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Higher-order Terms in the Brueckner-Goldstone Perturbation Expansions

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Higher-order terms in the perturbation expansions for energy and for expectation values of some frequently occurring one- and two-particle operators are studied in the framework of the standard Brueckner-Goldstone theory in oscillator basis. For the case of the ^{4}He nucleus explicit formulae are derived making it possible to calculate the binding energy up to the third order and other basic ground-state characteristics (r.m.s. radius, form factor), as well as the expectation value of the centre-of-mass Hamiltonian, up to the second order.

Члены более высоких порядков в рядах теории возмущений Бракнера-Голдстоуна. — Рассматриваются члены более высоких порядков рядов Бракнера-Голдстоуна для энергии и средних значений некоторых одно- и двухчастичных операторов в осциляторном базисе. В случае ядра ^{4}He получены явные выражения, при помощи которых можно вычислить энергию связи до третьего порядка и другие характеристики основного состояния (среднеквадратичный радиус, форм-фактор) и также энергию движения центра масс ядра, до второго порядка.

Členy vyšších řádů v Brueckenerových-Goldstoneových poruchových rozvojích. — V rámci standardní Brueckenrovy-Goldstoneovy teorie v oscilátorové bázi jsou studovány členy vyšších řádů v poruchovém rozvoji pro energii a střední hodnoty některých často se vyskytujících jednočásticových a dvoučásticových operátorů. Pro případ jádra ^{4}He jsou odvozeny explicitní formule umožňující vypočítat jeho vazebnou energii do třetího řádu a některé další charakteristiky základního stavu (středněkvadratický poloměr, tvarový faktor), jakož i střední hodnotu energie těžišťového pohybu, do druhého řádu.

Introduction

In the last decade many studies appeared dealing with the Brueckner-Goldstone (BG) theory in oscillator basis and with its applications for calculating the ground-state properties of light magic nuclei [1 – 11]. The attention was focused first of all on the binding energy (b.e.). Strong dependence of results of earlier second-order calculations on quantities parametrizing the single-particle (s.p.) spectrum [1] suggested that one cannot get a reliable value of the b.e. without taking into account

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higher-order diagrams of the BG expansion for energy. That's why the third-order diagrams were studied in detail. It appeared that all these diagrams, as shown in Fig. 1[1]), separate into three groups:

(i) diagrams 1(a, b): these diagrams significantly influence the b.e. and their contributions should be calculated as accurately as possible;

(ii) diagrams 1(c – g): all these diagrams contain at least one particle-hole composite interaction and their contributions can be made small by a suitable choice of the oscillator frequency ω [4, 5, 15];

(iii) diagrams 1(h, i): they represent the lowest order terms of the three-particle cluster expansion in powers of t. As the question of whether, and how rapidly this expansion converges is still open[2]), it is of little use to calculate the contributions of 1(h, i). Only the total contribution of the three-particle cluster is of interest; this quantity was found to be rather small, less than 10% of the total b.e. [13, 14] – within this accuracy diagrams 1(h, i) can be neglected.

The most important diagrams 1(a, b) involve infinite summations over particle states and usually a cut-off was used for calculating them [5, 7, 10, 11]. However, it is possible to express them in a closed form via the correlated two-particle function that satisfies the Bethe-Goldstone equation. Explicit formulae were firstly obtained by Kallio and Day [2] for an unrealistic case (central s-wave N – N potential). Later on, Clement [8] considered a more realistic case (s- and d-wave separable potentials) but applied several simplifying approximations in his calculation. It is one of the purposes of the present paper to derive exact formulae that can be applied for a general static N – N potential with a hard or soft core. To this end the formalism developed recently [15] is used (see sect. 1 for a brief review) and in the case of the ^{4}He nucleus explicit formulae are obtained for the contributions of diagrams 1(a, b) and 1(c – e) (sect. 2)[3]). The latter three diagrams were considered in order that we might verify that a reasonable value of ω can be found for which the diagrams of the second group become negligible. The numerical results reported in ref. [15] confirm that this really is the case.

[1]) In order to reduce the number of diagrams, we join the t-interaction bubbles inserted into a hole line or creating/annihilating a particle-hole pair with the corresponding V-interactions to a "composite" interaction. For example, diagram 1(d) contains one composite interaction and replaces two diagrams having at the top a t-bubble and a V-interaction respectively. Matrix elements of the s.p. potential V between any pair of hole states are assumed to obey the Brueckner-Hartreė-Fock (BHF) conditions; the corresponding matrix elements of the composite interaction then vanish and hence the diagrams containing composite interactions inserted between a pair of hole lines are omitted in Fig. 1.

[2]) While there is no convergence in the case of nuclear matter [12], some authors suggest that, in view of specific properties of the oscillator basis, the situation for light magic nuclei may be different [7, 13].

[3]) We limit ourselves to ^{4}He because the method used works best for this nucleus, e.g. the Pauli corrections to the most important matrix elements of t vanish (see ref. [15] for details).

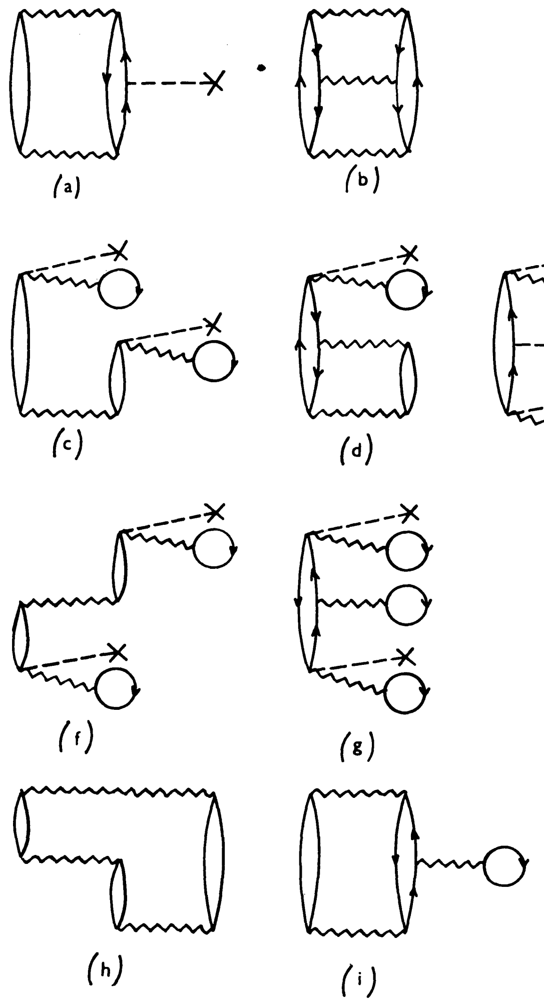

Fig. 1. Third-order diagrams occurring in the BG expansion for energy. All the t-interactions are on the energy shell except the middle one in diagrams (f)—(i). The diagrams containing a composite interaction inserted between a pair of hole lines as well as those "adjoint" to (c) and (d) (with inverse order of interactions) are not drawn

In contrast to energy relatively little attention has been paid to the BG expansions for expectation values $\langle O \rangle$ [4]). This is partly due to the fact that convergence depends on the operator considered and very little can be said about it in general. In the case of the BG expansions for $\langle O \rangle^{(k)}$, $k = 1, 2$, which have similar structure as the BG

[4]) Linked-cluster expansion for the expectation value of a general k-particle operator $O^{(k)}$ (with respect to the ground state of the total Hamiltonian of A-fermion system) is derived e.g. in ref. [16].

expansion for energy, one can use the same methods that improve convergence of the energy expansion (putting t-interactions on the energy shell wherever possible, application of the BHF conditions, etc.); however, in principle one cannot avoid the assumption that a few lowest-order diagrams yield the main contribution.

This assumption should be tested and this can be achieved by calculating for $N = 0, 1, \ldots$ the N-th approximation $\langle \mathsf{O} \rangle^{(N)}$ that includes all the diagrams of the BG expansion for $\langle \mathsf{O} \rangle$ up to the N-th order (in t interactions). To this purpose we derive in sect. 3 explicit formulae for contributions of diagrams up to the second order for several important one- and two-particle operators. Besides the operators corresponding to the r.m.s. radius and form factor attention is paid to the Hamiltonian H_{CM} that describes the centre-of-mass motion of the nucleus (A-fermion system) and can be expressed via simple one- and two-particle operators. The reason for considering the H_{CM} is the following: when calculating the b.e., we must subtract $\langle \mathsf{H}_{CM} \rangle$ from the ground-state energy E of the total A-nucleon Hamiltonian, the latter quantity being given by the BG energy expansion. Now, in the case of ^{4}He the E and $\langle \mathsf{H}_{CM} \rangle$ are comparable quantities and hence it is important to calculate H_{CM} with the same accuracy as E. The formulae given in sect. 3 allow to calculate the $\langle \mathsf{H}_{CM} \rangle$ up to the second order both in the "elementary" approach when $\mathsf{H}_{CM} = \mathsf{T}_{CM}$ (the c.m. kinetic energy operator) and in the Lipkin's approach [17] when H_{CM} contains an additional operator of the harmonic-oscillator potential energy.

1. Preliminaries

Our calculations of higher-order diagrams in the next two sections are based on the method of ref. [15] that enables one to obtain the t-matrix elements as well as the solution to the Bethe-Goldstone equation with a very good accuracy. Several features of this method, which are essential in the following, will be briefly summarized in this section.

1.1. The Single-particle Spectrum

The standard modification of the harmonic-oscillator (h.o.) spectrum is used (cf. refs. [1, 5, 7, 9–11]). The modified spectrum is pure point, the corresponding s.p. Hamiltonian h acting on the s.p. Hilbert space $\boldsymbol{H}$ has the same eigenvectors as the h.o. Hamiltonian

$$\mathsf{h}_{\mathrm{osc}} = \mathsf{T} + \mathsf{V}_{\mathrm{osc}}$$

and is related to it by

$$\mathsf{h} = \mathsf{T} + \mathsf{V} = \mathsf{h}_{\mathrm{osc}} - \frac{\omega}{2}\left[C\mathsf{I} - \sum_{\nu=0}^{\nu(F)} \eta_\nu \mathsf{P}_\nu\right] = \sum_{\nu=0}^{\infty} \varepsilon_\nu \mathsf{P}_\nu \,.\ ^{5)} \tag{1.1}$$

[5]) The system of units is used in which $h/(2\pi) = c = 1$.

The quantities occurring here have the following meaning:

1. I ... the unity operator on $\boldsymbol{H}$;

2. P_ν ... projection on the subspace of $\boldsymbol{H}$ spanned by eigenvectors of $\mathsf{h}_{\rm osc}$ belonging to the eigenvalue $\varepsilon_{\rm osc}(\nu) = (\omega/2)(2\nu + 3)$. In the standard notation one has

$$\mathsf{P}_\nu = \sum_{2n+l=\nu} \sum_{m=-l}^{1} \sum_{\sigma,\tau=\pm 1/2} \left|nlm; \sigma\tau\right\rangle \left\langle nlm; \sigma\tau\right| . \tag{1.2}$$

Clearly, $\mathsf{P}_\nu \boldsymbol{H}$ is also an eigenspace of h belonging to its eigenvalue

$$\varepsilon_\nu = \varepsilon_{\rm osc}(\nu) - \frac{\omega}{2}\begin{Bmatrix}(C+\eta) & \ldots & 0 \leqq \nu \leqq \nu(F) \\ C & \ldots & \nu > \nu(F)\end{Bmatrix};$$

3. $\nu(F)$ ... the maximum of occupied shell quantum numbers;

4. C, η_ν ... real dimensionless parameters determining an overall shift of the h.o. spectrum and shifts of occupied-state h.o. energies respectively.

In the case of ^{4}He we have $\nu(F) = 0$ and thus the s.p. spectrum depends on three parameters ω, C and $\eta \equiv \eta_0$; the occupied (hole) states differ only with respect to spin and isospin quantum numbers

$$\left|h\right\rangle \equiv \left|000; \sigma_h\tau_h\right\rangle$$

and all of them belong to the same s.p. energy

$$\varepsilon(h) \equiv \varepsilon_0 = \frac{\omega}{2}(3 - \eta - C) . \tag{1.3}$$

1.2. The Two-particle Hilbert Space $\boldsymbol{H}_2$

Two realizations of $\boldsymbol{H}_2$ will be used. First of them is the usual tensor-product realization $\boldsymbol{H} \otimes \boldsymbol{H}$; the set

$$\boldsymbol{E}_{IP} = \{\left|q_1q_2\right\rangle \equiv \left|n_1l_1m_1; \sigma_1\tau_1\right\rangle \otimes \left|n_2l_2m_2; \sigma_2\tau_2\right\rangle \mid n_i, l_i = 0, 1, \ldots; \\ m_i = -l_i, \ldots, l_i; \sigma_i, \tau_i = \pm 1/2\} \tag{1.4}$$

is an orthonormal basis in $\boldsymbol{H} \otimes \boldsymbol{H}$. With the help of projections corresponding to this basis (see Eq. (1.2)) the Pauli operator $\mathsf{A}(w)$ is conveniently expressed:

$$\mathsf{A}(w) = \sum_{\nu=\nu(F)+1}^{\infty} \sum_{\mu=\mu(F)+1}^{\infty} \frac{\mathsf{P}_\nu \otimes \mathsf{P}_\mu}{w - \varepsilon_\nu - \varepsilon_\mu} .$$

The starting energy w cannot exceed max $\{\varepsilon_\nu + \varepsilon_\mu \mid \nu, \mu = 0, 1, \ldots, \nu(F)\}$ and hence the right-hand-side is always well-defined.

As the second realization the Hilbert space of vector-valued functions $L^2(\mathbf{M}, \mu; \boldsymbol{G})$ is chosen. Here $\boldsymbol{G}$ is the Hilbert space related to angular, spin and isospin degrees of freedom of a nucleon pair, whereas elements of $L^2(\mathbf{M}, \mu)$ are complex functions on $\mathbf{M} = [0, \infty) \times [0, \infty)$ such that

$$\int_{\mathbf{M}} |f|^2 \, \mathrm{d}\mu = \int_0^\infty \int_0^\infty |f(r, R)|^2 \, r^2 R^2 \, \mathrm{d}r \, \mathrm{d}R \tag{1.5}$$

exists. The r, R are dimensionless radial coordinates of the nucleon pair with respect to its c.m. system and are related to radius vectors $\mathbf{x}_i$ $(i = 1, 2)$ of individual nucleons by

$$r = \frac{1}{b\sqrt{2}} |\mathbf{x}_1 - \mathbf{x}_2| , \quad R = \frac{1}{b\sqrt{2}} |\mathbf{x}_1 + \mathbf{x}_2| , \quad b = (m_N \omega)^{-1/2} . \tag{1.6}$$

In the space $L^2(\mathbf{M}, \mu; G)$ we shall work with the basis E_{CM} that is obtained using:
1. The basis in G in which the partial-wave decomposition of the Bethe-Goldstone equation can be performed exactly for a general N–N potential [3] and which correspond to couplings $\mathbf{l} + \mathbf{L} = \mathbf{\Lambda}$, $\mathbf{\Lambda} + \mathbf{S} = \mathbf{J}$:

$$\{g_{[((l,L)\lambda,S)JM;TM(T)]} \mid l, \quad L = 0, 1, \ldots ; \quad S, T = 0, 1 ; \\ M = -J, \ldots, J ; \quad M(T) = -T, \ldots, T\} .^{6)} \tag{1.7}$$

2. The basis in $L^2(\mathbf{M}, \mu)$ that is for any given pair of quantum numbers l, L formed by the functions

$$R_{nN}^{(l,L)}(r, R) = R_{nl}(r)/r \, . \, R_{NL}(R)/R \; n , \; N = 0, 1, \ldots ,$$

the R_{nl}'s being usual radial h.o. eigenfunctions that satisfy the normalization

$$\int_0^\infty R_{nl}^2(r) \, \mathrm{d}r = 1.$$

Now, the basis $E_{CM} \subset L^2(\mathbf{M}, \mu; G)$ can be constructed according to general properties of Hilbert spaces of vector-valued functions [18]:

$$E_{CM} = \{\varphi_{\langle((nl,NL)\lambda,S)JM;TM(T)\rangle} \mid n, l, N , \; L = 0, 1, \ldots ; \\ S, T = 0, 1 ; \quad M = -J, \ldots, J ; \quad M(T) = -T, \ldots, T\} , \tag{1.8}$$

the mapping $\varphi_{\langle\ldots\rangle} : \mathbf{M} \to G$ being given by

$$\varphi_{\langle((nl,NL)\lambda,\ldots\rangle}(r, R) = R_{nN}^{(l,L)}(r, R) \cdot g_{[((l,L)\lambda,\ldots]} .$$

We shall also use the Dirac's notation

$$|((l, L)\, \lambda, S)\, JM; TM(T)] \equiv g_{[((l,L)\lambda,S)JM;TM(T)]}$$
$$|((nl, NL)\, \lambda, S)\, JM; TM(T)\rangle \equiv \varphi_{\langle((nl,NL)\lambda,S)JM;TM(T)\rangle} .$$

[6]) Quantum numbers l, L refer to relative and c.m. orbital angular momenta of the nucleon pair, S and T to its total spin and isospin respectively.

The unitary transformation connecting the bases E_{CM} and E_{IP} is expressed via Moshinsky brackets [19] and vector-coupling coefficients.

In our further considerations we shall frequently use the subspace $H^{(occ)} \subset H_2$ that is spanned by all the vectors of E_{IP} satisfying $0 \leqq 2n_i + l_i \leqq \nu(F)$, $i = 1, 2$. This subspace is *not spanned by any subset of* E_{CM} *except the case* $\nu(F) = 0$, when vectors

$$\varphi^{(0)}_{SMTM(T)} \equiv |((00, 00)\, 0, S)\, SM;\, TM(T)\rangle \; S, T = 0, 1\,; \quad M = -S, \ldots, S\,;$$
$$M(T) = -T, \ldots, T$$

form a basis in $H^{(occ)}$. In this case the projection $\mathsf{P}^{(occ)}$ onto $H^{(occ)}$ can be expressed via one-dimensional projections $\mathsf{P}^{(0)}_{SMTM(T)}$ corresponding to vectors $\varphi^{(0)}_{SMTM(T)}$:

$$\mathsf{P}^{(occ)} = \sum_{hh'} |hh'\rangle\, \langle hh'| = \sum_{S,T=0}^{1} \sum_{M,M(T)} \mathsf{P}^{(0)}_{SMTM(T)}\,. \tag{1.9}$$

Similarly, if $\nu(F) = 0$, then it holds for the "antisymmetrized" trace of any two-particle operator $\mathsf{O}^{(2)}$ on $H^{(occ)}$:

$$\mathrm{Tr}^{(occ)}_a \mathsf{O}^{(2)} \equiv \sum_{hh'} \langle hh'|\, \mathsf{O}^{(2)} |\, hh'\rangle_a =$$
$$= \sum_{S,T=0}^{1} \sum_{M,M(T)} [1 - (-1)^{S+T}]\, (\varphi^{(0)}_{SMTM(T)}, \mathsf{O}^{(2)} \varphi^{(0)}_{SMTM(T)})\,. \tag{1.10}$$

1.3. The Reaction Matrix and Related Quantities in a Diagonal Approximation

In view of properties of the N – N potential v, the $L^2(\mathbf{M}, \mu; G)$ realization of H_2 has to be used when solving the reaction matrix equation

$$\mathsf{t}_w = \mathsf{v} + \mathsf{v}\mathsf{A}(w)\, \mathsf{t}_w\,,$$

the matrix elements of t having the simplest form in the E_{CM} basis. However, the Pauli operator $\mathsf{A}(w)$ given by Eq. (1.5) cannot be expressed via one-dimensional projections corresponding to vectors of E_{CM} and hence its matrix representation in this basis is not diagonal. This fact causes serious complications and therefore one usually proceeds in two steps: (i) introducing some diagonal approximation $\mathsf{A}_D(w)$ of $\mathsf{A}(w)$ and solving the corresponding operator equation for the "diagonal" reaction matrix $\mathsf{t}^{(D)}$, (ii) calculating the non-diagonal corrections to $\mathsf{t}^{(D)}$ with the help of the BBP relation [20] or other methods.

In ref. [15] earlier approaches [1–3] were generalized and a diagonal approximation was developed that appeared to be very accurate especially in the ^{4}He case. Matrix elements of $\mathsf{t}^{(D)}$ in the E_{CM} basis are diagonal with respect to all the quantum numbers except n, l, λ and do not depend on M, T and $M(T)$.[7]) In this paper we

[7]) The Coulomb interaction is not included in v.

shall consider only on-energy-shell matrix elements

$$\langle((nl, NL)\,\lambda, S)\,JM;\,TM(T)|\;\mathrm{t}^{(D)}_{\bar{w}(h,h')}\;|((\bar{n}\bar{l}, \bar{N}\bar{L})\,\bar{\lambda}, S)\,JM;\,TM(T)\rangle\,,$$

which means that

$$\bar{w}(h, h') = \varepsilon(h) + \varepsilon(h') = \frac{\omega}{2}\left[4\bar{n} + 2\bar{l} + 4\bar{N} + 2\bar{L} + 6 - \eta_h - \eta_{h'} - 2C\right].$$

The set $\boldsymbol{J}$ of pairs (l, λ) obeying the relations (for given J, S, $\bar{L}, \bar{l}$)

$$|J - S| \leqq \lambda \leqq J + S\,, \quad |\bar{L} - \lambda| \leqq l \leqq \bar{L} + \lambda\,, \quad (-1)^l = (-1)^{\bar{l}} \tag{1.11}$$

is obviously finite; if one chooses the order of pairs so that $(\bar{l}, \bar{L})$ is the first, one has

$$\boldsymbol{J} = (l_i, \lambda_i) \quad i = 1, 2, \ldots, Z\,, \quad (l_1, \lambda_1) = (\bar{l}, \bar{\lambda})\,.$$

Then, on-energy-shell matrix elements of $\mathrm{t}^{(D)}$ in the $\boldsymbol{E}_{CM}$ basis can be written as follows:

$$\langle((nl, NL)\,\lambda, S)\,JM;\,TM(T)|\;\mathrm{t}^{(D)}_{\bar{w}}|((\bar{n}\bar{l}, \bar{N}\bar{L})\,\bar{\lambda}, \bar{S})\,\bar{J}\bar{M};\,\bar{T}M(\bar{T})\rangle =$$

$$= \frac{\omega}{2}\,t^{\langle 0\rangle}_{in}\,\delta_{N\bar{N}}\delta_{L\bar{L}}\delta_{S\bar{S}}\delta_{J\bar{J}}\delta_{M\bar{M}}\delta_{M(T)M(\bar{T})} \tag{1.12}$$

where $(l_i, \lambda_i) = (l, \lambda)$, $\bar{w}$ stands instead of $\bar{w}(h, h')$ and $\langle 0\rangle$ represents the set of quantum numbers $\bar{n}\bar{l}\bar{N}\bar{L}\bar{\lambda}SJ$ (the quantum numbers M, T and $M(T)$ are omitted since the $\mathrm{t}^{(D)}$ matrix elements do not depend on them).

Similar notation can be used for the components of the two-particle correlated function: let $\psi^{\langle 0\rangle}_{\bar{w}} \in L^2(\mathbf{M}, \mu; \boldsymbol{G})$ satisfy the "diagonal" Bethe-Goldstone equation

$$\psi^{\langle 0\rangle}_{\bar{w}} = \varphi_{\langle 0\rangle} + \mathrm{A}^{(D)}_{\bar{w}}\mathrm{v}\psi^{\langle 0\rangle}_{\bar{w}}\,, \tag{1.13}$$

the quantities $\psi^{\langle 0\rangle}_{\bar{w}}$ and $\mathrm{t}^{(D)}_{\bar{w}}$ being related by $\mathrm{t}^{(D)}_{\bar{w}}\varphi_{\langle 0\rangle} = \mathrm{v}\psi^{\langle 0\rangle}_{\bar{w}}$. The $\psi^{\langle 0\rangle}_{\bar{w}}$ is a vector-valued function assigning to each r, $R \in \mathbf{M}$ a vector $\psi^{\langle 0\rangle}_{\bar{w}}(r, R) \in \boldsymbol{G}$. Now, the diagonal approximation ensures that the following simple partial-wave decomposition holds:

$$\psi^{\langle 0\rangle}_{\bar{w}}(r, R) = \sum_{i=1}^{Z}|((l_i, \bar{L})\,\lambda_i, S)\,J\ldots]\,.\,\frac{1}{R}\,R_{NL}(R)\frac{1}{r}\,\psi^{\langle 0\rangle}_i(r)\,. \tag{1.14}$$

From Eq. (1.13) one then obtains a system of ordinary second-order differential equations for the functions $\psi^{\langle 0\rangle}_i(r)$.

In the ^{4}He case the condition $v(F) = 0$ implies $\bar{n} = \bar{l} = \bar{N} = \bar{L} = 0$, which further gives $J = S = 0, 1$, and thus the single quantum number S fully identifies the set $\langle 0\rangle$. Similarly, the starting energy $\bar{w}$ assumes the same value for all pairs of hole states (cf. Eq. (1.3))

$$\bar{w} = 2\varepsilon_0 = \frac{\omega}{2}(6 - 2\eta - 2C)\,. \tag{1.15}$$

Finally, the conditions (1.11) imply $l_i = \lambda_i = 0, 2$, the value $l_i = 2$ occurring only in the triplet case $S = 1$; thus the number Z of admissible pairs (l_i, λ_i) is equal to $S + 1$ and it holds

$$l_i = \lambda_i = 2(i - 1) \quad i = 1, \ldots, S + 1 .$$

Concluding this summary of the method of ref. [15] let us mention explicit formulae for contributions of the "composite" interactions inserted between two hole lines or creating/annihilating a particle-hole pair. In general, this contribution reads

$$\sum_{h'} \langle qh' | \, \mathrm{t}_{\overline{w}(h,h')} | hh' \rangle_a - \langle q | \, \mathrm{V} | h \rangle \equiv \frac{\omega}{2} Z(q, h) \tag{1.16}$$

where $|q\rangle \equiv |n_q l_q m_q; \sigma_q \tau_q\rangle$ is an arbitrary s.p. state and $|h\rangle \equiv |n_h l_h m_h; \sigma_h \tau_h\rangle$ is a hole state. The BHF condition for $\langle q| \, \mathrm{V} |h\rangle$ then becomes $Z(q, h) = 0$. Applying the diagonal approximation, the following simple formulae are obtained for the ^{4}He case ($n_h = l_h = m_h = 0$ for all hole states):

$$Z(h, h') = \delta_{hh'} [\tfrac{3}{2}(t_{10}^{(0)} + t_{10}^{(1)} - 1) + \eta + C] , \tag{1.17}$$

$$\frac{Z(p, h)}{\varepsilon(h) - \varepsilon(p)} = - \frac{2}{\omega} \delta_{l0} \delta_{m0} \delta_{\sigma\sigma'} \delta_{\tau\tau'} \, S(n) \tag{1.18}$$

where $|p\rangle \equiv |nlm; \sigma\tau\rangle$ is a particle state $(2n + l > 0)$, $\sigma' \equiv \sigma_h$, $\tau' \equiv \tau_h$ and

$$S(n) = \frac{1}{4n + \eta} [\tfrac{3}{2} 2^{-n} (t_{1n}^{(0)} + t_{1n}^{(1)}) + \delta_{n1} \sqrt{\tfrac{3}{2}}] \quad n = 1, 2, \ldots . \tag{1.19}$$

It follows from Eq. (1.17) that *the BHF conditions for any pair of different hole states are identically fulfilled, whereas for $h = h'$ they do not depend on h and are equivalent to the single condition*

$$\tfrac{3}{2}(t_{10}^{(0)} + t_{10}^{(1)}) = \tfrac{3}{2} - \eta - C .$$

This condition reduces the number of free parameters to two (usually C and ω are left free) and rules out each diagram that contains at least one composite interaction inserted between any pair of hole lines.

2. Contributions of Third-order Diagrams in the BG Expansion for Energy

In this section the contributions $E_j^{(3)}$, $j = 2, \ldots, 5$ of diagrams 1(b–e) are calculated (the $E_3^{(3)}$, $E_4^{(3)}$ contain also the contributions of diagrams adjoint to 1(c, d)). For completeness the derivation of the contribution $E_1^{(3)}$ of diagram 1(a) is reproduced from ref. [15].

We proceed as follows: the contribution of a given diagram is firstly expressed according to the general rules for BG diagrams [16] in the "abstract" notation, using symbols $|h\rangle$ and $|p\rangle$ for hole and particle states (eigenstates of the s.p. Hamiltonian h) and $\varepsilon(h)$, $\varepsilon(p)$ for their respective energies, the shortened notation (1.16) being used wherever possible. As all the t-interactions are on the energy shell, we omit writing the starting energies. Then we put $\mathsf{t} = \mathsf{t}^{(D)}$, $\mathsf{V} = \mathsf{h} - \mathsf{T}$ and pass to the ^{4}He case so that everything is expressed via quantities $t_{in}^{(S)}$, $\psi_i^{(S)}$ and $S(n)$; eventual summations over hole states are performed with the help of Eqs. (1.9, 10).

$$E_1^{(3)} = -\tfrac{1}{4}\sum_{h_1h_2}\sum_{p_1p_2p_3p_4} \frac{\langle h_1h_2|\,\mathsf{t}\,|p_1p_2\rangle_a \langle p_1p_2|\,\mathsf{V}\otimes\mathsf{I} + \mathsf{I}\otimes\mathsf{V}\,|p_3p_4\rangle}{(\varepsilon(h_1) + \varepsilon(h_2) - \varepsilon(p_1) - \varepsilon(p_2))} \cdot$$

$$\cdot \frac{\langle p_3p_4|\,\mathsf{t}\,|h_1h_2\rangle_a}{(\varepsilon(h_1) + \varepsilon(h_2) - \varepsilon(p_3) - \varepsilon(p_4))} =$$

$$= -\tfrac{1}{2}\sum_{h_1h_2} \langle h_1h_2|\,\mathsf{t}\mathsf{A}(\varepsilon(h_1) + \varepsilon(h_2))\,\mathsf{V}^{(2)}\mathsf{A}(\varepsilon(h_1) + \varepsilon(h_2))\,\mathsf{t}\,|h_1h_2\rangle_a$$

where $\mathsf{V}^{(2)} = \mathsf{V}_{osc}\otimes\mathsf{I} + \mathsf{I}\otimes\mathsf{V}_{osc} - \omega C\,\mathsf{I}\otimes\mathsf{I}$.[8])

Let $\mathsf{A}_D(w)$ be the diagonal approximation of $\mathsf{A}(w)$ [15], i.e.

$$\mathsf{A}(w) = \mathsf{A}_D(w) + \Delta\mathsf{A}(w)\,.$$

This decomposition is substituted into (A) and the term containing $(\Delta\mathsf{A}(w))^2$ is neglected. For the ^{4}He case and $\mathsf{t} = \mathsf{t}^{(D)}$ we then get

$$E_1^{(3)} = (E_1^{(3)})_D + (E_1^{(3)})_P\,,$$

the first term representing the diagonal approximation of $E_1^{(3)}$, the second one the Pauli correction:

$$(E_1^{(3)})_D = -\tfrac{1}{2}\,\mathrm{Tr}_a^{(occ)}[\mathsf{t}^{(D)}\mathsf{A}_D(\bar{w})\,\mathsf{V}^{(2)}\mathsf{A}_D(\bar{w})\,\mathsf{t}^{(D)}]$$

$$(E_1^{(3)})_P = -\,\mathrm{Re}\,\mathrm{Tr}_a^{(occ)}[\mathsf{t}^{(D)}\,\Delta\mathsf{A}(\bar{w})\,\mathsf{V}^{(2)}\,\mathsf{A}_D(\bar{w})\,\mathsf{t}^{(D)}]\,.$$

Further we make use of the identity (see Eq. (1.6))

$$\tfrac{1}{2}m_N\omega^2(|\mathbf{x}_1|^2 + |\mathbf{x}_2|^2) = \frac{\omega}{2}(r^2 + R^2)$$

which yields

$$(\mathsf{V}^{(2)}\varphi)(r, R) = \frac{\omega}{2}(r^2 + R^2 - 2C)\,\varphi(r, R)\,.$$

It is useful to define a more general operator $\mathsf{V}_{\alpha,\beta,C}^{(2)}$

$$(\mathsf{V}_{\alpha,\beta,C}^{(2)}\varphi)(r, R) = \frac{\omega}{2}(\alpha r^2 + \beta R^2 - 2C)\,\varphi(r, R) \tag{2.1}$$

[8]) The projections $\mathsf{P}_0\otimes\mathsf{I}$, $\mathsf{I}\otimes\mathsf{P}_0$, which are contained in $\mathsf{V}\otimes\mathsf{I} + \mathsf{I}\otimes\mathsf{V}$, need not be included into $\mathsf{V}^{(2)}$ since they give zero if multiplied by $\mathsf{A}(w)$.

and introduce for $S = 0, 1$ the quantities

$$K_D^{(S)}(\alpha, \beta, C) = \frac{2}{\omega} \sum_{M=-S}^{S} \sum_{T,M(T)} [1 - (-1^{S+T}] \times$$

$$\times \left(\varphi^{(0)}_{SM\,TM(T)}, \mathsf{t}^{(D)}\, \mathsf{A}_D(\bar{w})\, \mathsf{V}^{(2)}_{\alpha,\beta,C}\, \mathsf{A}_D(\bar{w})\, \mathsf{t}^{(D)} \varphi^{(0)}_{SM\,TM(T)}\right)$$

$$K_P^{(S)}(\alpha, \beta, C) = \frac{2}{\omega} \sum_{M=-S}^{S} \sum_{T,M(T)} [1 - (-1)^{S+T}] \,.$$

$$. \left(\varphi^{(0)}_{SM\,TM(T)}, \mathsf{t}^{(D)}\, \Delta\mathsf{A}(\bar{w})\, \mathsf{V}^{(2)}_{\alpha,\beta,C}\, \mathsf{A}_D(\bar{w})\, \mathsf{t}^{(D)} \varphi^{(0)}_{SM\,TM(T)}\right).$$

The diagonal Bethe-Goldstone equation (1.13) together with the partial-wave decomposition (1.14) imply

$$([((l_i, 0)\, l_i, S)\, SM;\, TM(T)|, (\mathsf{A}_D(\bar{w})\, \mathsf{t}^{(D)} \varphi^{(0)}_{SM\,TM(T)})\,(r, R)) =$$

$$= \frac{1}{R} \boldsymbol{R}_{00}(R) \frac{1}{r} \chi_i^{(S)}(r)\,, \quad \chi_i^{(S)} = \psi_i^{(S)} - \delta_{i1} \boldsymbol{R}_{00}\,. \tag{2.2}$$

Further it holds for any $r, R \in \mathbf{M}$ (see ref. [15] for details)

$$([((l_i, 0)\, l_i, S)\, SM;\, TM(T)|, (\Delta\mathsf{A}(\bar{w})\, \mathsf{t}^{(D)} \varphi^{(0)}_{SM\,TM(T)})\,(r, R)) =$$

$$= \sum_{n=1}^{\infty} \frac{1}{2\eta + 4n + 4i - 4} \frac{t_{in}^{(S)}}{2^{n+i-1}} \sum_{\substack{m+N=n \\ N>0}} 2\langle ml_i N0l_i|\, nl_i 00 l_i\rangle \frac{\boldsymbol{R}_{m\,2i-2}(r)}{r} \frac{\boldsymbol{R}_{N0}(R)}{R}\,. \tag{2.3}$$

With the help of reccurence relations for the M-brackets [19] and of the relation (see [21])

$$r^2 \boldsymbol{R}_{nl}(r) = (2n + l + \tfrac{3}{2})\, \boldsymbol{R}_{nl}(r) - b_{n+1}^{(l)} \boldsymbol{R}_{n+1,l}(r) - b_n^{(l)} \boldsymbol{R}_{n-1,l}(r)\,, \tag{2.4}$$

$$b_n^{(l)} = \sqrt{[n(n + l + \tfrac{1}{2})]}$$

the following expressions are obtained:

$$K_D^{(S)}(\alpha, \beta, C) = 6 \sum_{i=1}^{S+1} \left\{ [\tfrac{3}{2}\beta - 2C] \int_0^\infty |\chi_i^{(S)}(r)|^2\, dr + \alpha \int_0^\infty |r\, \chi_i^{(S)}(r)|^2\, dr \right\}$$

$$K_P^{(S)}(\alpha, \beta, C) = -6\beta \sqrt{\tfrac{3}{2}} \sum_{i=1}^{S+1} \sum_{n=1}^{\infty} \frac{t_{in}^{(S)}}{2\eta + 4n + 4i - 4} \frac{1}{2^{2n+2i-3}} \times$$

$$\times \sqrt{\left(\frac{n(2n + 4i - 3)}{3}\right)} \int_0^\infty \boldsymbol{R}_{n-1,2i-2}(r)\, \chi_i^{(S)}(r)\, dr\,. \tag{2.5}$$

The series occurring here converges better than $\sum_{n=1}^{\infty} n 2^{-n}$ since the quantities

$$c_{in}^{(S)} = \frac{t_{in}^{(S)}}{2\eta + 4n + 4i - 4} \tag{2.6}$$

are proportional to the Fourier cofficients of $\psi_i^{(S)} \in L^2(0, \infty)$ with respect to the basis $\{R_{n,2i-2} | n = 0, 1, \ldots\}$ [9]) and hence $c_{in}^{(S)} \xrightarrow[n\to\infty]{} 0$. The final formula for $E_1^{(3)}$ thus reads

$$E_1^{(3)} = (E_1^{(3)})_D + (E_1^{(3)})_P = \frac{\omega}{2} \sum_{S=0}^{1} [-\tfrac{1}{2}K_D^{(S)}(1, 1, C) - \operatorname{Re} K_P^{(S)}(1, 1, C)] .$$

$$E_2^{(3)} = \tfrac{1}{8}\sum_{h_1h_2} \sum_{p_1p_2} \sum_{h_3h_4} \frac{\langle h_3h_4| \mathrm{t} |p_1p_2\rangle_a \langle h_1h_2| \mathrm{t} |h_3h_4\rangle_a \langle p_1p_2| \mathrm{t} |h_1h_2\rangle_a}{(\varepsilon(h_3) + \varepsilon(h_4) - \varepsilon(p_1) - \varepsilon(p_2))(\varepsilon(h_1) + \varepsilon(h_2) - \varepsilon(p_1) - \varepsilon(p_2))} =$$

$$= \tfrac{1}{2}\sum_{h_1h_2} \langle h_1h_2| [\mathrm{t} \sum_{h_3h_4} |h_3h_4\rangle \langle h_3h_4| \mathrm{t}\mathsf{A}(\varepsilon(h_3) + \varepsilon(h_4)) \mathsf{A}(\varepsilon(h_1) + \varepsilon(h_2)) \mathrm{t}] |h_1h_2\rangle_a .$$

For the ^{4}He case and $\mathrm{t} = \mathrm{t}^{(D)}$ we get with the help of Eqs. (1.9,10)

$$E_3^{(2)} = \tfrac{1}{2} \operatorname{Tr}_a^{(occ)}[\mathrm{t}^{(D)}\mathsf{P}^{(occ)}\mathrm{t}^{(D)}(\mathsf{A}(\bar{w}))^2 \mathrm{t}^{(D)}] =$$

$$= \tfrac{1}{2} \sum_{S,T=0}^{1} \sum_{M,M(T)} [1 - (-1)^{S+T}] \sum_{S',T'=0}^{1} \sum_{M',M(T')}$$

$$(\varphi_{SM\,TM(T)}^{(0)}, \mathrm{t}^{(D)}\varphi_{S'M'T'M(T')}^{(0)}) (\varphi_{S'M'\,T'M(T')}^{(0)}, \mathrm{t}^{(D)}(\mathsf{A}(\bar{w}))^2 \mathrm{t}^{(D)}\varphi_{SM\,TM(T)}^{(0)}) .$$

Now, Eq. (1.12) implies $S = S'$, $T = T'$, $M = M'$, $M(T) = M(T')$ and thus we can proceed as in the preceding case:

$$E_2^{(3)} = (E_2^{(3)})_D + (E_2^{(3)})_P$$

$$(E_2^{(3)})_D = \frac{\omega}{2} \sum_{S=0}^{1} t_{10}^{(S)} \tfrac{1}{2}K_D^{(S)}(0, 0, -\tfrac{1}{2}) = \frac{3\omega}{2} \sum_{S=0}^{1} t_{10}^{(S)} \sum_{i=0}^{S+1} \int_0^\infty |\chi_i^{(S)}(r)|^2 \,\mathrm{d}r$$

$$(E_2^{(3)})_P = \frac{\omega}{2} \sum_{S=0}^{1} t_{10}^{(S)} \operatorname{Re} K_P^{(S)}(0, 0, -\tfrac{1}{2}) = 0 .$$

$$E_3^{(3)} = 2 \operatorname{Re} \sum_{h_1h_2} \sum_{p_1p_2} \frac{\frac{\omega}{2} Z(h_1p_1) \frac{\omega}{2} Z(h_2p_2) \langle p_1p_2| \mathrm{t} |h_1h_2\rangle_a}{(\varepsilon(h_1) - \varepsilon(p_1))(\varepsilon(h_1) + \varepsilon(h_2) - \varepsilon(p_1) - \varepsilon(p_2))} ;$$

for the ^{4}He case and $\mathrm{t} = \mathrm{t}^{(D)}$ we get with the help of Eq. (1.18).

$$E_3^{(3)} = 2 \operatorname{Re} \sum_{n,m=1}^{\infty} S(n) S(m) \frac{4m + \eta}{4(n + m) + 2\eta} \times$$

$$\times \sum_{\sigma\sigma'\tau\tau'} \langle n00\sigma\tau; m00\sigma'\tau'| \mathrm{t}^{(D)} |000\sigma\tau; 000\sigma'\tau'\rangle_a .$$

By passing to the E_{CM} basis, one easily expresses the matrix elements of $\mathrm{t}^{(D)}$ in terms of $t_{in}^{(S)}$ and Moshinsky brackets; then the $E_3^{(3)}$ becomes

$$E_3^{(3)} = 6\omega \sum_{n,m=1} S(n) S(m) \frac{4m + \eta}{4(n + m) + 2\eta} \langle n + m0000 \mid n0m00\rangle \sum_{S=0}^{1} t_{1n+m}^{(S)} =$$

[9]) This follows from Eq. (1.13) — see [15].

$$= 6\omega \sum_{r=2} \frac{t_{1r}^{(0)} + t_{1r}^{(1)}}{4r + 2\eta} 2^{-r} \sum_{m=1}^{r-1} 2^{r-m} S(r-m)\, 2^m S(m)\,(4m+\eta)\,\langle r0000 \mid r - m0m00\rangle .$$

Now Eqs. (1.19) and (2.6) show that $2^n S(n) \sim c_{1n}^{(0)} + c_{1n}^{(1)}$ and hence there is some $K > 0$ such that $|2^n S(n)| < K$, $n = 1, 2, \ldots$. Using the Schwartz inequality and unitary properties of the M-brackets, we arrive at the following estimate

$$\left|\sum_{m=1}^{r-1} 2^{r-m} S(r-m)\, 2^m S(m)\,(4m+\eta)\,\langle r0000 \mid r - m0m00\rangle\right| \leqq$$

$$\leqq 4K^2 \left\{\sum_{m=1}^{r-1} \left(m + \frac{\eta}{4}\right)^2 \sum_{n+n'+1=r} \langle r0000 \mid nln'l0\rangle^2\right\}^{1/2} = \frac{4K^2}{3}\,(r^{3/2} + O(r)) .$$

As the set $\{(t_{1r}^{(0)} + t_{1r}^{(1)})/(4r + 2\eta) \mid r = 1, 2, \ldots\}$ is bounded (cf. (2.6)), the series (2.7) converges better than $\sum_{r=1}^{\infty} r^{3/2}\, 2^{-r}$.

$$E_4^{(3)} = 2\,\mathrm{Re}\left[-\tfrac{1}{2} \sum_{h_1h_2h_3} \sum_{p_1p_2} \frac{Z(h_3p_1)\frac{\omega}{2}}{\varepsilon(h_3) - \varepsilon(p_1)} \frac{\langle h_1h_2|\, t\, |h_3p_2\rangle_a \langle p_1p_2|\, t\, |h_1h_2\rangle_a}{\varepsilon(h_1) + \varepsilon(h_2) - \varepsilon(p_1) - \varepsilon(p_2)}\right].$$

For the ^{4}He case and $t = t^{(D)}$ it holds

$$E_4^{(3)} = \mathrm{Re} \sum_{m=1}^{\infty} S(m)\,(-2\,\mathrm{Tr}_a^{(occ)}[t^{(D)}(-Q_m)\, t^{(D)}] \tag{2.8}$$

where the operator Q_m on H_2 is defined by

$$Q_m = \frac{2}{\omega} \sum_{\sigma\tau} \sum_{v=1}^{\infty} \frac{|000\sigma\tau\rangle \langle m00\sigma\tau| \otimes P_v}{2\eta + 4m + 2v} .$$

For evaluating the trace in (2.8) we use Eq. (1.12) which implies

$$t^{(D)} \varphi_{SM\,TM(T)}^{(0)} = \frac{\omega}{2} \sum_{n=0}^{\infty} \sum_{i=1}^{S+1} t_{in}^{(S)} |((nl_i, 00)\, l_i, S)\, SM;\, TM(T)\rangle . \tag{2.9}$$

Thus the only matrix elements of Q_m we need are

$$\langle((nl_i, 00)\, l_i, S)\, SM;\, TM(T)|\, Q_m |((n'l_j, 00)\, l_j, S)\, SM;\, TM(T)\rangle \equiv \frac{2}{\omega}\, T_{in;jn'}^{(SM\,TM(T))}(m) .$$

These quantities do not depend on $S, M, T, M(T)$ and are simply expressed via M-brackets:

$$T_{in;jn'}(m) \equiv T_{in;jn'}^{(SM\,TM(T))}(m) =$$

$$= \delta_{ij}\delta_{n,n'-m} \frac{\langle nl_i00l_i \mid 00nl_il_i\rangle \langle n + ml_i00l_i \mid m0nl_il_i\rangle}{2\eta + 4(n+m) + 2l_i}\, \vartheta(2n + l_i - 1)$$

where

$$\vartheta(x) = 1 \ldots x \geqq 0\,, \quad \vartheta(x) = 0 \ldots x < 0\,. \tag{2.10}$$

Then the trace becomes

$$\mathrm{Tr}_a^{(occ)}[\mathrm{t}^{(D)}\mathrm{Q}_m\mathrm{t}^{(D)}] = \frac{\omega}{2}\,6\sum_{S=0}^{1}\sum_{i=1}^{S+1}\sum_{n=2-i}^{\infty}\frac{t_{in}^{(S)}t_{in+m}^{(S)}T_{in;in+m}(m)}{2\eta + 4(n+m) + 2l_i}. \tag{2.11}$$

By substituting this into (2.8) a twofold series arises. In order to estimate its convergence we make use of the formula (see [19])

$$\langle nl00l \mid 00nll\rangle = 2^{-n-l/2} \quad n = 0, 1, \dots \quad l = 0, 2, \dots \tag{2.12}$$

and introduce a new summation index $r = n + m$:

$$E_4^{(3)} = -6\omega\sum_{S=0}^{1}\sum_{i=1}^{S+1}\sum_{r=3-i}^{\infty}\frac{t_{ir}^{(S)}}{2\eta + 4r + 4i - 4}\,\frac{1}{2^{r+i-1}}\sum_{n=2-i}^{r-1}2^{r-n}\,S(r-n)\,t_{in}^{(S)} \times$$
$$\times\ \langle rl_i00l_i \mid r - n0nl_il_i\rangle\,.$$

The sum over n can be estimated in the same way as in Eq. (2.7), which implies that the whole series is again dominated by $\sum_r r^{3/2}\,2^{-r}$.

$$E_5^{(3)} = -\sum_{h_1p_1p_2}\frac{\frac{\omega}{2}\,Z(h_1p_2)}{\varepsilon(h_1) - \varepsilon(p_2)}\,\langle p_2|\,\mathrm{V}|p_1\rangle\,\frac{\frac{\omega}{2}\,Z(p_1h_1)}{\varepsilon(h_1) - \varepsilon(p_1)}\,.$$

The matrix elements of V occurring here are immediately evaluated with the help of the reccurence relation (2.4). Then it holds for ^{4}He and $\mathrm{t} = \mathrm{t}^{(D)}$

$$E_5^{(3)} = -2\omega\sum_{n=1}^{\infty}\{S(n)^2\,[(2n + \tfrac{3}{2}) - C] - 2\,S(n)\,S(n+1)\sqrt{((n+1)(n+\tfrac{3}{2}))}\}\,.$$

As to the convergence, Eqs. (1.19), (2.6) imply that the series is dominated by $\sum_n n\,2^{-n}$

3. The BG Expansions for Expectation Values of Some One- and Two-particle Operators

Let $\mathrm{O}^{(k)}$, $k = 1, 2$, be a k-particle operator describing an observable of the A-nucleon system ($A \geqq 2$). The state Hilbert space $\boldsymbol{H}_A$ of the system is the A-fold tensor product of the s.p. Hilbert spaces $\boldsymbol{H} = L^2(\boldsymbol{R}^3) \otimes \boldsymbol{H}_{\sigma\tau}$ or, more precisely, the antisymmetrical subspace $\boldsymbol{H}_A^{(a)}$ of $\boldsymbol{H}_A$. The operator $\mathrm{O}^{(k)}$ acts on $\boldsymbol{H}_A$ and is reduced by the subspace $\boldsymbol{H}_A^{(a)}$. Each one-particle operator $\mathrm{O}^{(1)}$ is fully determined by an operator $\mathrm{O}(1)$ on $\boldsymbol{H}$:

$$\mathrm{O}^{(1)} = \frac{1}{A}\sum_{j=1}^{A}\mathrm{O}_j\,,\quad \mathrm{O}_j = \underbrace{\mathrm{I}\otimes\mathrm{I}\otimes\dots\otimes\mathrm{I}}_{j-1}\otimes\mathrm{O}(1)\otimes\mathrm{I}\otimes\dots\otimes\mathrm{I}\,. \tag{3.1}$$

Similarly, each two-particle operator is determined by an operator $\mathrm{O}(2)$ on the two-particle Hilbert space $\boldsymbol{H}_2$:

$$\mathrm{O}^{(2)} = \frac{1}{A}\sum_{1\leqq j<k\leqq A}\mathrm{O}_{jk}\,. \tag{3.2}$$

In order to define the operators O_{jk} let us take a basis $\{\varphi_\mu\} \subset \boldsymbol{H}$; then $\boldsymbol{E}_2 = \{\varphi_{\mu(1)} \otimes \varphi_{\mu(2)}\}$ is a basis in $\boldsymbol{H}_2 = \boldsymbol{H} \otimes \boldsymbol{H}$ and $\boldsymbol{E}_A = \{\varphi_{\mu(1)} \otimes \ldots \otimes \varphi_{\mu(A)}\}$ is a basis in $\boldsymbol{H}_A$ [18]. It is then sufficient to define matrix elements of O_{jk} with respect to $\boldsymbol{E}_A$: [10])

$$\left(\varphi_{\mu(1)} \otimes \ldots \otimes \varphi_{\mu(A)}, \mathsf{O}_{jk}\varphi_{\nu(1)} \otimes \ldots \otimes \varphi_{\nu(A)}\right) = \\ = \prod_{\substack{i=1 \\ i \neq j,k}}^{A} \delta_{\mu(i),\nu(i)}\left(\varphi_{\mu(j)} \otimes \varphi_{\mu(k)}, \mathsf{O}(2)\, \varphi_{\nu(j)} \otimes \varphi_{\nu(k)}\right). \tag{3.3}$$

The set of n-th order diagrams in the BG expansion for $\langle \mathsf{O}^{(k)} \rangle$ is obtained from the set of $(n + 1)$-th order diagrams in the expansion for energy according to well-known rules [16]. In this section diagrams up to the second order contributing to $\langle \mathsf{O}^{(k)} \rangle$ are calculated. The same procedure as in sect. 2 is applied. General formulae for a rather wide class of one-particle operators are obtained, the specification being performed for the operators $\mathsf{R}^{(1)}$, $\mathsf{D}^{(1)}$ and $\mathsf{F}^{(1)}(\mathsf{q})$ (see below Eqs. (3.5, 6, 15)). As to two-particle operators, we limit ourselves to those appearing in the centre-of-mass Hamiltonian

$$\mathsf{H}_{CM}^{(\alpha)} = \frac{\mathsf{P}_{CM}^2}{2m_N A} + \tfrac{1}{2} m_N A \alpha^2 \omega^2 \mathsf{X}_{CM}^2 = \frac{\omega}{2}\left[\alpha^2(\mathsf{R}^{(1)} + 2\mathsf{R}^{(2)}) - \mathsf{D}^{(1)} - 2\mathsf{D}^{(2)}\right],$$

$$0 \leqq \alpha \leqq 1\,,^{11)} \quad \mathbf{X}_{CM} = \frac{1}{A}\sum_{j=1}^{A} \mathbf{x}_j\,, \quad \mathbf{P}_{CM} = \sum_{j=1}^{A} \mathbf{p}_j\,. \tag{3.4}$$

The operators $\mathsf{D}^{(1)}$ and $\mathsf{R}^{(1)}$ are constructed according to Eq. (3.1) from the Laplace operator Δ on $L^2(\mathbf{R})$ and the harmonic oscillator potential V_{osc} respectively:

$$\mathsf{D}(1) = \Delta \otimes \mathsf{I}_{\sigma\tau}\,, \tag{3.5}$$

$$\mathsf{R}(1) = \mathsf{R}_{orb} \otimes \mathsf{I}_{\sigma\tau}\,, \quad \mathsf{R}_{orb} = 2\omega\, \mathsf{V}_{osc}\,, \tag{3.6}$$

where $\mathsf{I}_{\sigma\tau}$ is the unity operator on the s.p. spin and isospin Hilbert space $\boldsymbol{H}_{\sigma\tau}$.

The operators $\mathsf{D}(2)$ and $\mathsf{R}(2)$ that determine $\mathsf{D}^{(2)}$ and $\mathsf{R}^{(2)}$ (see Eqs. (3.2,3)) are defined in the $\boldsymbol{H} \otimes \boldsymbol{H}$ realization of $\boldsymbol{H}_2$ via variables $\boldsymbol{r}_i \equiv \{r_i^{(\mu)} \mid \mu = 1, 2, 3\} = \mathbf{x}_i/b$ ($i = 1, 2$ – cf. (1.6)):

$$\left(\mathsf{R}(2)\, \psi_{\sigma(1)\tau(1);\sigma(2)\tau(2)}\right)(\boldsymbol{r}_1, \boldsymbol{r}_2) = \sum_{\mu=1}^{3} r_1^{(\mu)} r_2^{(\mu)} \psi_{\sigma(1)\tau(1);\sigma(2)\tau(2)}(\boldsymbol{r}_1, \boldsymbol{r}_2) \tag{3.7}$$

$$\left(\mathsf{D}(2)\, \psi_{\sigma(1)\tau(1);\sigma(2)\tau(2)}\right)(\boldsymbol{r}_1, \boldsymbol{r}_2) = \sum_{\mu=1}^{3} \frac{\partial^2 \psi_{\sigma(1)\tau(1);\sigma(2)\tau(2)}}{\partial x_1^{(\mu)}\, \partial x_2^{(\mu)}}(\boldsymbol{r}_1, \boldsymbol{r}_2)\,. \tag{3.8}$$

[10]) In fact this can be done only if $\mathsf{O}(2)$ is a bounded operator on O_2; for the general case see ref. [22].

[11]) By means of parameter α both the "elementary" and the Lipkin's approaches of treating the c.m. motion are covered: the former for $\alpha = 0$, the latter for $\alpha = 1$.

For the $L^2(\mathbf{M}, \mu, \boldsymbol{G})$ realization of $\boldsymbol{H}_2$ the relations (1.6) imply

$$(\mathsf{R}(2)\,\varphi)\,(r, R) = \tfrac{1}{2}(R^2 - r^2)\,\varphi(r, R)\,. \tag{3.9}$$

Analogously the $\mathsf{D}(2)$ becomes $\frac{1}{2}(\Delta^{(CM)} - \Delta^{(rel)})$ where $\Delta^{(CM)}$ is the Laplace operator with respect to the c.m. coordinates $R^{(\mu)} = (r_1^{(\mu)} + r_2^{(\mu)})/\sqrt{2}$, $\mu = 1, 2, 3$, and similarly $\Delta^{(rel)}$ is related to the relative coordinate $r^{(\mu)} = (r_1^{(\mu)} - r_2^{(\mu)})/\sqrt{2}$. Now, $L^2(\mathbf{M}, \mu, \boldsymbol{G})$ is the space of functions depending on spherical c.m. and relative coordinates and thus the action of $\mathsf{D}(2)$ is described by means of the basis (1.7) in $\boldsymbol{G}$ as follows:

$$(g_{[((l,L)\lambda,\ldots]}, (\mathsf{D}(2)\,\varphi)\,(r, R)) = \tfrac{1}{2}[(\Delta_L^{(CM)} f_{[((l,L)\lambda,\ldots]})\,(r, R) - (\Delta_l^{(rel)} f_{[((l,L)\lambda,\ldots]})\,(r, R) \tag{3.10}$$

where

$$f_{[((l,L)\lambda,\ldots]}(r, R) = (g_{[((l,L)\lambda,\ldots]}, \varphi(r, R)) \in L^2(\mathbf{M}, \mu)$$

and

$$(\Delta_L^{(CM)} f)\,(r, R) = \frac{1}{R}\left(\frac{\partial^2}{\partial R^2}\,Rf\right)(r, R) - \frac{L(L+1)}{R^2}\,f(r, R) \tag{3.11}$$

$$(\Delta_l^{(rel)} f)\,(r, R) = \frac{1}{r}\left(\frac{\partial^2}{\partial r^2}\,rf\right)(r, R) - \frac{l(l+1)}{r^2}\,f(r, R)\,. \tag{3.12}$$

Notice that the r.m.s. radius can be expressed via $\langle \mathsf{R}^{(1)} \rangle$ and $\langle \mathsf{R}^{(2)} \rangle$ [15].

3.1. One-particle Operators

The diagrams we have to consider are shown in Fig. 2 where the conventions introduced in Fig. 1 are used: especially the BHF conditions $Z(h, h') = 0$ (cf. Eqs. (1.16, 17)) are assumed to be fulfilled so that all the diagrams containing a "composite" interaction inserted between a pair of hole lines are omitted. As to diagrams containing a composite interaction creating/annihilating a particle-hole pair, we can expect their contributions to be small when the oscillator frequency ω is chosen self-consistently (see the discussion in Introduction). However, except diagram 2(k) where an off-energy-shell t-interaction appears, all these contributions can easily be calculated. The explicit formulae we give below can be used for examining how these diagrams depend on ω and checking that they actually become small for the self-consistent value of ω.

We shall consider only such $\mathsf{O}^{(1)}$ that are constructed from operators $\mathsf{O}(1)$ of the form (cf. Eqs. (3.5, 6))

$$\mathsf{O}(1) = \mathsf{O}_{orb} \otimes \mathsf{I}_{\sigma\tau} \tag{3.13}$$

where O_{orb} is an operator on $L^2(\mathbf{R}^3)$. Then, for $A = 4$, matrix elements of $\mathsf{O}(1)$ for any pair of hole states read

$$\langle h|\,\mathsf{O}(1)\,|h'\rangle = \delta_{hh'}\langle 000|\,\mathsf{O}_{orb}|000\rangle\,.$$

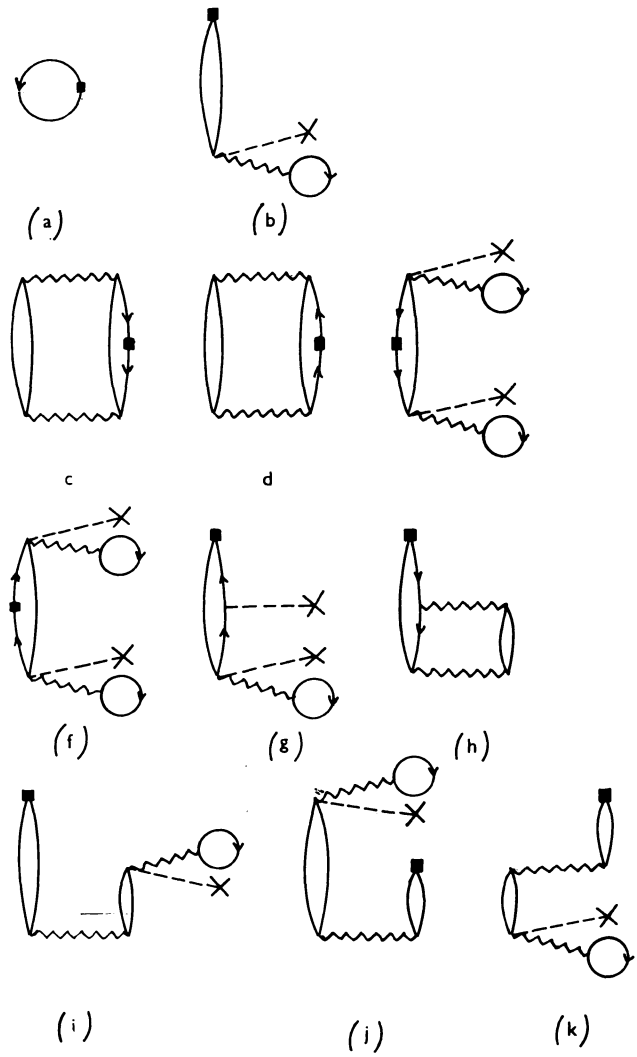

Fig. 2. Diagrams up to the second order in the BG expansion for $\langle O^{(1)} \rangle$. All the t-interactions are on the energy shell except the middle one in diagram (k). The diagrams adjoint to (b, g, h, i, j, k) are not drawn

For the orbital operators corresponding to R(1) and D(1) it follows from Eqs. (3.5, 6)

$$\langle nlm | \mathrm{R}_{orb} - \Delta | n'l'm' \rangle = \delta_{nn'} \delta_{ll'} \delta_{mm'} (4n + 2l + 3) \,. \tag{3.14}$$

Combining this result with the reccurence relation (2.4), we see that the operators R_{orb} and Δ have identical non-diagonal matrix elements, whereas the diagonal matrix elements are of opposite signs. Thus, in most cases it is sufficient to consider only one of these operators, say $\mathrm{R}^{(1)}$.

In addition to $R^{(1)}$, $D^{(1)}$ we shall derive explicit formulae also for the operator $F^{(1)}(\boldsymbol{q})$ that is needed when calculating the form factor [15] and is determined by the following operator $F(1; \boldsymbol{k})$ on $\boldsymbol{H}$:

$$F(1; \boldsymbol{k}) = F_{orb}(\boldsymbol{k}) \otimes I_{\sigma\tau}, \quad (F_{orb}(\boldsymbol{k})\, \psi)(\boldsymbol{r}) = \exp(i\boldsymbol{kr})\, \psi(\boldsymbol{r}),$$
$$\psi \in L^2(\mathbf{R}^3), \quad \boldsymbol{k} = b\boldsymbol{q}. \tag{3.15}$$

The generating function for the Laguerre polynomials [21] can be used when calculating the matrix elements of $F_{orb}(\boldsymbol{k})$:

$$\frac{\sin kr}{kr} = \exp\left(-\frac{k^2}{4}\right) \sum_{n=0}^{\infty} \frac{(k^2/2)^n}{(2n+1)!!} L_n^{(1/2)}(r^2) =$$
$$= \exp\left(-\frac{k^2}{4}\right) \sum_{n=0}^{\infty} \frac{(k^2/2)^n}{\sqrt{(2n+1)!}} \frac{R_{n0}(r)}{R_{00}(r)}. \tag{3.16}$$

Explicit expressions for matrix elements $\langle n00|\, O_{orb} |000\rangle$, $n = 0, 1, \ldots$ that frequently occur in the following calculations read

$$\langle n00|\, R_{orb} |000\rangle = \tfrac{3}{2}\delta_{n0} - \tfrac{3}{2}\delta_{n1},$$
$$\langle n00|\, F_{orb}(\boldsymbol{k})\, |000\rangle = \int_0^{\infty} R_{n0}(r) \frac{\sin kr}{kr} R_{00}(r)\, dr = \frac{\exp(-k^2/4)\, k^{2n}}{2^n \sqrt{(2n+1)!}}. \tag{3.17}$$

1. Contributions of diagrams 2(a–c):

These quantities, which we denote $\langle O^{(1)}\rangle^{(0)}$, $\langle O^{(1)}\rangle^{(1)}$ and $\langle O^{(1)}\rangle_1^{(2)}$, are simply related to matrix elements (3.17):

$$\langle O^{(1)}\rangle^{(0)} = \sum_h \langle h|\, \tfrac{1}{4} O(1)\, |h\rangle = \langle 000|\, O_{orb} |000\rangle,$$

$$\langle O^{(1)}\rangle^{(1)} = 2\, \mathrm{Re} \sum_{ph} \langle h|\, \tfrac{1}{4} O(1)\, |p\rangle \frac{Z(p, h)\, \dfrac{\omega}{2}}{\varepsilon(h) - \varepsilon(p)} =$$
$$= -2\, \mathrm{Re} \sum_{n=1}^{\infty} S(n)\, \langle 000|\, O_{orb} |n\, 00\rangle,$$

$$\langle O^{(1)}\rangle_1^{(2)} = -\tfrac{1}{2} \sum_{h_1 h_2 h} \sum_{p_1 p} \frac{\langle hh_2|\, t\, |pp_1\rangle_a \langle h_1|\, \tfrac{1}{4} O(1)\, |h_2\rangle \langle pp_1|\, t\, |hh_1\rangle_a}{(\varepsilon(h) + \varepsilon(h_2) - \varepsilon(p) - \varepsilon(p_1))(\varepsilon(h) + \varepsilon(h_1) - \varepsilon(p) - \varepsilon(p_1))} =$$
$$= -\tfrac{1}{8} \langle 000|\, O_{orb} |000\rangle\, 2\, \mathrm{Tr}_a^{(occ)} [t^{(D)} (A(\bar{w}))^2\, t^{(D)}].$$

The trace can be expressed via $K_D^{(S)}(0, 0, -1/2)$ and $K_P^{(S)}(0, 0, -1/2)$ (see (2.5)) proceeding as in sect. 2, we get:

$$\langle O^{(1)}\rangle_1^{(2)} = (\langle O^{(1)}\rangle_1^{(2)})_D + (\langle O^{(1)}\rangle_1^{(2)})_P,$$
$$(\langle O^{(1)}\rangle_1^{(2)})_D = -\tfrac{3}{4} \langle 000|\, O_{orb} |000\rangle \sum_{S=0}^{1} \sum_{i=1}^{S+1} \int_0^{\infty} |\chi_i^{(S)}(r)|^2\, dr,$$
$$(\langle O^{(1)}\rangle_1^{(2)})_P = 0.$$

2. Contribution of diagram 2(d):

$$\langle \mathsf{O}^{(1)} \rangle_2^{(2)} = \tfrac{1}{2} \sum_{h_1 h} \sum_{p_1 p_2 p} \frac{\langle hh_1 | \mathsf{t} | pp_2 \rangle_a \langle p_2 | \tfrac{1}{4}\mathsf{O}(1) | p_1 \rangle \langle pp_1 | \mathsf{t} | hh_1 \rangle_a}{(\varepsilon(h) + \varepsilon(h_1) - \varepsilon(p) - \varepsilon(p_2))(\varepsilon(h) + \varepsilon(h_1) - \varepsilon(p) - \varepsilon(p_1))} =$$

$$= \tfrac{1}{8} \mathrm{Tr}_a^{(occ)} [\mathsf{t}^{(D)} \mathsf{A}(\bar{w}) (\mathsf{I} \otimes \mathsf{O}(1) + \mathsf{O}(1) \otimes \mathsf{I}) \mathsf{A}(\bar{w}) \mathsf{t}^{(D)}] .$$

If $\mathsf{O}^{(1)} = \mathsf{R}^{(1)}$, it holds $\mathsf{I} \otimes \mathsf{O}(1) + \mathsf{O}(1) \otimes \mathsf{I} = (2/\omega) \mathsf{V}_{1,1,0}^{(2)}$ and hence the result is the same as in the case of $E_1^{(3)}$ for $C = 0$, i.e.

$$\langle \mathsf{R}^{(1)} \rangle_2^{(2)} = \tfrac{1}{8} \sum_{S=0}^{1} [K_D^{(S)}(1, 1, 0) + 2 \,\mathrm{Re}\, K_P^{(S)}(1, 1, 0)] .$$

As in $\langle \mathsf{O}^{(1)} \rangle_2^{(2)}$ both diagonal and non-diagonal matrix elements of $\mathsf{O}(1)$ occur, we cannot obtain the formula for $\langle \mathsf{D}^{(1)} \rangle_2^{(2)}$ directly from that for $\langle \mathsf{R}^{(1)} \rangle_2^{(2)}$. Let us denote

$$\Phi_{SM\,TM(T)} = [\mathsf{I} \otimes \mathsf{D}(1) + \mathsf{D}(1) \otimes \mathsf{I}] \,\mathsf{A}_D(\bar{w})\, \mathsf{t}^{(D)} \varphi_{SM\,TM(T)}^{(0)} ;$$

Eqs. (2.2), (3.10–12) now imply

$$F_i^{(S)}(r, R) \equiv \sum_{T=0}^{1} [1 - (-1)^{S+T}] \sum_{MM(T)} ([(l_i, 0)\, l_i, S)\, SM;\, TM(T)|, \Phi_{SM\,TM(T)}(r, R)) =$$

$$= 6 \left[\frac{1}{r} \chi_i^{(S)}(r) \left(\Delta_0^{(CM)} \frac{R_{00}}{R} \right)(R) + \frac{1}{R} R_{00}(R) \left(\Delta_{2i-2}^{(rel)} \frac{\chi_i^{(S)}}{r} \right)(r) \right] .$$

Further Eqs. (1.14, 17) yield

$$(\langle \mathsf{D}^{(1)} \rangle_2^{(2)})_D = \tfrac{1}{8} \sum_{S=0}^{1} \sum_{i=1}^{S+1} \int_0^\infty \int_0^\infty \frac{1}{rR} R_{00}(r)\, \chi_i^{(S)}(r)\, F_i^{(S)}(r, R)\, r^2 R^2 \,\mathrm{d}r \,\mathrm{d}R =$$

$$= \tfrac{3}{4} \sum_{S=0}^{1} \sum_{i=1}^{S+1} \int_0^\infty \frac{1}{r} \chi_i^{(S)}(r) \left(\Delta_{2i-2}^{(rel)} \frac{\chi_i^{(S)}}{r} \right)(r)\, r^2 \,\mathrm{d}r - \frac{3}{2} \int_0^\infty |\chi_i^{(S)}(r)|^2 \,\mathrm{d}r .$$

The Pauli correction contains integrals

$$J_i^{(S)}(n, N) = \int_0^\infty \int_0^\infty \frac{1}{rR} R_{N0}(R)\, R_{n-N,2i-2}(r)\, F_i^{(S)}(r, R)\, r^2 R^2 \,\mathrm{d}r \,\mathrm{d}R \qquad n, N = 1, 2, \ldots .$$

Using orthogonality of functions R_{N0}, $N = 0, 1, \ldots$, and Eqs. (3.14, 17), we get

$$J_i^{(S)}(n, N) = -\delta_{N1} \sqrt{\frac{3}{2}} \int_0^\infty R_{n-1,2i-2}(r)\, \chi_i^{(S)}(r) \,\mathrm{d}r .$$

Now, comparison with the formula (2.5) for $K_P^{(S)}(1,1,0)$ shows that

$$(\langle \mathsf{D}^{(1)} \rangle_2^{(2)})_P = (\langle \mathsf{R}^{(1)} \rangle_2^{(2)})_P .$$

If $O^{(1)} = F^{(1)}(\boldsymbol{q})$, the calculation is much more difficult and we shall limit ourselves only to the diagonal term. As in the previous case we introduce

$$\Psi^{(\boldsymbol{k})}_{SM\,TM(T)} = [\mathsf{I} \otimes \mathsf{F}(1; \boldsymbol{k}) + \mathsf{F}(1; \boldsymbol{k}) \otimes \mathsf{I}]\ \mathsf{A}_D(\overline{w})\ \mathsf{t}^{(D)} \varphi^{(0)}_{SM\,TM(T)}$$

and

$$G_i^{(S)}(\boldsymbol{k}; r, R) \equiv$$

$$\equiv \sum_{T=0}^{1} [1 - (-1)^{S+T}] \sum_{MM(T)} ([((l_i, 0)\, l_i, S)\, SM;\ TM(T)|,\ \Psi^{(\boldsymbol{k})}_{SM\,TM(T)}(r, R))$$

so that

$$(\langle \mathsf{F}^{(1)}(\boldsymbol{q})\rangle_2^{(2)})_D = \tfrac{1}{8} \sum_{S=0}^{1} \sum_{i=1}^{S+1} \int_0^\infty \int_0^\infty \frac{1}{rR}\, R_{00}(R)\, \chi_i^{(S)}(r)\, G_i^{(S)}(\boldsymbol{k}; r, R)\, r^2 R^2\, \mathrm{d}r\, \mathrm{d}R\ .$$

Now, Eqs. (3.15) and (1.6) imply that it holds for any vector $\varphi \in L^2(\mathbf{M}, \mu; \boldsymbol{G})$

$$([\mathsf{F}(1; \boldsymbol{k}) \otimes \mathsf{I} + \mathsf{I} \otimes \mathsf{F}(1; \boldsymbol{k})]\ \varphi)\,(r, R) = \mathsf{f}_{12}(k; r, R)\ \varphi(r, R)$$

where $\mathsf{f}_{12}(k; r, R)$ is the bounded operator on $\boldsymbol{G}$ that multiplies each vector of $\boldsymbol{G}$ by product of functions $F^{(kR)}$ and $f^{(kr)}$ of the c.m. and relative angular variables of a nucleon pair:

$$F^{(kR)}(\Theta) = \exp\left(\frac{ikR}{\sqrt{2}} \cos \Theta\right), \quad f^{(kr)}((\vartheta) = 2 \cos\left(\frac{kr}{\sqrt{2}} \cos \vartheta\right).$$

Using once more Eqs. (1.14) and (2.2) we get

$$(*) \qquad G_i^{(S)}(\boldsymbol{k}; r, R) = \sum_{j=1}^{S+1} G_{ij}^{(S)}(k; r, R)\, \frac{1}{rR}\, R_{00}(R)\, \chi_j^{(S)}(r)$$

where

$$G_{ij}^{(S)}(k; r, R) = \sum_{T=0}^{1} [1 - (-1)^{S+T}]\ .$$

$$.\ \sum_{M,M(T)} [((l_i, 0)\, l_i, S)\, SM;\ TM(T)\, |\mathsf{f}_{12}(k; r, R)|\ ((l_j, 0)\, l_j, S)\, SM;\ TM(T)] =$$

$$= \sum_{T=0}^{1} [1 - (-1)^{S+T}]\,(2T + 1) \sum_{M} \sum_{\mu\mu'} (l_i\mu, SM - \mu \mid SM)\,(l_j\mu', SM - \mu' \mid SM) \times$$

$$\times\ \delta_{\mu\mu'} \int_\Omega F^{(kR)} |Y_{00}|^2\, \mathrm{d}\Omega \int_\Omega f^{(kr)} \overline{Y}_{2i-2,\mu} Y_{2j-2,\mu'}\, \mathrm{d}\Omega\ .$$

Now, the sum over M can be performed: symmetry properties and orthogonality relations of Clebsh coefficients yield the factor $\delta_{ij}(2S + 1)/(2l_i + 1)$. Then the summation over μ is carried out with the help of the addition theorem for the spherical harmonics, which gives

$$G_{ij}^{(S)}(k; r, R) = \delta_{ij}(2S + 1) \sum_{T=0}^{1} [1 - (-1)^{S+T}]\,(2T + 1)\, \frac{1}{4\pi} \int_\Omega F^{(kR)}\, \mathrm{d}\Omega\, \frac{1}{4\pi} \int_\Omega f^{(kr)}\, \mathrm{d}\Omega$$

$$= 12\delta_{ij} \frac{\sin(kR/\sqrt{2})}{kR/\sqrt{2}} \frac{\sin(kr/\sqrt{2})}{kr/2}.$$

Then (*) is transformed to

$$G_i^{(S)}(\mathbf{k}; r, R) = 12 \frac{\sin(kR/\sqrt{2})}{kR/\sqrt{2}} \frac{\sin(kr/\sqrt{2})}{kr/\sqrt{2}} \frac{1}{rR} \boldsymbol{R}_{00}(R)\, \chi_i^{(S)}(r)$$

and, using the expansion (3.16), the final result is obtained:

$$(\langle \mathsf{F}^{(1)}(\mathbf{q})\rangle_2^{(2)})_D = \tfrac{3}{2} \sum_{S=0}^{1} \sum_{i=1}^{S+1} \int_0^\infty \boldsymbol{R}_{00}^2(R) \frac{\sin(kR/\sqrt{2})}{kR/\sqrt{2}}\, dR \int_0^\infty \frac{\sin(kr/\sqrt{2})}{kr/\sqrt{2}} |\chi_i^{(S)}(r)|^2\, dr =$$

$$= \tfrac{3}{2} \exp\left(\frac{-k^2}{4}\right) \sum_{n=0}^{\infty} \frac{(k^2/4)^n}{\sqrt{(2n+1)!}} \sum_{S=0}^{1} \sum_{i=1}^{S=1} \int_0^\infty \frac{|\chi_i^{(S)}(r)|^2}{\boldsymbol{R}_{00}(r)} \boldsymbol{R}_{n0}(r)\, dr.$$

As $\chi_i^{(S)}(r) \sim \boldsymbol{R}_{00}(r)$ for large r and $|\chi_i^{(S)}(r)|^2/\boldsymbol{R}_{00}(r)$ tends to zero for $r \to 0$, it holds $|\chi_i^{(S)}|^2/\boldsymbol{R}_{00} \in L^2(0, \infty)$; hence the integrals on the right-hand-side of the last equation converge to zero for $n \to \infty$ and consequently the series is convergent for all values of k.

3. Contributions of diagrams 2(e – j)

These quantities will be denoted $\langle \mathsf{O}^{(1)}\rangle_j^{(2)}$, $j = 3, 4, \ldots, 8$; for $j \geqq 5$ each of them contains also the contribution of the corresponding adjoint diagram. The calculation is analogous as in section 2, this analogy referring also to the question of convergence of eventual infinite series. In case that the resulting formula for $\langle \mathsf{O}^{(1)}\rangle_j^{(2)}$ depends on $\mathsf{O}(1)$ only via matrix elements $\langle n00|\mathsf{O}_{orb}|\,000\rangle$, we shall not perform specification for the operators $\mathsf{R}^{(1)}$ and $\mathsf{F}^{(1)}(\mathbf{q})$: explicit expressions are obtained by substituting from Eqs. (3.17).

$$\langle \mathsf{O}^{(1)}\rangle_3^{(2)} = -\sum_{h_1 h_2 p} \frac{(\omega/2)\, Z(h_2 p)}{\varepsilon(h_2) - \varepsilon(p)} \langle h_1|\, \tfrac{1}{4}\mathsf{O}(1)\, |h_2\rangle \frac{(\omega/2)\, Z(p h_1)}{\varepsilon(h_1) - \varepsilon(p)} =$$

$$= -\langle 000|\, \mathsf{O}_{orb}|\, 000\rangle \sum_{n=1}^{\infty} (S(n))^2.$$

$$\langle \mathsf{O}^{(1)}\rangle_4^{(2)} = \sum_{p_1 p_2 h} \frac{(\omega/2)\, Z(h p_2)}{\varepsilon(h) - \varepsilon(p_2)} \langle p_2|\, \tfrac{1}{4}\mathsf{O}(1)|p_1\rangle \frac{(\omega/2)\, Z(p_1 h)}{\varepsilon(h) - \varepsilon(p_1)} =$$

$$= \sum_{n,m=1}^{\infty} S(n)\, S(m)\, \langle n00|\, \mathsf{O}_{orb}|m00\rangle.$$

In particular, we get (cf. the calculation of $E_5^{(3)}$)

$$\langle \mathsf{R}^{(1)}\rangle_4^{(2)} = \sum_{n=1}^{\infty} [(2n + 3/2)(S(n))^2 - 2\, S(n)\, S(n+1) \sqrt{((n+1)(n+3/2))}],$$

$$\langle \mathsf{D}^{(1)}\rangle_4^{(2)} = -\sum_{n=1}^{\infty} [(2n + 3/2)(S(n))^2 + 2\, S(n)\, S(n+1) \sqrt{(([n+1)(n+3/2))}].$$

For the operator $\mathsf{F}^{(1)}(\boldsymbol{q})$ Eq. (3.15) yields

$$\langle \mathsf{F}^{(1)}(\boldsymbol{q})\rangle_4^{(2)} = \sum_{n,m=1}^{\infty} S(n)\, S(m) \int_0^{\infty} \boldsymbol{R}_{n0}(r)\, \boldsymbol{R}_{m0}(r) \frac{\sin kr}{kr}\, \mathrm{d}r\,.$$

Further the inequality

$$\left|\int_0^{\infty} \boldsymbol{R}_{n0}(r)\, \boldsymbol{R}_{m0}(r) \frac{\sin kr}{kr}\, \mathrm{d}r\right|^2 \leqq \int_0^{\infty} |\boldsymbol{R}_{n0}(r)|^2 \left|\frac{\sin kr}{kr}\right|^2 \mathrm{d}r \int_0^{\infty} |\boldsymbol{R}_{m0}(r)|^2\, \mathrm{d}r \leqq 1$$

implies that the twofold series is dominated by $\sum_n (S(n))^2$ and thus the convergence is very rapid for all k.

$$\langle \mathsf{O}^{(1)}\rangle_5^{(2)} = -2\,\mathrm{Re} \sum_{p_1 p_2 h} \frac{\langle h|\, \tfrac{1}{4}\mathsf{O}(1)\, |p_2\rangle}{\varepsilon(h) - \varepsilon(p_2)} \langle p_2|\, \mathsf{V} |p_1\rangle \frac{(\omega/2)\, Z(p_1 h)}{\varepsilon(h) - \varepsilon(p_1)} =$$

$$= -2\,\mathrm{Re} \sum_{n,m=1}^{\infty} \frac{\langle 000|\, \mathsf{O}_{orb} |n00\rangle}{-(4n + \eta)} \langle n00|\, \mathsf{R}_{orb} - C\mathsf{I}\, |m00\rangle\, (-S(m)) =$$

$$= -2\,\mathrm{Re} \sum_{n=1}^{\infty} \frac{\langle 000|\, \mathsf{O}_{orb} |n00\rangle}{4n + \eta} \times$$

$$\times \left[(2n + 3/2 - C)\, S(n) - \vartheta(n - 2) \sqrt{[n(n + 1/2)]} \times \right.$$

$$\left. \times\, S(n - 1) - \sqrt{[(n + 1)(n + 3/2)]}\, S(n + 1)\right].$$

$$\langle \mathsf{O}^{(1)}\rangle_6^{(2)} = 2\,\mathrm{Re}(-\tfrac{1}{2}) \sum_{p'p} \sum_{h_1 h_2 h} \frac{\langle h_2|\, \tfrac{1}{4}\mathsf{O}(1)\, |p\rangle\, \langle h_1 h|\, \mathsf{t} |h_2 p'\rangle_a \langle pp'|\, \mathsf{t} |h_1 h\rangle_a}{\varepsilon(h_2) - \varepsilon(p)\quad \varepsilon(h_1) + \varepsilon(h) - \varepsilon(p) - \varepsilon(p')} =$$

$$= -\,\mathrm{Re} \sum_{v=1}^{\infty} \sum_{2n+l=v} \sum_{m=-l}^{l} \frac{\langle 000|\, \tfrac{1}{4}\mathsf{O}_{orb} |nlm\rangle}{(\omega/2)(2v + \eta)}\, 2\mathrm{Tr}_a^{(occ)}[\mathsf{t}^{(D)} \mathsf{Q}_{nlm} \mathsf{t}^{(D)}]\,. \tag{3.18}$$

The calculation is similar as in the case of $E_4^{(3)}$; however, we have to treat a more complicated operator

$$\mathsf{Q}_{nlm} = \frac{2}{\omega} \sum_{\sigma\tau} \sum_{v'=1}^{\infty} \sum_{2n'+l'=v'} \sum_{m'=-l'}^{l'} \sum_{\sigma'\tau'} \frac{|000\sigma\tau\rangle \langle nlm\sigma\tau| \otimes |n'l'm'\sigma'\tau'\rangle \langle n'l'm'\sigma'\tau'|}{4n + 2l + 2v' + 2\eta}$$

because matrix elements of O_{orb} need not be diagonal with respect to angular quantum numbers l, m. The calculation again reduces to evaluation of

$$\langle ((rl_i, 00)\, l_i, S)\, SM;\, TM(T)\, |\mathsf{Q}_{nlm}| ((r'l_j, 00)\, l_j, S)\, SM;\, TM(T)\rangle\,.$$

As these matrix elements are diagonal with respect to M, it is clear that they vanish for $m \neq 0$. For $m = 0$ it is possible to perform the summation over M (cf. (1.10)) which gives the factor $\delta_{ij}(2S + 1)/(2l_i + 1)$. Then, with the help of symmetry properties of Clebsh coefficients, the sum over m' is carried out:

$$\sum_{m'} (l0,\, l_i m' \mid l_i m') = \delta_{l0}(2l_i + 1)\,. \tag{3.19}$$

Thus the trace in Eq. (3.18) is zero unless $l = m = 0$, and the formula for $\langle \mathrm{O}^{(1)}\rangle_6^{(2)}$ is obtained from that for $E_4^{(3)}$ if one replaces $S(r-n)$ by

$$(2/\omega)\,\langle 000|\,\tfrac{1}{4}\mathrm{O}_{orb}|r-n00\rangle/(4r-4n+\eta)$$

$$\langle \mathrm{O}^{(1)}\rangle_6^{(2)} = -3\sum_{S=0}^{1}\sum_{i=1}^{S+1}\sum_{r=3-i}^{\infty}\frac{t_{ir}^{(S)}}{2\eta+4r+4i-4}\,2^{-r-(i-1)}\sum_{n=2-i}^{r-1}2^{r-n}\times$$

$$\times\frac{\langle 000|\,\mathrm{O}_{orb}|r-n00\rangle}{4(r-n)+\eta}\,t_{in}^{(S)}\langle rl_i00l_i\,|\,r-n0nl_il_i\rangle\,.$$

Finally, Eqs. (3.17) show that

$$2^n\langle 000|\,\mathrm{O}_{orb}|n00\rangle/(4n+\eta)\xrightarrow[n\to\infty]{}0 \qquad (3.20)$$

for both R_{orb} and $\mathrm{F}_{orb}(\boldsymbol{k})$; consequently, the estimate of convergence performed for $E_4^{(3)}$ is valid.

$$\langle \mathrm{O}^{(1)}\rangle_7^{(2)} = 2\mathrm{Re}\sum_{h_1h}\sum_{p_1p}\frac{\langle h|\,\frac{1}{4}\mathrm{O}(1)\,|p\rangle}{\varepsilon(h)-\varepsilon(p)}\,\frac{\omega}{2}\,Z(h_1p_1)\,\frac{\langle pp_1|\,\mathrm{t}|hh_1\rangle_a}{\varepsilon(h)+\varepsilon(h_1)-\varepsilon(p)-\varepsilon(p_1)}\,.$$

As the quantities $Z(h, p)$ and $\langle h\,|\mathrm{O}(1)\,|p\rangle$ are diagonal with respect to spin and isospin quantum numbers, the calculation reduces to evaluation of the following sum

$$\sum_{\sigma_1\sigma\tau_1\tau}\langle(nlm\sigma\tau)\otimes(n_100\sigma_1\tau_1)\,|\mathrm{t}^{(D)}|(000\sigma\tau)\otimes(000\sigma_1\tau_1)\rangle_a \equiv \boldsymbol{S}_{nlm}(n_1)\,.$$

Passing to the basis $\boldsymbol{E}_{CM}$ and using Eqs. (1.12), (3.19), we find

$$\boldsymbol{S}_{nlm}(n_1) = 6\delta_{l0}\delta_{m0}(t_{1r}^{(0)}+t_{1r}^{(0)})\,\langle r0000|n0n_100\rangle\,,\quad r = n+n_1\,.$$

Then

$$\langle \mathrm{O}^{(1)}\rangle_7^{(2)} = 3\,\mathrm{Re}\sum_{r=2}^{\infty}\frac{t_{1r}^{(0)}+t_{1r}^{(1)}}{4r+2\eta}\sum_{n=1}^{r-1}\frac{\langle 000|\,\mathrm{O}_{orb}|n00\rangle}{4n+\eta}\times$$

$$\times\,S(r-n)\,(4r-4n+\eta)\,\langle r0000|n0r-n00\rangle\,.$$

In view of (3.20) we can apply the estimate of convergence for $E_3^{(3)}$ (see Eq. (2.7)).

$$\langle \mathrm{O}^{(1)}\rangle_8^{(2)} = 2\,\mathrm{Re}\sum_{h_1h}\sum_{p_1p}\frac{(\omega/2)\,Z(h,p)}{\varepsilon(h)-\varepsilon(p)}\,\langle h_1|\,\tfrac{1}{4}\mathrm{O}(1)\,|p_1\rangle\,\frac{\langle pp_1|\,\mathrm{t}|hh_1\rangle_a}{\varepsilon(h)+\varepsilon(h_1)-\varepsilon(p)-\varepsilon(p_1)} =$$

$$= 3\,\mathrm{Re}\sum_{r=2}^{\infty}\frac{t_{1r}^{(0)}+t_{1r}^{(1)}}{4r+2\eta}\sum_{n=1}^{r-1}\langle 000|\,\mathrm{O}_{orb}|n00\rangle\,S(r-n)\,\langle r0000|n0r-n00\rangle$$

(the same procedure as in the previous case).

3.2. Two-particle Operators

Only operators $\mathrm{R}^{(2)}$ and $\mathrm{D}^{(2)}$, Eqs. (3.7–12), will be considered. The zero- and first-order diagrams in the BG expansions for $\langle \mathrm{O}^{(2)}\rangle$ are shown in Fig. 3; their respective contributions will be denoted $\langle O^{(2)}\rangle^{(0)}$, $\langle O^{(2)}\rangle_1^{(1)}$, $\langle O^{(2)}\rangle_2^{(1)}$, the first-order quantities containing also contributions of diagrams adjoint to 3(b, c).

The operators R(2), D(2) act on the orbital part of $\boldsymbol{H}_2$ only; it is convenient to work with the "coupled" basis in $(\boldsymbol{H} \otimes \boldsymbol{H})_{orb}$:

$$|(n_1 l_1, n_2 l_2)\, l_{12} m_{12}\} = \sum_{m_1+m_2=m_{12}} (l_1 m_1, l_2 m_2 |\, l_{12} m_{12})\, |(n_1 l_1 m_1) \otimes (n_2 l_2 m_2)\rangle \,.$$

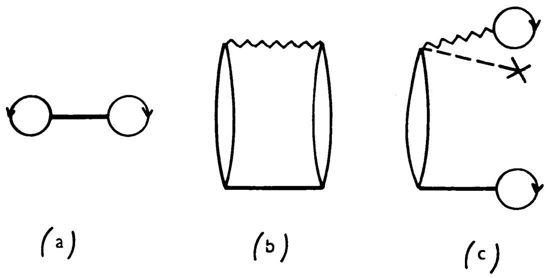

Fig. 3. The zero- and first-order diagrams in the BG expansion for $\langle O^{(2)}\rangle$. Horizontal thick lines represent O(2) "interactions". The diagrams adjoint to (b, c) are not drawn

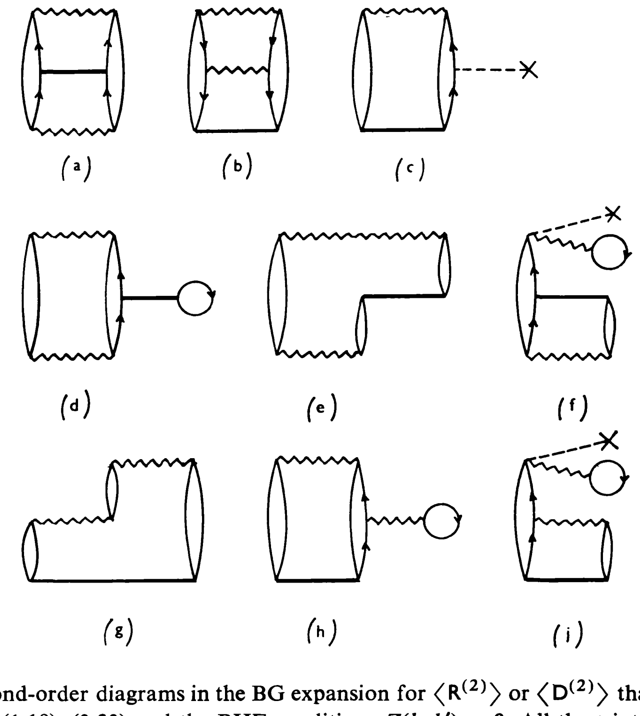

Fig. 4. The second-order diagrams in the BG expansion for $\langle R^{(2)}\rangle$ or $\langle D^{(2)}\rangle$ that do not vanish in view of Eqs. (1.18), (3.23) and the BHF conditions $Z(h, h') = 0$. All the t-interactions are on the energy shell except the middle ones in diagrams (g—i). The diagrams adjoint to (b, c, f—i) are not drawn

For calculating the matrix elements of $\mathsf{O}(2) = \mathsf{R}(2), \mathsf{D}(2)$ in this basis we use Eqs. (3.7,8) showing that each of these operators is the scalar product of two identical vector operators

$$\mathsf{O}(2) = (\mathbf{o} \otimes \mathbf{o}) = \sum_{q=-1}^{1} (-1)^q \, \mathsf{o}_q \otimes \mathsf{o}_{-q}, \quad \mathbf{o} = \mathbf{r}, \mathbf{d}, \tag{3.21}$$

where r_q is the operator that multiplies each $\psi(\boldsymbol{r}) \in L^2(\boldsymbol{R}^3)$ by the q-th component of $\boldsymbol{r}$ and similarly the d_q's are spherical components of the gradient operator. The well-known rules of tensor-operator algebra [23] then lead to the following selection rule:

$$\{(n'_1 l'_1, n'_2 l'_2)\, l'_{12} m'_{12}|\, \mathsf{O}(2)\, |(n_1 l_1, n_2 l_2)\, l_{12} m_{12}\} = 0 \quad \text{unless}$$

$$l_{12} = l'_{12}, m_{12} = m'_{12}, \quad |l_1 - 1| \leqq l'_1 \leqq l_1 + 1, \quad |l_2 - 1| \leqq l'_2 \leqq l_2 + 1. \tag{3.22}$$

This rule together with Eq. (1.18) causes that it holds

$$\langle \mathsf{R}^{(2)} \rangle^{(0)} = \langle \mathsf{D}^{(2)} \rangle^{(0)} = 0, \quad \langle \mathsf{R}^{(2)} \rangle_2^{(1)} = \langle \mathsf{D}^{(2)} \rangle_2^{(1)} = 0$$

and of the second-order diagrams only those shown in Fig. 4 may be non-zero. Further, in the remaining diagrams 3(b), 4(a−i) only two type of $\mathsf{O}(2)$ matrix elements occur. In view of (3.21) the standard formula [23] can be applied giving the following expression in terms of reduced matrix elements of $\mathbf{o}$:

$$(*) \quad \{(n1, n'1)\, 00|\, \mathsf{O}(2)\, |(\bar{n}0, 00)\, 00\} = -1/\sqrt{3}\, (n1 \| \mathbf{o} \| \bar{n}0)\, (n'1 \| \mathbf{o} \| 00)$$

$$(**) \quad \{(n1, 00)\, 1m|\, \mathsf{O}(2)\, |(00, n'1)\, 1m\} = -\tfrac{1}{3}(n1 \| \mathbf{o} \| 00)\, (00 \| \mathbf{o} \| n'1).$$

The reduced matrix elements are easily obtained using the expression of operators r_0, d_0 in spherical coordinates [23]:

$$\left(\mathsf{r}_0 \frac{1}{r} \boldsymbol{R}_{nl} Y_{lm}\right)(r, \vartheta, \varphi) = \sqrt{\frac{4\pi}{3}}\, \boldsymbol{R}_{nl}(r)\, Y_{lm}(\vartheta, \varphi)\, Y_{10}(\vartheta, \varphi)$$

$$\left(\mathsf{d}_0 \frac{1}{r} \boldsymbol{R}_{nl} Y_{lm}\right)(r, \vartheta, \varphi) = \cos\vartheta\, Y_{lm}(\vartheta, \varphi) \frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{1}{r} \boldsymbol{R}_{nl}\right)(r) - \frac{\sin\vartheta}{r^2} \frac{\partial}{\partial\vartheta} Y_{lm}(\vartheta, \varphi)$$

and the following relations for the $\boldsymbol{R}_{nl}$'s [21]

$$r\boldsymbol{R}_{n0}(r) = \sqrt{(n + 3/2)}\, \boldsymbol{R}_{n1}(r) - \sqrt{(n)}\, \boldsymbol{R}_{n-1,1}(r)$$

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{1}{r} \boldsymbol{R}_{n0}\right)(r) = -\frac{1}{r}\left[\sqrt{(n + 3/2)}\, \boldsymbol{R}_{n1}(r) + \sqrt{(n)}\, \boldsymbol{R}_{n-1,1}(r)\right].$$

Then

$$(n1 \| \mathbf{r} \| \bar{n}0) = -(\bar{n}0 \| \mathbf{r} \| n1) = \sqrt{(n + 3/2)}\, \delta_{n\bar{n}} - \sqrt{(\bar{n})}\, \delta_{n,\bar{n}-1}$$

$$(n1 \| \mathbf{d} \| \bar{n}0) = (\bar{n}0 \| \mathbf{d} \| n1) = -\sqrt{(n + 3/2)}\, \delta_{n\bar{n}} - \sqrt{(\bar{n})}\, \delta_{n,\bar{n}-1}.$$

By substituting into (*), (**) we finally get (the upper sign refers to **r**, the lower one to **d**):

$$\{(n1, n'1)\, 00|\, \mathrm{O}(2)\, |(\bar{n}0, 00)\, 00\} = \pm \frac{\delta_{n'0}}{\sqrt{2}} [\sqrt{(\bar{n})}\, \delta_{n,\bar{n}-1} \mp \sqrt{(n + 3/2)}\, \delta_{n\bar{n}}] \qquad (3.23)$$

$$\{(n1, 00)\, 1m|\, \mathrm{O}(2)\, |(00, n'1)\, 1m\} = \pm \tfrac{1}{2}\delta_{n0}\delta_{n'0}\,. \qquad (3.24)$$

The contributions of diagrams 4(g−i) that contain t-interactions off the energy shell will not be calculated for the following reasons: (i) diagrams 4(g, h) can be regarded as the lowest-order terms of the "three-particle cluster" in $\langle \mathrm{O}^{(2)} \rangle$ which arises from the three-particle cluster in the BG expansion for energy by replacing in each diagram the bottom t-interaction by the O(2) interaction. One can thus expect that the total contribution of the three-particle cluster in $\langle \mathrm{O}^{(2)} \rangle$ is small and then the diagrams 4(g, h) can be neglected (cf. Introduction); (ii) the contribution of diagram 4(i) is small since this diagram contains a "composite" interaction[12]).

Explicit formulae for the contributions of diagrams 3(b), 4(a−f) will now be derived.

1. Contribution of diagram 3(b):

$$\langle \mathrm{O}^{(2)} \rangle_1^{(1)} = 2\,\mathrm{Re}\,\tfrac{1}{4} \sum_{p'p} \sum_{h'h} \frac{\langle hh'|\, \mathrm{t}\, |pp'\rangle_a \langle pp'|\, \tfrac{1}{4}\mathrm{O}(2)\, |hh'\rangle_a}{\varepsilon(h) + \varepsilon(h') - \varepsilon(p) - \varepsilon(p')} =$$

$$= -\frac{1}{4}\frac{\sqrt{3}}{2}\,\mathrm{Re} \sum_{\sigma\tau} \sum_{\sigma'\tau'} \frac{\langle (000\sigma\tau) \otimes (000\sigma'\tau')|\, \mathrm{t}^{(D)} |\{(01, 01)\, 00\} \otimes (\sigma\tau, \sigma'\tau')\rangle_a}{-(\omega/2)\,(4 + 2\eta)}\,.$$

Passing to the E_{CM} basis we get

$$\langle \mathrm{R}^{(2)} \rangle_1^{(1)} = \langle \mathrm{D}^{(2)} \rangle_1^{(1)} = \tfrac{3}{4}\sqrt{(3)}\, \langle 10000\, |\, 01010\rangle \frac{t_{11}^{(0)} + t_{11}^{(1)}}{4 + 2\eta}$$

where $\langle 10000\, |\, 01010\rangle = -1/\sqrt{2}$ (see below Eq. (3.25).

2. Contribution of diagram 4(a):

$$\langle \mathrm{O}^{(2)} \rangle_1^{(2)} = \tfrac{1}{8} \sum_{p_1p_2p_3p_4} \sum_{h'h} \frac{\langle hh'|\, \mathrm{t}\, |p_1p_2\rangle_a \langle p_1p_2|\, \tfrac{1}{4}\mathrm{O}(2)\, |p_3p_4\rangle_a \langle p_3p_4|\, \mathrm{t}\, |hh'\rangle_a}{(\varepsilon(h) + \varepsilon(h') - \varepsilon(p_1) - \varepsilon(p_2))\,(\varepsilon(h) + \varepsilon(h') - \varepsilon(p_3) - \varepsilon(p_4))} =$$

$$= \tfrac{1}{2}\,\mathrm{Tr}_a^{(occ)}[\mathrm{t}^{(D)}\, \mathrm{A}(\bar{w})\, \tfrac{1}{4}\mathrm{O}(2)\, \mathrm{A}(\bar{w})\, \mathrm{t}^{(D)}]\,.$$

We shall limit ourselves to the diagonal approximation only: $\mathrm{A}(\bar{w}) = \mathrm{A}_D(\bar{w})$. Then Eqs. (3.9−12) and (2.2) imply (cf. the calculation of $(\langle \mathrm{R}^{(1)} \rangle_2^{(2)})_D$ and $(\langle \mathrm{D}^{(1)} \rangle_2^{(2)})_D$):

$$(\langle \mathrm{R}^{(2)} \rangle_1^{(2)})_D = \tfrac{3}{4} \sum_{S=0}^{1} \sum_{i=1}^{S+1} \frac{1}{2} \left[\frac{3}{2} \int_0^\infty |\chi_i^{(S)}(r)|^2\, \mathrm{d}r - \int_0^\infty |\chi_i^{(S)}(r)|^2\, r^2 \mathrm{d}r \right]$$

[12]) Unlike the case of diagrams 4(g, h), the calculation of 4(i) would not be difficult since the starting energy of the middle t-interaction is again $\bar{w}$ (see Eq. (1.15)) and further the selection rule (3.23) implies that the quantum numbers of both incoming particle lines are $n_1 = n_2 = 0$ $l_1 = l_2 = 1$, $l_{12} = m_{12} = 0$.

$$(\langle D^{(2)}\rangle_1^{(2)})_D = \tfrac{3}{4}\sum_{S=0}^{1}\sum_{i=1}^{S+1}\frac{1}{2}\left[-\frac{3}{2}\int_0^\infty |\chi_i^{(S)}(r)|^2\,\mathrm{d}r - \int_0^\infty \frac{1}{r}\chi_i^{(S)}(r)\left(\Delta_{2i-2}^{(rel)}\frac{\chi_i^{(S)}}{r}\right)(r)\,r^2\,\mathrm{d}r\right].$$

By comparing this result to the formulae for $\langle O^{(1)}\rangle_k^{(2)}$, $k = 1, 2$, we get

$$2(\langle O^{(2)}\rangle_1^{(2)})_D + (\langle O^{(1)}\rangle_1^{(2)})_D + (\langle O^{(1)}\rangle_2^{(2)})_D = 0 \quad O = R, D\,.$$

The expression (3.4) then shows that in the framework of the diagonal approximation the contributions of diagrams 2(c, d) and 4(a) to $\langle H_{CM}^{(\alpha)}\rangle$ cancel out.

3. Contributions of diagrams 4(b, c):

The matrix elements of O(2) occurring in these diagrams are of the type (3.23) (for $\bar{n} = 0$) and hence the same results are obtained for $R^{(2)}$ and $D^{(2)}$: $\langle R^{(2)}\rangle_k^{(2)} = \langle D^{(2)}\rangle_k^{(2)}$, $k = 2, 3$.

$$\langle R^{(2)}\rangle_2^{(2)} = 2\,\mathrm{Re}\,\tfrac{1}{8}\sum_{p'p}\sum_{h_1h_2h_3h_4}\frac{\langle pp'|\,\tfrac{1}{4}R(2)\,|h_1h_2\rangle_a\,\langle h_1h_2|\,t\,|h_3h_4\rangle_a}{\varepsilon(h_1)+\varepsilon(h_2)-\varepsilon(p)-\varepsilon(p')}\times$$

$$\times\frac{\langle h_3h_4|\,t\,|pp'\rangle_a}{\varepsilon(h_3)+\varepsilon(h_4)-\varepsilon(p)-\varepsilon(p')} =$$

$$= -\frac{1}{4}\frac{\sqrt{3}}{2}\frac{1}{(4+2\eta)^2}\,\mathrm{Re}\,\mathrm{Tr}_a^{(occ)}\left[\frac{2}{\omega}\,t^{(D)}\sum_{\sigma\tau\sigma'\tau'}|\{(01,01)\,00\}\otimes(\sigma\tau,\sigma'\tau')\rangle\,.\right.$$

$$\left.\cdot\,\langle\{(00,00)\,00\}\otimes(\sigma\tau,\sigma'\tau')|\,\frac{2}{\omega}\,t^{(D)}\right]$$

$$= -\frac{3}{2}\frac{\sqrt{3}}{2}\frac{\langle 10000\,|\,01010\rangle}{(4+2\eta)^2}\sum_{S=0}^{1}t_{11}^{(S)}t_{10}^{(S)} = \frac{\tfrac{3}{4}\sqrt{\tfrac{3}{2}}}{(4+2\eta)^2}\sum_{S=0}^{1}t_{11}^{(S)}t_{10}^{(S)}\,.$$

$$\langle R^{(2)}\rangle_3^{(2)} =$$

$$= -2\,\mathrm{Re}\,\tfrac{1}{2}\sum_{p_1p'p}\sum_{h_1h}\frac{\langle pp_1|\,\tfrac{1}{4}R(2)\,|hh_1\rangle_a\,\langle p'|\,V\,|p\rangle\,\langle h_1h|\,t\,|p_1p'\rangle_a}{(\varepsilon(h)+\varepsilon(h_1)-\varepsilon(p)-\varepsilon(p_1))\,(\varepsilon(h)+\varepsilon(h_1)-\varepsilon(p_1)-\varepsilon(p'))} =$$

$$= (-2)\frac{1}{4}\left(\frac{-\sqrt{3}}{2}\right)\sum_{n'=0}^{\infty}\frac{\langle n'10|\,R_{orb}-C\,|\,010\rangle}{(4+2\eta)(4+2\eta+4n')}\times$$

$$\times\sum_{\sigma_1\tau_1\sigma\tau}\left\langle(000\sigma_1\tau_1)\otimes(000\sigma\tau)\left|\frac{2}{\omega}\,t^{(D)}\right|\{(01,n'1)\,00\}\otimes(\sigma_1\tau_1,\sigma\tau)\right\rangle_a.$$

The reccurence relation (2.4) rules out all terms except those for $n' = 0, 1$:

$$\langle R^{(2)}\rangle_3^{(2)} = \frac{3\sqrt{3}}{2}\frac{1}{4+2\eta}\times$$

$$\times\left[(\tfrac{5}{2}-C)\frac{t_{11}^{(0)}+t_{11}^{(1)}}{4+2\eta}\langle 10000\,|\,01010\rangle - \sqrt{\tfrac{5}{2}}\,\frac{t_{12}^{(0)}+t_{12}^{(1)}}{8+2\eta}\langle 20000\,|\,01110\rangle\right].$$

With the help of Eq. (3:25) we get

$$\langle \mathrm{R}^{(2)} \rangle_3^{(2)} = \frac{-\frac{3}{2}\sqrt{\frac{3}{2}}}{4 + 2\eta} \sum_{S=0}^{1} \left[(\tfrac{5}{2} - C) \frac{t_{11}^{(S)}}{4 + 2\eta} - \frac{\sqrt{5}}{2} \frac{t_{21}^{(S)}}{8 + 2\eta} \right].$$

4. Contributions of diagrams 4(d–f):

These quantities are denoted $\langle \mathrm{O}^{(2)} \rangle_j^{(2)}$, $j = 4, 5, 6$. The formulae for $\mathrm{R}^{(2)}$ and $\mathrm{D}^{(2)}$ differ at most in sign; in the following the upper sign always refers to $\mathrm{R}^{(2)}$ and the lower one to $\mathrm{D}^{(2)}$. As a result of transformation between the E_{CM} and E_{IP} bases M brackets of the following three types appear; all of them can be expressed in a closed form with the help of the recurrence and symmetry relations [19]:

$$\alpha_n = \langle n0000 \mid n-11010 \rangle = \langle n0000 \mid 01n-110 \rangle = -2^{1-n} \sqrt{\frac{n}{2}} \tag{3.25}$$

$$\beta_n = \langle n2002 \mid n1012 \rangle = -2^{-n} \sqrt{\frac{2n + 5}{10}} \tag{3.26}$$

$$\gamma_n = \langle n2002 \mid n-13012 \rangle = -2^{-n} \sqrt{\frac{3n}{10}}. \tag{3.27}$$

$$\langle \mathrm{O}^{(2)} \rangle_4^{(2)} = \tfrac{1}{2} \sum_{h_1 h} \sum_{p_1 p' p} \frac{\langle p_1 p |\, \mathrm{t} \,| h_1 h \rangle_a \sum_{h'} \langle p' h' |\, \tfrac{1}{4} \mathrm{O}(2) \,| p_1 h' \rangle_a \langle h_1 h |\, \mathrm{t} \,| p' p \rangle_a}{(\varepsilon(h) + \varepsilon(h_1) - \varepsilon(p) - \varepsilon(p_1))(\varepsilon(h) + \varepsilon(h_1) - \varepsilon(p) - \varepsilon(p'))}.$$

Now Eqs. (3.22, 24) imply

$$\langle \mathrm{O}^{(2)} \rangle_4^{(2)} = \mp \tfrac{1}{8} \mathrm{Tr}_a^{(occ)} \left[\frac{2}{\omega} \mathrm{t}^{(D)} \mathrm{B} \frac{2}{\omega} \mathrm{t}^{(D)} \right], \quad \mathrm{B} = \sum_{p'p} \frac{|p'p\rangle \langle p'p|}{(4n + 2l + 2 + 2\eta)^2} \delta_{n'0} \delta_{l'1}.$$

In view of (1.10), (2.9) only the following matrix elements of B are needed when evaluating the trace:

$$\langle ((rl_i, 00)\, l_i, S)\, SM; TM(T) |\mathrm{B}| (r'l_j, 00)\, l_j, S)\, SM; TM(T) \rangle =$$
$$= \frac{\delta_{ij} \delta_{rr'}}{(4r + 2l_i + 2\eta)^2} \vartheta(2r + l_i - 2) \sum_{2n+l+1=2r+l_i} \langle rl_i 00 l_i \mid nl01 l_i \rangle^2 .$$

Using Eqs. (3.25–27) we get the final result

$$\langle \mathrm{O}^{(2)} \rangle_4^{(2)} = \mp \frac{3}{4} \left[\sum_{r=1}^{\infty} \left(\frac{\alpha_r}{4r + 2\eta} \right)^2 \sum_{S=0}^{1} (t_{1r}^{(S)})^2 + \sum_{r=0}^{\infty} \left(\frac{t_{2r}^{(1)}}{4r + 2\eta + 4} \right)^2 (\beta_r^2 + \vartheta(r-1) \gamma_r^2) \right]$$
$$= \mp \frac{3}{2} \sum_{r=1}^{\infty} \frac{r 2^{-2r}}{(4r + 2\eta)^2} \left[\sum_{S=0}^{1} (t_{1r}^{(S)})^2 + (t_{2,r-1}^{(1)})^2 \right].$$

This series is dominated by $\sum_r r\, 2^{-2r}$ (see Eq. (2.6)).

$$\langle \mathrm{O}^{(2)} \rangle_5^{(2)} = \sum_{p_1 p_2 p} \sum_{h_1 h_2 h} \frac{\langle p_1 p |\, \mathrm{t} \,| h_1 h \rangle_a \langle h_1 p_2 |\, \tfrac{1}{4} \mathrm{O}(2) \,| p_1 h_2 \rangle_a \langle h_2 h |\, \mathrm{t} \,| p_2 p \rangle_a}{(\varepsilon(h_1) + \varepsilon(h) - \varepsilon(p_1) - \varepsilon(p))(\varepsilon(h_2) - \varepsilon(h) - \varepsilon(p_2) - \varepsilon(p))}.$$

Here the O(2) matrix element is of the type (3.24); only the direct part contributes – the exchange part vanishes in view of (3.22). Passing to the E_{CM} basis we get with the help of (2.9)

$$\langle O^{(2)}\rangle_5^{(2)} = \pm\tfrac{1}{8}\sum_{\sigma\tau\bar\sigma\bar\tau}\sum_{S,T=0}^{1}\sum_{S',T'=0}^{1}[1-(-1)^{S+T}][1-(-1)^{S'+T'}]\sum_{i=1}^{S+1}\sum_{r=0}^{\infty}t_{ir}^{(S)}\times$$
$$\times\sum_{j=1}^{S'+1}\sum_{r'=0}^{\infty}t_{jr'}^{(S')}\sum_{2n+l=1}\sum_{\lambda=|l-1|}^{l+1}\delta_{2i-2,\lambda}\delta_{2j-2,\lambda}\Pi(\bar\sigma,\sigma,S,\lambda)\times$$
$$\times\Pi(\bar\sigma,\sigma,S',\lambda)\,\Pi(\bar\tau,\tau,T,0)\,\Pi(\bar\tau,\tau,T',0)\frac{\langle r\lambda 00\lambda\,|\,01nl\lambda\rangle\langle r'\lambda 00\lambda\,|\,01nl\lambda\rangle}{(4n+2l+2+2\eta)^2}$$

where

$$\Pi(\bar\sigma,\sigma,S,\lambda) =$$
$$= \sum_{\sigma'}(\tfrac{1}{2}\sigma',\tfrac{1}{2}\bar\sigma\,|\,S\sigma'+\bar\sigma)(\tfrac{1}{2}\sigma',\tfrac{1}{2}\sigma\,|\,S\sigma'+\sigma)(\lambda\bar\sigma-\sigma,S\sigma'+\sigma\,|\,S\sigma'+\bar\sigma).$$

It can be shown [4] that this quantity is proportional to the 6-j symbol $\begin{Bmatrix}1/2 & 1/2 & S\\ S & \lambda & 1/2\end{Bmatrix}$ so that it vanishes unless $\lambda = 0, 1$. As the latter possibility does not occur in our case, we have

$$\Pi(\bar\sigma,\sigma,S,\lambda) = \delta_{\lambda 0}\,\Pi(\bar\sigma,\sigma,S,0) = \delta_{\lambda 0}\delta_{\bar\sigma\sigma}\frac{2S+1}{2}.$$

With the help of Eq. (3.25) we then get the result

$$\langle O^{(2)}\rangle_5^{(2)} = \pm\tfrac{9}{4}\sum_{r=1}^{\infty}\frac{r\,2^{-2r}}{(4r+2\eta)^2}\Big[\sum_{S=0}^{1}t_{1r}^{(S)}\Big]^2.$$

The same estimate of convergence as in the previous case holds.

$$\langle O^{(2)}\rangle_6^{(2)} = 2\,\tfrac{1}{2}\,\mathrm{Re}\sum_{pp'\bar p}\sum_{h'h}\frac{\langle p'p|\,t\,|h'h\rangle_a\langle\bar p h'|\,\tfrac{1}{4}O(2)\,|pp'\rangle_a}{\varepsilon(h)+\varepsilon(h')-\varepsilon(p)-\varepsilon(p')}\frac{(\omega/2)\,Z(h,\bar p)}{\varepsilon(h)-\varepsilon(\bar p)}.$$

Applying Eq. (1.18) we see that the matrix element of O(2) occurring here is of the type (3.23), which implies

$$\langle O^{(2)}\rangle_6^{(2)} = \pm\frac{1}{4}\frac{1}{\sqrt{2}}2\sum_{\bar n=1}^{\infty}\sum_{n=0}^{\infty}(-S(\bar n))\,[\sqrt{(\bar n)}\,\delta_{n,\bar n-1}\mp\sqrt{(n+3/2)}\,\delta_{n\bar n}]\times$$
$$\times\,6\sum_{S=0}^{1}\sum_{i=1}^{S+1}\sum_{r=0}^{\infty}\delta_{i1}+\frac{\langle r0000\,|\,01n10\rangle}{-(4n+4+2\eta)}t_{1r}^{(S)}.$$

Finally, using (3.25) we get

$$\langle O^{(2)}\rangle_6^{(2)} = \tfrac{3}{2}\sum_{n=1}^{\infty}S(n)\,n\,2^{-n}\left[\sqrt{\left(\left(1+\frac{1}{n}\right)\left(1+\frac{3}{2n}\right)\right)}\frac{t_{1n+1}^{(0)}+t_{1n+1}^{(1)}}{4n+4+2\eta}\mp 2\,\frac{t_{1n}^{(0)}+t_{1n}^{(1)}}{4n+2\eta}\right].$$

The considerations done when estimating Eq. (2.7) show that the series converges better than $\sum_n n\, 2^{-2n}$.

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