle_{(2\ldots k)}Y(1)\} \tag{17}$$

and it gives the correlation correction to the single-particle Fock–Dirac density matrix:

$$\tilde{\rho}_1(1)=\rho(1)+\Delta(1). \tag{18}$$

This can be seen either by a reduction with respect to particle (2) in Eq. (16) or by an independent calculation using relations similar to (11)-(13). Equations (16)-(18) hold under the normalization condition imposed on T_k,

$$T_0^2+\frac{1}{2}\sum_{1\leqslant k\leqslant N}\langle T_k^2\rangle=1. \tag{19}$$

Note also that the product T_kY is anti-Hermitian because of (6), and with regard to the unspecified particle number for the operator Y there is the same arbitrariness as for the product $T_k\rho$.

The relations (16)-(18), which constitute one of the principal results of this paper, enable us, in particular, at sufficiently small Δ to carry out, instead of a reduction with respect to N − 1 and N − 2 particles, a contraction with the smaller number k − 1 and k − 2 of particles. As a special case, these formulas contain the previously found [5] one- and two-particle density matrices for the superposition of Φ with singly and doubly excited configurations.

4. Equation for Transition Operators

We now consider a system of fermions described by a Hamiltonian containing only the single-particle $\sum_{1\leqslant i\leqslant N}h(i)$ and two-particle $\sum_{1\leqslant i<j\leqslant N}g(ij)$ interactions. Application of the variational principle to the energy functional

$$E(T)=\langle h(1)\tilde{\rho}_1(1)\rangle+\langle g(12)\tilde{\rho}_2(12)\rangle,$$

calculated by means of (16)-(18) with allowance for the normalization (19), the "transition" conditions (5), and the self-consistency $f\rho=\rho f$, where $f(1)=h(1)+2\langle g^{A}(12)\rho(2)\rangle_{(2)}$ is the Fock operator and $g^{A}(12)=A_2(12)g(12)$, gives a system of equations that determine the operators T_k and the correlation energy $\lambda = E(T) - E(T_0 = 1)$. The equation for the transition operator T_k is "coupled" to the equations for $T_{k\pm1}$ and $T_{k\pm2}$ and can be represented in the explicit form

$$\hat{\Pi}_k[T_k]+A_k\sum_{1\leqslant i<j\leqslant k}\{T_{k-1}(1\ldots j\ldots k)w(ij)+T_{k-1}(1\ldots\hat{i}\ldots k)w(ji)+w^{+}(ij)T_{k-1}(1\ldots\hat{j}\ldots k)+$$

$$w^{+}(ji)T_{k-1}(1\ldots\hat{i}\ldots k)+{}^{1}/{}_{2}v(ij)T_{k-2}(1\ldots\hat{i}\ldots\hat{j}\ldots k)+$$

$$^{1}/_{2}z(ij)T_{k-2}Y(1\ldots\hat{i}\ldots\hat{j}\ldots k)\}+\sum_{1\leqslant i\leqslant k}\langle w(i,k+1)T_{k+1}(1\ldots k+1)+T_{k+1}(1\ldots k+1)w^{+}(i,k+1)\rangle_{(k+1)}+$$

$$\frac{(k+1)(k+2)}{2}\langle v(k+1,k+2)T_{k+2}(1\ldots k+2)\rangle_{(k+1,k+2)}=\lambda T_k(1\ldots k). \tag{20}$$

In (20), we have used the following notation. The superoperator $\hat{\Pi}_k$ acts on an arbitrary k-particle transition operator $X(1 \ldots k)$, which satisfies (4), in accordance with the rule

$$\hat{\Pi}_k[X(1\ldots k)]=\Big[\sum_{1\leqslant i\leqslant k}|f(i)|+\sum_{1\leqslant i<j\leqslant k}(g^{A}_{\circ\circ,\circ\circ}(ij)+$$

$$g^{A}_{\ominus\ominus,\ominus\ominus}(ij)),X(1\ldots k)\Big]_{+}+2kA_k\sum_{1\leqslant i\leqslant k}\langle u(i,k+1)X(1\ldots\hat{i}\ldots k)\rangle_{(k+1)}, \tag{21}$$

where the symbol $\wedge$ over an index means that this index is omitted; for example, $X(1\ldots\hat{i}\ldots k)=X(1\ldots i-1, i+1\ldots k)$. Further, the two-particle potentials $u(ij)$, $g^{A}_{\circ\circ,\circ\circ}$, etc, are different cases of particle–hole interactions in the clusters described by the operators T_k. The symbol $\circ$ denotes projection onto filled states, and the symbol $\ominus$ projection onto vacant states $(\rho_\ominus=I-\rho)$; for example, $g^{A}_{\circ\ominus,\circ\circ}(12)=\rho(1)\rho_\ominus(2)g^{A}(12)\rho(1)\rho(2)$. In this notation, the potential $u(12)$ is defined as

$$u(12)=g^{A}_{\circ\ominus,\ominus\circ}(12)+g^{A}_{\ominus\circ,\circ\ominus}(12) \tag{22}$$

and it reflects the interaction of the fermions and holes for clusters of a given particle number k ($u(ij)$ enters only in each superoperator $\hat{\Pi}_k$). The operator

$$w(12)=g^{A}_{\ominus\circ,\ominus\ominus}(12)-g^{A}_{\circ\ominus,\circ\circ}(12) \tag{23}$$

describes the correlation interaction between clusters that differ by only one particle, and is therefore neither Hermitian nor symmetric with respect to the operation of permutation $P_{1,2}$ of particles. Finally, the potentials $v(12)$ and $z(12)$ characterize the Hermitian and skew-Hermitian components of the fermion–hole interaction of clusters that differ by two particles:

$$v(12)=g^{A}_{\circ\circ,\ominus\ominus}(12)+g^{A}_{\ominus\ominus,\circ\circ}(12), \tag{24}$$

$$z(12)=g^{A}_{\circ\circ,\ominus\ominus}(12)-g^{A}_{\ominus\ominus,\circ\circ}(12). \tag{25}$$

In the cases $k = 0, 1, 2$, Eqs. (20) go over into Eqs. (22)-(24) of [5] for the superposition of the single-determinant function with one- and two-fold excited configurations (because of (19), it is necessary to make the substitution $T_0 \rightarrow 2T_0$).

We consider the other special case $k = 1, 2, 3$, which is characteristic of an excited state which reflects the interaction of single-particle clusters with two- and three-particle clusters. For convenience, we make the renotation $T_1(1)=D(1)$, $T_2(12)=T(12)$, $T_3(123)=X(123)$ and, using (20), we write down the system of equations for these quantities:

$$\hat{\Pi}_1[D]+2\langle w(12)T(12)\hat{T}(12)w^{+}(12)\rangle_{(2)}+3\langle v(23)X(123)\rangle_{(23)}=\lambda D(1),$$

$$\hat{\Pi}_2[T]+D(1)w(12)+D(2)w(21)+w^{+}(12)D(1)+w^{+}(21)D(2)+3\langle[w(13)+w(23)]X(123)+$$

$$X(123)[w^{+}(13)+w^{+}(23)]\rangle_{(3)}=\lambda T(12), \tag{26}$$

$$\hat{\Pi}_3[X]+A_3\{T(12)[w(13)+w(23)]+T(23)[w(21)+w(31)]+T(13)[w(12)+w(32)]+\text{herm. con.}+{}^{1}/{}_{2}[v(12)D(3)+$$

$$v(13)D(2)+v(23)D(1)+z(12)DY(3)+z(13)DY(2)+z(23)DY(1)]\}=\lambda X(123).$$

Leaving aside here a discussion of the methods of solution and simplification of the system (26), which are similar in spirit to those proposed in [5], we obtain one more helpful consequence of these equations, which is associated with the calculation of the energy dispersion of the Tamm–Dancoff excited state Φ_* as a superposition of only singly excited configurations [12]. This means that for such an excited state we proceed from a single-particle transition operator D that satisfies corresponding Tamm–Dancoff equations of the form

$$\hat{\Pi}_1[D]=\pi D, \tag{27}$$

where π is the excitation energy. If the system (26) did not contain other terms with D, Eq. (27) would correspond to the exact solution for the total Hamiltonian H_N. It is natural to estimate the deviation of the Tamm–Dancoff solution (27) from the exact one by means of the square of the norm of the "superfluous" terms with D in (26). A more detailed analysis shows that because of the normalization (19) we necessarily obtain, to within a coefficient $\frac{1}{2}$, an expression for the energy dispersion of the excited state defined by

$$\sigma_*^2=\langle\Phi_*|H_N^2|\Phi_*\rangle-\langle\Phi_*|H_N|\Phi_*\rangle^2. \tag{28}$$

After a number of simple transformations, we obtain an explicit expression for the required dispersion in terms of the correlation operators v(12) and w(12):

$$\sigma_*^2=\sigma^2+2\langle[w(12)w^+(12)-v^2(12)]D^2(1)+w(12)w^+(21)D(1)D(2)\rangle_{(12)}+2\langle\langle v(12)D(2)\rangle_{(2)}^2\rangle_{(1)}, \tag{29}$$

where $\sigma^2={}^1/_2\langle v^2\rangle$ is the dispersion of the single-determinant function [4, 5]. In the derivation of (29) for arbitrary two-particle operator B(12) = B(21) and single-particle operator C(1), we have used an identity that can be readily established by means of (15) and (15′):

$$3\langle B(12)C(3)A_3(123)\rangle_{(123)}=\langle B\rangle\langle C\rangle-2\langle B(12)C(2)\rangle_{(12)},$$

and the property $w^2(12) = w(12)w(21) = 0$, which follows from the definition (23). Using the expression for σ_*^2, we can readily make an indirect estimate of the correlation effects for excited states found in the Tamm–Dancoff approximation (27). But if the operator D is found with neglect of the series of terms in $\hat{\Pi}_1$, then in (29) we must include with the coefficient $\frac{1}{2}$ the squares of the norms of the omitted terms. In the general case, qualitative conclusions about the interactions of clusters containing different numbers of particles can be obtained prior to the solution of the system (22) by comparing the norms $\|u\|$, $\|v\|$, $\|w\|$ of the potentials, which can be readily calculated in each concrete case.

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