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TWO-PARTICLE GREEN FUNCTIONS AND NUCLEAR STRUCTURE

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Abstract: The two-particle Green function is studied in terms of the ladder approximation and applied to the two-particle shell model. The resulting non-Hermitian eigenvalue problem is solved in a simple schematic model, and conclusions are drawn regarding electromagnetic transition probabilities and the cross sections for two-particle transfer reactions.

1. Introduction

The Green function method and related approaches have been used by several authors for the calculation of spherical nuclear structures on the basis of the independent particle model. These methods have generally led to extensions of the conventional shell model and to a deeper understanding of collective states.

In the present paper the two-particle Green function (defined in sect. 2) is considered. It provides information about systems having $A \pm 2$ particles, where A is the number of particles in a chosen reference system or core. Conventional shell-model calculations have been made [1,2]) for cases where the core is a magic nucleus. These assume that the core is completely inert. The general Green function equation which is just that of Bethe and Salpeter [3]), gives the properties of both systems of $(A+2)$ and $(A-2)$ particles together. This coupling between the two systems implies virtual excitations in the ground state of the core.

The lowest-order approximation in which the core excitation effects appear is the linear or ladder approximation (LA). In this approximation the core is excited by promoting pairs of particles across the Fermi level. The Green function equation reduces in this case to a linear eigenvalue problem. The corresponding secular equation is derived in sect. 3.

The pairing correlations between particles are very important and in the case when the residual two-body interaction is large compared to the spacing between the independent-particle levels lead to superconductivity†. This behaviour is indicated by the

† See ref. [4]) for a discussion of this transition in the many-electron case.

occurrence of poles of the Green function off the real axis. In the present work interest centres on the case when the core is a magic or semi-magic nucleus, so that there is a wide separation between the levels available for particles and holes. Thus the poles should occur at real energies. Indeed if this were not the case, the shell model could have little validity.

In sect. 4 a formula is presented for the matrix element for electromagnetic decay. In sect. 5 the theory is applied to a simple schematic model, and conclusions are drawn about transition probabilities between collective states and the cross sections for two-particle transfer reactions.

2. Two-particle Green functions

The nucleon levels in a given, spherical potential well U are chosen as basic states of the second quantization representation. The orbitals associated with U are denoted by the set of quantum numbers $\{k\} = \{nljm\}$ and the corresponding single-particle energies by ε_k. Where necessary, the isospin projection may be included in $\{k\}$ and adds no essential complication to the development. The Fermi operators C_k^+ and C_k create and destroy a particle in the state $\{k\}$.

The time-dependent Green functions or propagators are defined as expectation values of time-ordered products of Heisenberg operators taken with respect to the exact ground state $|0\rangle$ of an A-particle system. The Hamiltonian may be written as

$$H = \sum_i T_i + \sum_i U_i + \sum_{i<j} V_{ij}, \tag{1}$$

where T_i represents the kinetic energy of particle i and V_{ij} is the residual interaction between the particles i and j. The number A is assumed to be even, and the ground state $|0\rangle$ of even parity and vanishing total angular momentum.

The single-particle Green functions [5]) provide information about the $(A+1)$- and $(A-1)$-particle systems and give a reasonably rigorous mathematical basis to the concept of a quasi-particle. These Green functions are assumed to be diagonal, which is justifiable in the nuclear case where orbitals differing in the quantum number n are well-separated in energy.

The particle-hole Green functions have been used to study the vibrations of closed-shell nuclei in terms of coherent mixing of particle-hole configurations [6]).

The two-particle Green function may be defined as

$$G(12, 1'2'; J; t-t') = i\langle 0|T\{A_-(12; J; t)A_+(1'2'; J; t')\}|0\rangle, \tag{2}$$

with the notation

$$\begin{aligned} A_+(12; J) &= N(12; J) \sum_m (-1)^{j_1-j_2}(2J+1)^{\frac{1}{2}} \begin{pmatrix} j_1 & j_2 & J \\ m & -m & 0 \end{pmatrix} C^+_{j_1 m} C^+_{j_2 -m}, \\ A_-(12; J) &= (A_+(12; J))^+, \\ N(12; J) &= (1+(-1)^J \delta_{j_1 j_2})^{-\frac{1}{2}}. \end{aligned} \tag{3}$$

The symbol T denotes the Wick chronological ordering operator, and the time-dependent operators $A_-(12; J; t)$ and $A_+(12; J; t)$ are in the Heisenberg picture. The 3-j symbol in the first of eqs. (3) serves to couple the two particles to a definite total spin J.

The Fourier transforms of the time-dependent Green functions give the energy-dependent ones. By going over to the Schrödinger picture and taking the Fourier transform of eq. (2), the Lehmann spectral representation is obtained:

$$G(12; 1'2'; J; E)$$
$$= -\sum_{n(+)} \frac{X(12; n(+)J)X^*(1'2'; n(+)J)}{E - w_{n(+)J} + i\alpha} + \sum_{n(-)} \frac{X^*(1'2'; n(-)J)X(12; n(-)J)}{E + w_{n(-)J} - i\alpha}, \quad (4)$$

where

$$\begin{aligned} X(rs; n(+)J) &= \langle 0|A-(rs; J)|n(+)J\rangle, \\ X(rs; n(-)J) &= \langle n(-)J|A-(rs; J)|0\rangle. \end{aligned} \quad (5)$$

These matrix elements for two-particle transfer satisfy the symmetry relation

$$X(rs; nJ) = (-1)^{1+j_r+j_s-J}X(sr; nJ). \quad (6)$$

In eq. (4), α is positive and tends to zero. The kets $|n(+)J\rangle$ and $|n(-)J\rangle$ represent the eigenstates of the Hamiltonian H for the $(A+2)$- and $(A-2)$-particle systems, respectively, and

$$w_{n(\pm)J} = E_{nJ}(A \pm 2) - E_0(A) \quad (7)$$

are their energies with respect to the ground state energy of the A-particle system.

The singularities of $G(12, 1'2'; J; E)$, as can be seen from eq. (4), are determined by the stationary energies of the $(A+2)$- and $(A-2)$-particle systems. To bound states correspond discrete poles while for unbound states the continuous series of poles gives rise to a branch cut.

3. The eigenvalue problem

The Green function (2) may be evaluated from a series expansion which can be described by Feynman diagrams. If the fermion lines are renormalized by the self-energy diagrams, the series is a sum of interaction diagrams such as those shown in fig. 1. The LA is given by the sum of the ladder diagrams which are the iterations of fig. 1(b). A second-order ladder diagram is shown in fig. 1(c). In figs. 1(d) and 1(e) are shown diagrams not included in the LA. Fig. 2 shows a ladder which doubles back in time; in the intermediate state at time t, two particle-hole pairs are excited from the A-particle system.

The LA leads to a simple eigenvalue problem as can be seen as follows: the time derivative of eq. (2) is

$$\frac{\partial}{\partial t} G(12, 1'2'; J; t-t') = i\delta_{11'}\delta_{22'}(1-n_1-n_2)\delta(t-t') - \langle 0|T\{[H, A_-(12; J; t)]A_+(1'2'; J; t')\}|0\rangle, \quad (8)$$

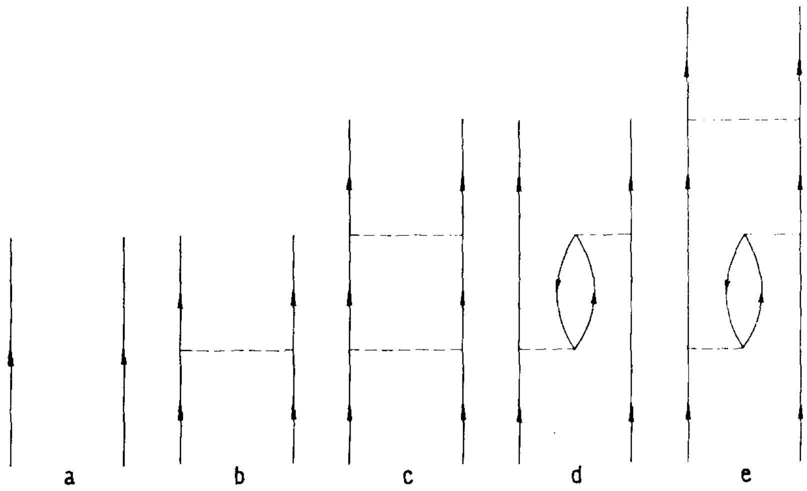

Fig. 1. Interaction diagrams. The continuous lines represent the renormalized single-particle propagators and the dashed lines the interaction matrix elements. The direction of increasing time is upwards.

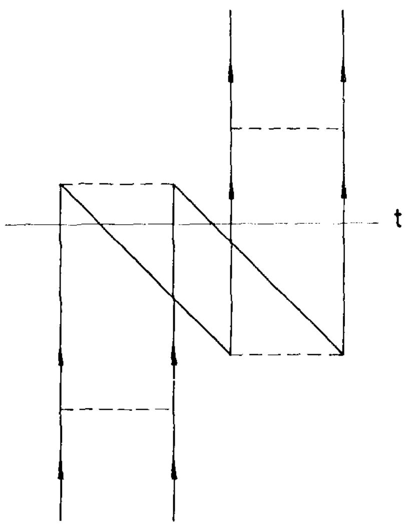

Fig. 2. Diagram with backward-going lines. At the time t, four particles and two holes are present.

where

$$n_k = (2j_k+1)^{-1} \sum_m \langle 0|C^{+}_{j_k m} C_{j_k m}|0\rangle. \tag{9}$$

The second member on the right of eq. (8) may now be approximated by making contractions of the four-operator products in the exact commutator so that the final result contains merely products of two. This procedure is known as the random phase approximation. It is equivalent to the LA. Hartree-Fock type contractions are presumed to be already included in the ε_k. The resulting expression for the commutator is

$$[H, A_-(12; J; t)] = -(\varepsilon_1+\varepsilon_2)A_-(12; J; t) - (1-n_1-n_2)\sum_{r\leqq s} \langle 12; J|V|rs; J\rangle A_-(rs; J; t), \tag{10}$$

where the interaction matrix element is now taken between the coupled, normalized and antisymmetrized kets $|rs; J\rangle$. Substituting eq. (10) into eq. (8) yields

$$\left[\frac{\partial}{\partial t}+i(\varepsilon_1+\varepsilon_2)\right] G(12, 1'2'; J; t-t') = i\delta_{11'}\delta_{22'}(1-n_1-n_2)\delta(t-t') - i(1-n_1-n_2)\sum_{r\leqq s} \langle 12; J|V|rs; J\rangle G(rs, 1'2'; J; t-t'), \tag{11}$$

which is readily converted to integral form using the unperturbed Green function which corresponds to fig. 1(a);

$$S(12; t-t') = i\{(1-n_1)(1-n_2)\theta(t-t')+n_1 n_2 \theta(t'-t)\} \exp[-i(\varepsilon_1+\varepsilon_2)(t-t')], \tag{12}$$

whereupon

$$G(12, 1'2'; J; t-t') = \delta_{11'}\delta_{22'}S(12; t-t') - \sum_{r\leqq s} \langle 12; J|V|rs; J\rangle \int S(12; t-t'')G(rs, 1'2'; J; t''-t')\mathrm{d}t''. \tag{13}$$

It is easily seen that the iteration solution of (13) corresponds to the sum of the ladder diagrams. The Fourier transform of eq. (13) is

$$\sum_{r\leqq s} [\{S(12; E)\}^{-1}\delta_{r1}\delta_{s2}+\langle 12; J|V|rs; J\rangle]G(rs, 1'2'; J; E) = \delta_{11'}\delta_{22'}, \tag{14}$$

where

$$S(12; E) = -\frac{(1-n_1)(1-n_2)}{E-(\varepsilon_{1(+)}+\varepsilon_{2(+)})+i\alpha} + \frac{n_1 n_2}{E+(\varepsilon_{1(-)}+\varepsilon_{2(-)})-i\alpha}. \tag{15}$$

In the last equation there has been a slight change of notation; the energies $\varepsilon_{k(+)}$ and $\varepsilon_{k(-)}$ have been introduced according to

$$\varepsilon_{k(\pm)} = \pm\varepsilon_k = E_k(A\pm 1)-E_0(A), \tag{16}$$

where $E_k(A\pm1)$ is the experimental energy of the quasi-particle or quasi-hole state with quantum numbers $\{k\}$ in the $(A+1)$- or $(A-1)$-particle system, respectively. Thus the single-particle energies are renormalized empirically. However, it should be remembered that the single-particle strength is distributed over various poles of the propagator [5]). The effects of this will not be included here. It follows that in eq. (9) the expectation value of the number operator is given by

$$n_k = 0 \quad \text{for} \quad \{k\} \text{ above the Fermi sea,}$$
$$n_k = 1 \quad \text{when } \{k\} \text{ is in the Fermi sea.}$$

By taking the residue of eq. (14) at the pole at energy E the following eigenvalue equation is obtained:

$$\sum_{r\leqq s}[\{-E\pm(\varepsilon_{1(\pm)}+\varepsilon_{2(\pm)})\}\delta_{r1}\delta_{s2}+(1-n_1-n_2)\langle 12;J|V|rs;J\rangle]X(rs;J) = 0. \quad (17)$$

Both sets of poles, at $E = \pm w_{n(\pm)J}$ in the systems with $A\pm2$ particles respectively are given by this equation. Eq. (17) may be written in matrix form as follows:

$$\begin{bmatrix} A & C \\ -C^+ & -B \end{bmatrix}\begin{bmatrix} X_+ \\ X_- \end{bmatrix} = E\begin{bmatrix} X_+ \\ X_- \end{bmatrix}, \quad (18)$$

where

$$\left.\begin{aligned}(A)_{12,rs} &= (\varepsilon_{1(+)}+\varepsilon_{2(+)})\delta_{1r}\delta_{2s}+\langle 12;J|V|rs,J\rangle,\\ (X_+)_{rs} &= X(rs;J),\end{aligned}\right\} \quad 12, rs \text{ all above Fermi sea}$$

$$\left.\begin{aligned}(B)_{12,rs} &= (\varepsilon_{1(-)}+\varepsilon_{2(-)})\delta_{1r}\delta_{2s}+\langle 12;J|V|rs;J\rangle,\\ (X_-)_{rs} &= X(rs;J),\end{aligned}\right\} \quad 12, rs \text{ all in Fermi sea}$$

$$(C)_{12,rs} = \langle 12;J|V|rs;J\rangle, \quad 12, \text{ above Fermi sea } rs \text{ in Fermi sea.} \quad (19)$$

It is seen that the matrix in eq. (18) is non-Hermitian and thus may have complex roots as already mentioned. The coupling of the eigenstates of the $(A+2)$- and $(A-2)$-particle systems is given by the matrix C, which arises from the inclusion of ladders which double-back as in fig. 2. The conventional shell-model procedure diagonalizes the matrices A and B and is thus equivalent to setting $C = 0$. The Green function in this case is given by the sum of ladders having a single direction in time.

To the order in which the calculation has been performed, the eigenvectors satisfy the following orthonormality relations:

$$\sum_n \pm X(rs;n(\pm);J)X^*(r's';n(\pm);J) = (1-n_r-n_s)\delta_{rr'}\delta_{ss'},$$
$$\sum_{r\leqq s}(1-n_1-n_2)X(rs;n(\pm);J)X^*(rs;n'(\pm);J') = \pm\delta_{nn'}\delta_{JJ'}. \quad (20)$$

The first of the relations (20) follows from the definition of the amplitudes $X(rs;n;J)$. For the second relation, orthogonality may be proved from eq. (18). The normalization then follows from the first relation.

It is worthwhile to note that if the condition $n_k = 1$ or 0 is released, as would happen if the one-particle propagators were renormalized by particle-hole vibrations [7]), a non-linear system of equations results.

4. State vector and transition probability

Any of the state vectors of the $(A+2)$- and $(A-2)$-particle systems which are connected to the state $|0\rangle$ by the two particle operators $A_+(rs; J)$ or $A_-(rs, J)$ can be written as a linear combination of the wave functions $A_+(rs, J)|0\rangle$ or $A_-(rs, J)|0\rangle$, respectively. Thus

$$\begin{aligned} |n(\pm); J\rangle &= Q_+(n(\pm); J)|0\rangle, \\ \langle n(\pm); J| &= \langle 0|Q_-(n(\pm); J), \end{aligned} \tag{21}$$

where

$$\begin{aligned} Q_+(n(\pm); J) &= \sum_{r \leqq s} \Gamma(rs; n(\pm)J)A_\pm(rs; J), \\ Q_-(n(\pm); J) &= (Q_+(n(\pm); J))^+. \end{aligned} \tag{22}$$

The orthonormality of the states $|n(\pm); J\rangle$ sets down a condition which must be satisfied by the amplitudes $\Gamma(rs; n(\pm); J)$, namely

$$\sum_{r \leqq s} \Gamma(rs; n(+); J)\langle n'J'|A_\pm(rs; J)|0\rangle = \delta_{n(\pm)n'}\delta_{JJ'}, \tag{23}$$

so that

$$\begin{aligned} \Gamma(rs; n(+); J) &= (1-n_r-n_s)X(rs; n(+); J), \\ \Gamma(rs; n(-); J) &= (1-n_r-n_s)X^*(rs; n(-); J). \end{aligned} \tag{24}$$

It can be shown that the linear treatment presented here is equivalent to the quasi-boson approximation, in fact

$$\langle 0|[A_-(r's'; J'), A_+(rs; J)]|0\rangle = (1-n_r-n_s)\delta_{rr'}\delta_{ss'}\delta_{JJ'}, \tag{25}$$

$$\langle 0|[Q_-(n'; J'), Q_+(n; J)]|0\rangle = \delta_{nn'}\delta_{JJ'}. \tag{26}$$

The approximate neglect of the exclusion principle in the quasi-boson method is reflected in the LA where the omission of some second-order diagrams in the expansion of the Green function implies a similar neglect.

In order to evaluate the transition probability for an electromagnetic decay, the matrix element of the transition operator

$$M(\sigma\lambda; \mu) = \sum_{j_p j_q} \langle j_p||M(\sigma\lambda)||j_q\rangle \sum_{m_p m_q} (-1)^{j_p - m_p} \begin{pmatrix} j_p & \lambda & j_q \\ -m_p & \mu & m_q \end{pmatrix} C^+_{j_p m_p} C_{j_q m_q} \tag{27}$$

between the initial and final states is needed. The expression for this matrix element for the two nuclei with $A \pm 2$ particles is

$$\langle nJ||M(\sigma\lambda)||n'J'\rangle = \sqrt{(2J+1)(2J'+1)} \sum_{j_p} \sum_{j_r \leqq j_s} (-1)^{j_p+j_s+J}(1-n_r-n_s)X(rs;\, n'J')$$
$$\times N(rs;\, J') \Big[\langle j_p||M(\sigma\lambda)||j_r\rangle N^{-1}(ps;\, J) \begin{Bmatrix} J & \lambda & J' \\ j_r & j_s & j_p \end{Bmatrix} X^*(ps, J)$$
$$+(-1)^{J'}\langle j_p||M(\sigma\lambda)||j_s\rangle N^{-1}(pr;\, J) \begin{Bmatrix} J & \lambda & J' \\ j_s & j_r & j_p \end{Bmatrix} X^*(pr;\, J) \Big]$$
$$+(-1)^{J+J'} \sum_{\beta} \langle nJ||Q_+(n'J')||\beta\lambda\rangle \langle\beta\lambda||M(\sigma\lambda)||0\rangle. \tag{28}$$

The state $|nJ\rangle$ contains even numbers of excited particle-hole pairs and will connect through the operator $Q_+(n'J')$ with states also having the same type of structure. Thus, the states $|\beta\lambda\rangle$ should be orthogonal to $M(\sigma\lambda)|0\rangle$ because the operator $M(\sigma\lambda)$ excites a single particle-hole pair. Critical to this argument is the observation that the correlations introduced into $|0\rangle$ by the method discussed here are of a pairing type. The second term in eq. (28) should therefore be zero. The first term may be called the effective transition matrix element within the framework of the LA.

5. Schematic model

Consider a system having two groups of degenerate single-particle levels at energies ε_+ and ε_-, respectively. The parity within each group of levels is constant. This model permits an especially simple solution if the residual interaction is factorable in terms of pairing operators, e.g.

$$V = -\tfrac{1}{2} \sum_{\lambda} G_\lambda \sum_{\mu} P^+_{\lambda\mu} P_{\lambda\mu}, \tag{29}$$

where

$$P^+_{\lambda\mu} = \sum_{r \leqq s} (-1)^f \alpha(rs, \lambda) A_+(rs;\, \lambda\mu). \tag{30}$$

Here,

$$\begin{aligned} f &= n_r + n_s + l_s + \tfrac{1}{2}(2\lambda + K - 1 + j_s - j_r), \\ K &= \lambda \qquad \text{if} \quad j_r + j_s + \lambda \quad \text{is even}, \\ K &= \lambda + 1 \quad \text{if} \quad j_r + j_s + \lambda \quad \text{is odd}, \end{aligned} \tag{31}$$

$$\alpha(rs, \lambda) = \left| P_\lambda(rs)(2-\delta_{j_r j_s})^{\frac{1}{2}} \sqrt{(2j_r+1)(2j_s+1)} \begin{pmatrix} j_r & j_s & \lambda \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \right|, \tag{32}$$

where $P_\lambda(rs)$ depends on the radial form of the interaction. This factorization is a suitable form for an interaction of short range [8]. In eq. (29) only one term is effective for each J, namely that for $\lambda = J$.

The $J = 0$ states arise only from configurations of the type $(j)^2$, and for the $J = 2$ states it will be assumed that other configurations are of little importance and are hence ignored. With this restriction formula (30) becomes

$$P^+_{\lambda\mu} = (-1)^{\frac{1}{2}\lambda} \sum_r (-1)^{l_r} \alpha(j_r^2, \lambda) A_+(j_r^2; \lambda\mu), \tag{33}$$

and the following dispersion formula is easily obtained for the energies of states with $J = \lambda$:

$$1 - \tfrac{1}{2} G_\lambda \sum_r \alpha^2(j_r^2, \lambda) S(rr; \omega) = 0. \tag{34}$$

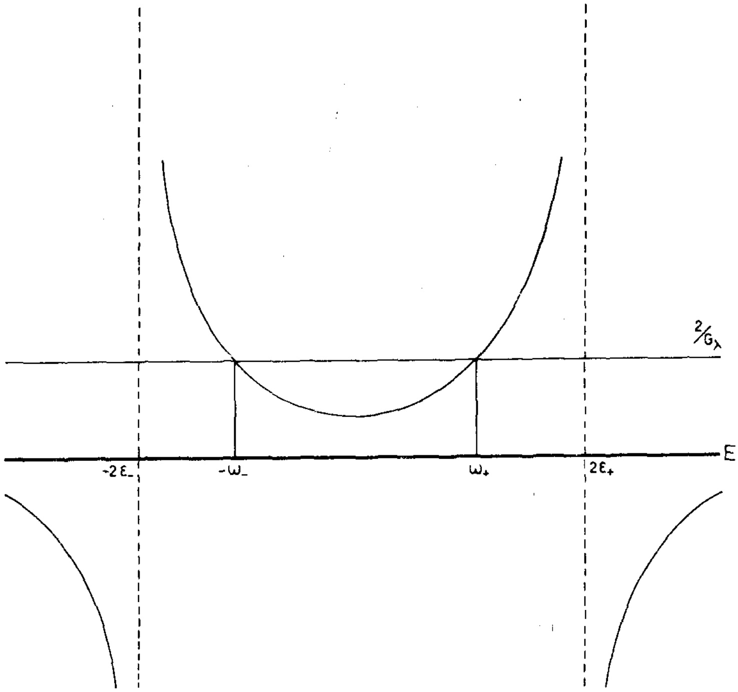

Fig. 3. Graphical solution of eq. (34). The collective states appear at energies $\pm\omega_\pm$ and the non-collective states at $\pm 2\varepsilon_\pm$.

This relation has two solutions corresponding to collective states, one in the $(A+2)$-particle system and the other in the $(A-2)$-particle system. These states decrease rapidly in energy with increasing G_λ. The rest of the states remain at the unperturbed positions $2\varepsilon_+$ and $2\varepsilon_-$. This is illustrated in fig. 3 where the second term in eq. (34) is shown as a function of ω. If there are as many levels above as in the Fermi sea, the collective states have real energies as long as

$$\delta = \varepsilon_+ + \varepsilon_- > G_\lambda \sum_r (1 - n_r) \alpha^2(j_r^2; \lambda). \tag{35}$$

When δ falls below the critical value, the eigenvalues corresponding to collective states become imaginary, and the gap equation for a superconducting system has a real solution [9]).

The general formula (28) leads to the following expression for the matrix element for emission of E2 radiation between collective states of $J = 2$ and $J = 0$:

$$\langle 2^+||M(\text{E2})||0^+\rangle = -2\sum_r (1-2n_r)\alpha(j_r^2, 2)\alpha(j_r^2, 0)\{S(rr;\,\omega_{J=2})Srr;\,\omega_{J=0})$$
$$\times (2j_r+1)^{-\frac{1}{2}}\langle j_r||M(\text{E2})||j_r\rangle R(\omega_{J=2};\,2)R(\omega_{J=0};\,0), \quad (36)$$

where

$$R(\omega_\pm;\,\lambda) = \left\{\mp\sum_r \alpha^2(j_r^2;\,\lambda)\frac{\text{d}}{\text{d}E}S(rr;\,E)|_{\pm\omega_\pm}\right\}^{-\frac{1}{2}}. \quad (37)$$

Formula (36) follows from the fact that the state vector is given by

$$X(rr;\,n(\pm)\lambda) = (-1)^{l_r+\frac{1}{2}\lambda}\alpha(j_r^2;\,\lambda)S(rr;\,\omega_\pm)R(\omega_\pm;\,\lambda). \quad (38)$$

It seen that there is coherent enhancement of the matrix element arising from the levels above the Fermi sea ($n_r = 0$) and a similar coherence from those in the Fermi sea ($n_r = 1$), but the two sets of terms interfere destructively.

The matrix element of the operator $P_{\lambda 0}^+$ between the ground state of the reference system and a collective state n is given by

$$\langle n\lambda||P_\lambda^+||0\rangle = \sum_r \alpha^2(rr;\,\lambda)S(rr;\,\omega)R(\omega;\,\lambda), \quad (39)$$

and it is easily seen that all terms in this expression contribute coherently. Consequently the matrix element may be considerably enhanced. This result may have important consequences for two-particle transfer reactions, e.g. (p, t). The cross section may be thought of as a sum over products of a nuclear dynamical factor, called the "spectroscopic factor", and another factor independent of the structure of the nuclear states[10]). In the present calculation the spectroscopic factor may be identified with the eigenvector (38), and if it is assumed that the second factor in the cross-section formula is approximately proportional to $\alpha(rr;\,\lambda)$, the collective states would be populated with very high probability in the reaction, in which two particles are dropped into the nucleus. In the inverse reaction the ground state of the A-particle nucleus would be populated largely through the collective states of the $(A+2)$-particle nucleus. The same enhancement has been found by Bès and Broglia [8]) for $J = 0$ states.

6. Conclusion

The Green function technique gives an extension to the two-particle shell model, which includes pair correlations in the core. There results an eigenvalue problem only slightly more complicated than that arising in conventional shell-model work.

There is a close correspondence between this eigenvalue problem and that discussed by Thouless [6]) in the particle-hole case. Both have non-Hermitian secular matrices, and the occurrence of complex eigenvalues indicates a transition in the system. In the particle-hole case this transition is from spherical to deformed shape, and in the two-particle case it is from a normal to a superconducting state.

Both theories admit of schematic solutions involving factorable potentials [6]), which show strong collective properties for correlated states. In the former case there is enhancement of electromagnetic transition probabilities, and in the latter the cross section for two particle transfer is enhanced.

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