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REMARKABLE PROPERTIES OF THE BROKEN PAIR MODEL

II RELATION WITH THE QUASI-PARTICLE SCHEME

by

B. LORAZO

Division de Physique Théorique*, Institut de Physique Nucléaire,
F-91406 ORSAY Cedex France

and

G. QUESNÉ*

Service de Physique Théorique et Mathématique
C.P.229, Université Libre de Bruxelles
Campus de la Plaine, Bd du Triomphe
B-1050 BRUXELLES, Belgique

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* Laboratoire associé au C.N.R.S.

* Maître de Recherches F.N.R.S.

Abstract

A non-spurious quasi-particle scheme is presented, its number-projection being exactly the broken-pair model. From this property, quantities needed in the broken-pair approach are easily evaluated by making use of the extreme simplicity of the quasi-particle algebra. Applications to the Hamiltonian operator and to one-body operators are presented for seniority $v = 0, 1$ and 2 .

1. Introduction

In a previous paper ¹⁾, henceforth referred to as I, the differential structure of the Broken Pair Model ²⁾ (BPM) has been exhibited. It was shown that for any n-pair α -state with well defined seniority $V^\alpha = \sum_i v_i^\alpha$ (see §3.1 of I for the notations) ⁺

$$|n\alpha; 0; p\rangle = \mathcal{J}_+^n |\alpha\rangle \quad (1)$$

where

$$\mathcal{J}_+ = \sum_i p_i S_i^\dagger \quad (2)$$

it was possible to factorize out the model parameters p_i in an exponential term. More precisely, the zero-broken-pair (0-b.p.) states (1) can be written as

$$|n\alpha; 0; p\rangle = \exp\left(\sum_i \hat{n}_i^\alpha \ln p_i\right) |n\alpha; 0\rangle \quad (3)$$

where $|n\alpha; 0\rangle$ corresponds to $|n\alpha; 0; p\rangle$ with $p_i = 1$ (i.e. $\mathcal{J}_+ \equiv S_+ = \sum_i S_i^\dagger$) and

$$\hat{n}_i^\alpha = \frac{1}{2} (\hat{N}_i - v_i^\alpha) \quad (4)$$

is the operator number of pairs in the orbit i , associated with the V^α -particle seniority- V^α α -state $|\alpha\rangle$ according to

$$\hat{n}_i^\alpha |\alpha\rangle = 0 \quad (5)$$

⁺The notation $|\dots\rangle$, unlike $|\dots\rangle$, means that the corresponding state is not normalized to unity.

The differential structure of BPM follows immediately from eq.(3) since the k-b.p. α -states are connected to the 0-b.p. α -states (1) through the differential relations (eq.I.39)

$$|(n-k)\alpha; \{i_k\}; \underline{p}\rangle = [(n-k)!/n!] \partial_{\{i_k\}}^{(k)} |n\alpha; 0; \underline{p}\rangle \quad (6)$$

with $\{i_k\} \equiv i_1 i_2 \dots i_k$ and $\partial_{i_k} = \partial/\partial p_{i_k}$. As mentioned in I, the b.p. number k is just the order of differentiation. This definition differs from that usually adopted ³⁾ but it has the great advantage of leading to a unified description of the k-b.p. subspaces $\mathcal{E}^{(k)}$, whatever the considered seniority v^α may be.

From relation (6) and for any operator \hat{O} independent of the parameters p_i , one then obtained

$$\hat{O} |(n-k)\alpha; \{i_k\}; \underline{p}\rangle = [(n-k)!/n!] \partial_{\{i_k\}}^{(k)} [\hat{O} |n\alpha; 0; \underline{p}\rangle] \quad (7)$$

which simply relates $\hat{O}[\mathcal{E}^{(k)}]$ to $\hat{O}[\mathcal{E}^{(0)}]$. Consequently, it appeared necessary to determine $\hat{O}[\mathcal{E}^{(0)}]$ only. As a result (eq. I.55)

$$\begin{aligned} \hat{O} |n\alpha; 0; \underline{p}\rangle &= \sum_k \sum_{\alpha' k' \{i_{k'}\}} [n!/n'!] b_{\{i_{k'}\}}^{(k')}(\alpha') [\hat{N}(\alpha')]_{\{i_{k'}\}}^{(k')} \\ & |n'\alpha'; 0; \underline{p}\rangle O_{\{i_{k'}\}}^{(k')}(\alpha'; k; \underline{p}) \end{aligned} \quad (8)$$

with

$$b_{\{i_{k'}\}}^{(k')}(\alpha') = \prod_{m=1}^{k'} [m(\Omega_{i_m}^\alpha + 1 - \sum_{\ell=1}^m \delta_{i_m i_\ell})]^{-1} \quad (9)$$

$$[N(\alpha)]_{\{i,k\}}^{(k)} = \prod_{m=1}^k (\hat{n}_{i_m}^{\alpha} + 1 - \sum_{l=1}^m \delta_{i_m \neq l}) \quad (10)$$

The quantities $O_{\{i,k\}}^{(k)}$ ($\alpha, k; p$) are n -independent and can be evaluated according to their explicit definition (eq. I.56) but, the simplest the way of determining them, the more powerful the equation (8). Indeed, this n -independency property enables one to evaluate them very easily. Without losing any generality, a meaningful example is provided by the seniority zero case. If the operator \hat{O} is the Hamiltonian operator \hat{H} , one has the simple equality

$$[\hat{H} \mathcal{J}_+^n |0\rangle]_{v=0} = \hat{\mathcal{H}}(p) \mathcal{J}_+^n |0\rangle \quad (11)$$

with (see eq. I.8)

$$\hat{\mathcal{H}}(p) = \sum_i \mathcal{H}_i^{(0)}(p) \frac{\hat{n}_i}{\Omega_i} + \frac{1}{2} \sum_{i,j} \mathcal{H}_{i,j}^{(2)}(p) \frac{\hat{n}_i(\hat{n}_j - \delta_{ij})}{\Omega_i(\Omega_j - \delta_{ij})} \quad (12)$$

Multiplying both sides of (eq. 11) with $1/n!$ and summing from $n = 0$ to $n = \infty$, one gets

$$[\hat{H} \exp \mathcal{J}_+ |0\rangle]_{v=0} = \hat{\mathcal{H}}(p) \exp \mathcal{J}_+ |0\rangle \quad (13)$$

and, consequently

$$\langle 0 | \exp \mathcal{J}_+^\dagger \hat{H} \exp \mathcal{J}_+ |0\rangle = \langle 0 | \exp \mathcal{J}_+^\dagger \hat{\mathcal{H}}(p) \exp \mathcal{J}_+ |0\rangle \quad (14)$$

Since $\exp \mathcal{J}_i |0\rangle$ is nothing but a zero-quasi-particle (0-q.p.) state ⁴⁾ (up to a normalization constant), it should be clear that the standard and well-known techniques of the Quasi-Particle Scheme (Q.P.S.) can be used to evaluate on the one-hand the l.h.s. of (14) and, on the other hand, the quantities ⁵⁾ (a general demonstration of this simple result is given below)

$$\langle 0 | \exp \mathcal{J}_i^\dagger \cdot \hat{n}_i \exp \mathcal{J}_i | 0 \rangle / \langle 0 | \exp \mathcal{J}_i^\dagger \cdot \exp \mathcal{J}_i | 0 \rangle = p_i^2 \sigma_i \Omega_i \quad (15)$$

$$\langle 0 | \exp \mathcal{J}_i^\dagger \cdot \hat{n}_i (\hat{n}_i - \delta_{ij}) \exp \mathcal{J}_i | 0 \rangle / \langle 0 | \exp \mathcal{J}_i^\dagger \cdot \exp \mathcal{J}_i | 0 \rangle = (p_i^2 \sigma_i) (p_j^2 \sigma_j) \Omega_i (\Omega_i - \delta_{ij}) \quad (16)$$

with

$$\sigma_i = (1 + p_i^2)^{-1} \quad (17)$$

Then, the unknown quantities $\mathcal{H}_{\sigma_i}^{(1)}(p)$ and $\mathcal{H}_{\sigma_{ij}}^{(1)}(p)$ are simply obtained by rewriting the l.h.s. result as a polynomial in the variables $(p_i^2 \sigma_i)$.

It is the aim of this paper to generalize this seniority zero example to the case of any operator \hat{O} and any seniority $\nu \neq 0$. As stressed out in I, because of the adopted b.p. number definition, the case $\nu \neq 0$ makes no difference with the case $\nu = 0$. As a consequence, the generalization turns out to be straightforward as will appear below. In sect.2, a non-spurious q.p. scheme is built up from BPM with the help of what is called the "exponentiation procedure". The problem of extracting from q.p. calculations the quantities $O_{k_1 k_2}^{(k)}(a'; k; p)$ needed in BPM is solved in sect.3. Results are presented for the Hamiltonian

operator and for any one-body operator.

2. The non-spurious quasi-particle scheme

In the following the definitions are those of I. As a general convention, for corresponding quantities, the notation adopted in BPM is used in QPS with an extra \sim (this does not apply to the one-particle and one-q.p. operators notation)

2.1. The subspace $\tilde{\mathcal{E}}(0)$

Let us consider in the N -particle 0-b.p. subspace $\tilde{\mathcal{E}}(0)$, the seniority- ν^α α -state, with $N = 2n + \nu^\alpha$

$$|n\alpha; 0; p\rangle = J_+^n |\alpha\rangle \quad (18)$$

where the ν^α -particle seniority- ν^α α -state $|\alpha\rangle$ writes

$$|\alpha\rangle = P_\alpha(a) |0\rangle \quad (19)$$

Multiplying both sides of (18) with $1/n!$ and summing from $n = 0$ to $n = \infty$ (this defines the "exponentiation procedure") one obtains

$$|\widetilde{\alpha}; 0; p\rangle = \exp J_+ |\alpha\rangle \quad (20)$$

*Rigorously, one should write n^α instead of n but, for simplicity of notations, the index α will be suppressed unless necessary.

or, equivalently, taking into account (19)

$$|\alpha; 0; p\rangle = P_{\alpha}(\alpha) |\widetilde{0; p}\rangle \tag{21}$$

By definition, the states (20) span the subspace $\mathcal{E}^{(0)}$. As above-mentioned, the state

$$|\widetilde{0; p}\rangle = \exp \mathcal{J}_+ |0\rangle \tag{22}$$

is an unnormalized 0-q.p. state which can be written as

$$|\widetilde{0; p}\rangle = \prod_{\substack{k, m_k > 0}} [1 + (-)^{\ell_k + j_k + \bar{m}_k} p_k a_k(i\bar{m}_k) a_k(im_k)] |0\rangle \tag{23}$$

The canonical Bogoliubov-Valatin⁶⁾ transformation associated with this 0-q.p. state is

$$d_k(im_k) = \sigma_k^{\frac{1}{2}} [a_k(im_k) + (-)^{\ell_k + j_k + \bar{m}_k} p_k a_k(i\bar{m}_k)] \tag{24}$$

Remark: the usual BCS wave function corresponds to the parametrization $p_k = v_k/u_k$ with the constraints $v_k^2 + u_k^2 = 1$, $\langle \text{BCS} | \hat{N} | \text{BCS} \rangle = 2 \sum_k v_k^2 \Omega_k = N$, together with the assumption that $\langle \text{BCS} | H - \lambda N | \text{BCS} \rangle$ be minimal.

Since the transformation (24) preserves seniority⁷⁾, the states (20) contain at least v^q q.p.. On the other hand, making use of the inverse transformation

$$a_k(im_k) = \sigma_k^{\frac{1}{2}} [d_k(im_k) + (-)^{\ell_k + j_k + \bar{m}_k} p_k d_k(i\bar{m}_k)] \tag{25}$$

in the equivalent definition (21), one sees immediately that they also contain at most \sqrt{N} q.p.. Hence, the states (20) are \sqrt{N} -q.p. states with well-defined seniority \sqrt{N} . Their expression in terms of q.p. operators is obtained by inserting the transformation (25) in the definition (21). The only term which survives is that one which corresponds to the replacement of $P_+(\alpha)$ with the operator

$$\left(\prod_i \sigma_i^{\frac{1}{2}\sqrt{N}} \right) \tilde{P}_+(\alpha) \quad (26)$$

deduced from $P_+(\alpha)$ by the substitution

$$a_i(\epsilon m_i) \rightarrow \sigma_i^{\frac{1}{2}} d_i(\epsilon m_i) \quad (27)$$

One thus obtains

$$|\alpha; 0; \underline{p}\rangle = \left(\prod_i \sigma_i^{\frac{1}{2}\sqrt{N}} \right) \tilde{P}_+(\alpha) |\widetilde{0}; \underline{p}\rangle \quad (28)$$

Comparison of eq. (28) with eq. (18) rewritten as

$$|n\alpha; 0; \underline{p}\rangle = P_+(\alpha) |n; 0; \underline{p}\rangle \quad (29)$$

clearly exhibits the similar structure of subspaces $\tilde{\mathcal{E}}(0)$ and $\mathcal{E}(0)$, i.e. one goes from $\mathcal{E}(0)$ to $\tilde{\mathcal{E}}(0)$ by substituting $|\widetilde{0}; \underline{p}\rangle$ to $|n; 0; \underline{p}\rangle$ and by making use of the transformation (27). The norm of the q.p. states (28) is simply evaluated according to

$$\begin{aligned} \langle \alpha; 0; \underline{p} | \alpha; 0; \underline{p} \rangle &= \left(\prod_i \sigma_i^{\sqrt{N}} \right) \langle \widetilde{0}; \underline{p} | \widetilde{0}; \underline{p} \rangle \\ &= \prod_i \sigma_i^{-2\sqrt{N}} \end{aligned} \quad (30)$$

the norm $\langle \widetilde{0; p} | \widetilde{0; p} \rangle$ being easily obtained from the particular expression (23) of $|\widetilde{0; p}\rangle$.

Finally, a useful expression of the $k = 0$ α -states (20) is obtained by applying the exponentiation procedure to both sides of eq.(3), namely

$$|\widetilde{\alpha; 0; p}\rangle = \exp\left(\sum_x \hat{n}_x^\alpha \ln p_x\right) |\alpha; 0\rangle \quad (31)$$

2.2 The differential structure of QPS

As in the case $k = 0$, the q.p. subspace $\widetilde{\mathcal{E}}(k)$ with $k \geq 1$ is deduced from the subspace $\mathcal{E}(k)$ by summing over the pair number. Consider the whole set of N -particle seniority- ν^k states belonging to $\mathcal{E}(k)$ -eq.(1.28)-

$$|(n-k)\alpha; \{i_k\}; p\rangle = \left(\prod_{m=1}^k S_m^{i_m}\right) J_+^{n-k} |\alpha\rangle \quad (32)$$

Multiplying both sides with $1/(n-k)!$ and summing from $n = k$ to $n = \infty$, one defines the new set of states

$$|\widetilde{\alpha; \{i_k\}; p}\rangle = \left(\prod_{m=1}^k S_m^{i_m}\right) |\widetilde{\alpha; 0; p}\rangle \quad (33)$$

which, by definition, belong to $\widetilde{\mathcal{E}}(k)$. From the definition (20) of $|\widetilde{\alpha; 0; p}\rangle$, one immediately obtains

$$|\widetilde{\alpha; \{i_k\}; p}\rangle = \mathcal{D}_{\{i_k\}}^{(k)} |\widetilde{\alpha; 0; p}\rangle \quad (34)$$

which clearly exhibits the differential structure of QPS.

This relation has to be compared with eq. (6), its equivalent in BPM.

At this point, in view of forthcoming calculations, it is not unuseful to realize how one goes from (6) to (34). Multiplying both sides of (6) with $1/(n-k)!$ and summing from $n = k$ to $n = \infty$, one gets

$$\overline{|\alpha; \{i_k\}; p\rangle} = \sum_{n=k}^{\infty} \frac{\partial_{i_k}^{(k)}}{k!} (1/n!) \mathcal{I}_+^n |\alpha\rangle \quad (35)$$

Since all the partial derivatives of \mathcal{I}_+^n vanish identically for $0 \leq n \leq k-1$, the lower limit $n = k$ in eq. (35) can be replaced by $n = 0$, restoring thereby the operator $\exp \mathcal{I}_+$

Even if relations (6) and (34) show that $\tilde{\mathcal{E}}(k)$ and $\mathcal{E}(k)$ have the same structure, there is however a small difference between them. For $k \gg 1$, subspaces $\mathcal{E}(k)$ are subject to the "summation" property

$$\sum_{i_k} P_{i_k} |(n-k) \alpha; \{i_k\}; p\rangle = |(n-k+1) \alpha; \{i_{k-1}\}; p\rangle \quad (36)$$

while this is not the case for subspaces $\tilde{\mathcal{E}}(k)$ as indicated by

$$\sum_{i_k} P_{i_k} \overline{|\alpha; \{i_k\}; p\rangle} = \mathcal{I}_+ \overline{|\alpha; \{i_{k-1}\}; p\rangle} \quad (37a)$$

$$\neq \overline{|\alpha; \{i_{k-1}\}; p\rangle} \quad (37b)$$

This minor lack of symmetry between the two formalisms is due to the fact that, for $k \gg 1$, states of $\tilde{\mathcal{E}}(k)$ have not

a well defined number of q.p.. It is sufficient to exhibit this point in the simplest case, i.e. $\tilde{\mathcal{E}}(1)$. Using

$$S_i^\alpha = \sigma_i (\tilde{S}_i^\alpha - 2p_i \tilde{S}_i^\alpha - p_i^2 \tilde{S}_i^\alpha) \quad (38)$$

where \tilde{S}_q^α is deduced from S_q^α by simply replacing the one-particle operators with the one-q.p. operators, any α -state of $\tilde{\mathcal{E}}(1)$ writes

$$|\alpha; \{i\}; \underline{p}\rangle = \sigma_i (\tilde{S}_i^\alpha - 2p_i \tilde{S}_i^\alpha - p_i^2 \tilde{S}_i^\alpha) |\alpha; 0; \underline{p}\rangle \quad (39)$$

$$= p_i^{-1} (\sigma_i p_i \tilde{S}_i^\alpha + \langle \alpha; 0; \underline{p} | \hat{n}_i^\alpha | \alpha; 0; \underline{p} \rangle) |\alpha; 0; \underline{p}\rangle \quad (40)$$

The last equality follows from seniority considerations. Also, use has been made of the relation (see eq. (53) below)

$$\langle \alpha; 0; \underline{p} | \hat{n}_i^\alpha | \alpha; 0; \underline{p} \rangle = p_i^2 \sigma_i \Omega_i^\alpha \quad (41)$$

Eq. (40) clearly shows that $\tilde{\mathcal{E}}(1)$ contains V^α and $(V^\alpha + 2)$ -q.p. states. More generally, subspace $\tilde{\mathcal{E}}(k)$ is built up from \tilde{N} -q.p. states with \tilde{N} ranging from V^α to $V^\alpha + 2k$. This mixing ensures that subspaces $\tilde{\mathcal{E}}(k)$ are non-spurious in the sense that the number projection of $\tilde{\mathcal{E}}(k)$ is simply $\tilde{\mathcal{E}}(k)$ - by construction! - i.e. the number-projection, (or its inverse the exponentiation procedure) establishes a one-to-one correspondence between $|\alpha; \{i\}_k; \underline{p}\rangle$ and $|\alpha; \{i\}_k; \underline{p}\rangle$.

3. Application

3.1 Determination of the unknown quantities $O_{\{i_k\}}^{(k)}(\alpha; k; p)$

Let δ be any p -independent operator. Its action on both sides of eq. (34) leads to

$$\delta \overline{|\alpha; i_k; p\rangle} = \partial_{i_k}^{(k)} [\delta \overline{|\alpha; 0; p\rangle}] \quad (42)$$

Thus, similarly to what is obtained in BPH, $\delta[\tilde{E}(k)]$ is simply related to $\delta[\tilde{E}(0)]$. It is then easy to establish the equivalent in QFS of eq. (8). Applying the "exponentiation procedure" $\sum_{n=0}^{\infty} 1/n!$ to both sides of eq. (I.52)*

$$\begin{aligned} \delta |n\alpha; 0; p\rangle &= \sum_k \binom{n}{k} \sum_{\alpha' k' \{i_{k'}\}} b_{\{i_{k'}\}}^{(k')}(\alpha') (\prod_{m=1}^{k'} S_m^{\alpha'}) J_{\alpha'}^{p-n-k} |\alpha'\rangle \\ &\times \langle \alpha' | (\prod_{m=1}^{k'} S_m^{\alpha'}) [\delta, J_{\alpha'}]^{(k)} | \alpha \rangle \quad (43) \end{aligned}$$

and remembering that, for fixed k , only terms with $n \geq k$ are non-zero in the r.h.s. - as required by the coefficient $\binom{n}{k}$ - one obtains

$$\begin{aligned} \delta \overline{|\alpha; 0; p\rangle} &= \sum_k \sum_{\alpha' k' \{i_{k'}\}} b_{\{i_{k'}\}}^{(k')}(\alpha') \overline{|\alpha'; i_{k'}; p\rangle} \\ &\times (1/k!) \langle \alpha' | (\prod_{m=1}^{k'} S_m^{\alpha'}) [\delta, J_{\alpha'}]^{(k)} | \alpha \rangle \quad (44) \end{aligned}$$

* In practice, the infinite summation over k is strongly limited by vanishing value of $[\delta, J_{\alpha'}]^{(k)}$.

or, using successively eqs. (34,31,10) and (I.56)

$$\begin{aligned} \widehat{0}|\alpha; 0; \underline{p}\rangle &= \sum_{kk'k''} b_{kk'}^{(k)}(\alpha) [\widehat{N}(\alpha)]_{kk'}^{(k)} \widehat{0}|\alpha'; 0; \underline{p}\rangle \\ &\quad \times O_{kk''}^{(k)}(\alpha'; k; \underline{p}) \end{aligned} \quad (45)$$

Since the ν^k -q.p. states $\widehat{0}|\alpha; 0; \underline{p}\rangle$ are pure seniority- ν^k states, eq. (45) can be used to deduce from standard q.p. calculations the coefficients $O_{kk''}^{(k)}(\alpha'; k; \underline{p})$ which are needed in BPM (see eq. 8). This can be done by considering the matrix element ⁺

$$\widehat{0}|\alpha'; 0; \underline{p}\rangle \widehat{0}|\alpha; 0; \underline{p}\rangle = \sum_{kk'k''} b_{kk'}^{(k)}(\alpha') \widetilde{\eta}_{kk''}^{(k)}(\alpha; \underline{p}) O_{kk''}^{(k)}(\alpha'; k; \underline{p}) \quad (46)$$

where the quantities

$$\widetilde{\eta}_{kk''}^{(k)}(\alpha; \underline{p}) = \widehat{0}|\alpha; 0; \underline{p}\rangle [\widehat{N}(\alpha)]_{kk''}^{(k)} \widehat{0}|\alpha; 0; \underline{p}\rangle \quad (47)$$

are connected to the $k=0$ α -state norm

$$\widetilde{\eta}^{(0)}(\alpha; \underline{p}) = \widehat{0}|\alpha; 0; \underline{p}\rangle \widehat{0}|\alpha; 0; \underline{p}\rangle \quad (48.a)$$

$$= \widehat{0}|\alpha; 0\rangle \exp\left(2 \sum_{\alpha} \widehat{n}_{\alpha} \ln p_{\alpha}\right) \widehat{0}|\alpha; 0\rangle \quad (48.b)$$

⁺ From seniority considerations, $[\widehat{N}(\alpha)]_{kk''}^{(k)}$ do not connect states $|\alpha\rangle$ and $|\alpha'\rangle$ such that $\alpha' \neq \alpha$.

through the differential relation (with $\mathcal{D}_i = \frac{1}{2} p_i \cdot \partial_i$)

$$\tilde{\eta}_{\{i_k\}}^{(k)}(\alpha; \underline{p}) = \left[\prod_{m=1}^k (\mathcal{D}_{i_m} + 1 - \sum_{\ell=1}^m \delta_{i_m i_\ell}) \right] \tilde{\eta}^{(0)}(\alpha; \underline{p}) \quad (49)$$

The last relation follows from the definition (10) and from the identity

$$(\mathcal{D}_i - \hat{n}_i^\alpha) \exp\left(2 \sum_j \hat{n}_j^\alpha \ln p_j\right) |\alpha; 0\rangle = 0 \quad (50)$$

Making use of the obvious recursion relation

$$\tilde{\eta}_{\{i_k\}}^{(k)}(\alpha; \underline{p}) = (\mathcal{D}_{i_k} + 1 - \sum_{\ell=1}^k \delta_{i_k i_\ell}) \tilde{\eta}_{\{i_{k-1}\}}^{(k-1)}(\alpha; \underline{p}) \quad (51)$$

and of the expression (30) for $\tilde{\eta}^{(0)}(\alpha; \underline{p})$, one gets

$$\tilde{\eta}_{\{i_k\}}^{(k)}(\alpha; \underline{p}) = [k! b_{\{i_k\}}^{(k)}(\alpha)]^{-1} \tilde{\eta}^{(0)}(\alpha; \underline{p}) \prod_{m=1}^k (p_{i_m}^2 \sigma_{i_m}) \quad (52)$$

or equivalently, using normalized q.p. states

$$\begin{aligned} \langle \alpha; 0; \underline{p} | \prod_{m=1}^k \left(\frac{\hat{n}_{i_m}^\alpha + 1 - \sum_{\ell=1}^m \delta_{i_m i_\ell}}{\Omega_{i_m}^\alpha + 1 - \sum_{\ell=1}^m \delta_{i_m i_\ell}} \right) | \alpha; 0; \underline{p} \rangle \\ = \prod_{m=1}^k (p_{i_m}^2 \sigma_{i_m}) \end{aligned} \quad (53-a)$$

$$= \prod_{m=1}^k \langle \alpha; 0; \underline{p} | \frac{\hat{n}_{i_m}^\alpha}{\Omega_{i_m}^\alpha} | \alpha; 0; \underline{p} \rangle \quad (53-b)$$

Having expressed \hat{O} in terms of q.p. operators with the help of the inverse Bogoliubov-Valatin transformation (25), the l.h.s. of eq.(46) is evaluated using standard Q.P.S. algebra and rewritten in terms of quantities (53) (care has to be taken of the fact that the q.p. states are unnormalized). Then a direct identification of that result with the r.h.s. of eq.(46) provides the unknown quantities $\hat{O}_{i'k'}^{(k)}(a'; k; \underline{p})$. Comparison of eq.(46) with eq.(I.57)⁺

$$(n'a'; 0; \underline{p} | \hat{O} | n\alpha; 0; \underline{p}) = (n!/n!) \sum_{kk'k''} b_{i'k'}^{(k)}(a') \eta_{i'k'}^{(k)}(n'a'; \underline{p}) \times \hat{O}_{i'k'}^{(k)}(a'; k; \underline{p}) \quad (54)$$

shows that the matrix elements of \hat{O} in $\tilde{\mathcal{E}}(0)$ can be deduced from the corresponding matrix elements in $\tilde{\mathcal{E}}(0)$ simply by replacing $\eta_{i'k'}^{(k)}(a'; \underline{p})$ with $(n!/n!) \eta_{i'k'}^{(k)}(n'a'; \underline{p})$, thus generalizing the results of the seniority zero case (see eqs.(I.1) and (I.6)). This comparison also provides the effective q.p. operator

$$\tilde{\hat{O}}_{\alpha\alpha'}(\underline{p}) = \sum_{kk'k''} b_{i'k'}^{(k)}(a') [\hat{N}_{\alpha\alpha'}]_{i'k'}^{(k)} \hat{O}_{i'k'}^{(k)}(a'; k; \underline{p}) \quad (55)$$

such that

$$(\alpha'; 0; \underline{p} | \hat{O} | \alpha; 0; \underline{p}) = (\alpha'; 0; \underline{p} | \tilde{\hat{O}}_{\alpha\alpha'}(\underline{p}) | \alpha; 0; \underline{p}) \quad (56)$$

⁺ From our general convention, $\eta_{i'k'}^{(k)}(n\alpha; \underline{p})$ is defined by eq.(47) with $|\alpha; 0; \underline{p}\rangle$ simply replaced with $|n\alpha; 0; \underline{p}\rangle$.

3.2 Results for some operators

We now present results for the most frequently used operators - the Hamiltonian operator and the one-body transition operators - in the seniority $v = 0, 1$ and 2 subspaces. Only operators which do not change the number of particles are considered here. In eq. (8), the summation indexes k and k' are related to the seniorities v^k and $v^{k'}$ according to relation (I.53) with $r = 0$

$$k' = k + \frac{1}{2}(v^{k'} - v^k) \quad (57)$$

and the constraint $k' \geq 0$. From hermiticity and complex conjugation considerations, it is sufficient to only consider the case of states $|k\rangle$ and $|k'\rangle$ such that $v^{k'} \geq v^k$. States $|k\rangle$ with seniority $v^k = 0, 1, 2$ are written as +

$$|k\rangle = \begin{cases} |0\rangle, & v^k = 0 \\ |a m_a\rangle \equiv a_+(a m_a)|0\rangle, & v^k = 1 \\ |abJM\rangle \equiv (1 + \delta_{ab})^{-\frac{1}{2}} [a_+(b) \otimes a_+(a)]_M^J |0\rangle, & v^k = 2 \end{cases} \quad (58)$$

In the following use is made of the notations $d_{ab}^j = (1 + \delta_{ab})^{-\frac{1}{2}}$, $\mathcal{P}_{abj} = (-)^{j_a + j_b - j + 1} p_{ab}$ and $\tilde{j} = (2j + 1)^{1/2}$.

3.2.1 The one-body operators

Let \hat{T}_Q^K be the most general (particle number conserving) one-body operator

+ The coupling convention is that of I.

$$\hat{T}_Q^K = \sum_{a,b} T(abK) [a_+(a) \otimes \bar{a}_-(b)]_Q^K \quad (59)$$

with

$$T(abK) = (-1)^{l_b + i_a + i_k - J} \hat{J}_a \hat{K}^{-1} \sum_{m_b, Q} \langle j_b K m_b Q | i_a m_a \rangle \langle a m_a | \hat{T}_Q^K | b m_b \rangle \quad (60)$$

for which the summation index k in eq. (8) takes the values 0 and

1. This operator cannot connect states $|a\rangle$ and $|a'\rangle$ such that

$|v^a - v^{a'}| > 2$. The unknown quantities are denoted by $\mathcal{G}_{k; i}^{(K)}(a'; k; p)$.

a) the case $|a\rangle = |a'\rangle \equiv |0\rangle$

$$\mathcal{G}_i^{(0)}(a'; 0; p) = 0 \quad (61.a)$$

$$\mathcal{G}_i^{(1)}(a'; 1; p) = \delta_{k0} \delta_{Q0} (-1)^{l_i+1} (2\Omega_i)^{\frac{1}{2}} T(i; 0) \quad (61.b)$$

b) the case $|a\rangle = |0\rangle$, $|a'\rangle = |abJM\rangle$

$$\mathcal{G}_i^{(0)}(a'; 1; p) = -\delta_{kT} \delta_{Q0} \mathcal{A}_{a'}^{(0)} (1 + \beta_{abT}) [P_a T(baJ)] \quad (62)$$

c) the case $|a\rangle = |am_b\rangle$, $|a'\rangle = |bm_b\rangle$

$$\mathcal{G}_i^{(0)}(a'; 0; p) = (-1)^{l_a + i_a + i_b - K} \hat{K} \hat{J}_b^{-1} \langle j_a K m_a Q | i_a m_a \rangle T(baK) \quad (63.a)$$

$$\mathcal{G}_i^{(1)}(a'; 1; p) = \delta_{a'a} \delta_{k0} \delta_{Q0} (-1)^{l_i+1} (2\Omega_i)^{\frac{1}{2}} T(i; 0)$$

$$+ \delta_{a'c} (-1)^{l_i} \hat{K} \hat{J}_i^{-1} \langle j_a K m_a Q | i_a m_a \rangle P_a^{-1} (1 + \beta_{abK}) [P_b T(abK)] \quad (63.b)$$

d) the case $|a\rangle \equiv |abJM\rangle$, $|a'\rangle \equiv |cdJ'M'\rangle$

$$\begin{aligned} \mathcal{G}^{(b)}(a'a; 0; p) &= d_a^p d_{a'}^p \langle JKMQ | J'M'\rangle \hat{K} \hat{J} (1 + \mathcal{O}_{abT})(1 + \mathcal{O}_{cdT'}) \\ &\times \left[\delta_{ac} (-1)^{l_a + j_a + j_a' + 1} \begin{Bmatrix} j_a & j_b & J \\ K & J' & j_a' \end{Bmatrix} T(abK) \right] \quad (64.a) \end{aligned}$$

$$\begin{aligned} \mathcal{G}_c^{(b)}(a'a; l; p) &= \delta_{a_0} \delta_{a_0'} \delta_{a a'} (-1)^{l_a + 1} (2\Omega_c)^{\frac{1}{2}} T(l < 0) \\ &+ d_a^p d_{a'}^p \langle JKMQ | J'M'\rangle \hat{K} \hat{J} (1 + \mathcal{O}_{abT})(1 + \mathcal{O}_{cdT'}) \\ &\times \left[\delta_{ac} \delta_{bc} (-1)^{l_a + j_a + j_a' + j_b + k} \begin{Bmatrix} j_a & j_b & J \\ K & J' & j_a' \end{Bmatrix} P_b^{-1} (1 + \mathcal{O}_{bdK}) [P_c T(bdK)] \right] \quad (64.b) \end{aligned}$$

3.2.2. The Hamiltonian operator

For a subspace with given seniority v , one has $k' = k = 0, 1, 2$ and the matrix elements of interest are given by relation (I.60). The Hamiltonian operator (for spherical systems of identical particles) writes

$$\begin{aligned} \hat{H} &= \sum_i \epsilon_i \hat{N}_i + \frac{1}{4} \sum_{abcdJ} U_J^{(b)}(ab, cd) \\ &\times \left[[a_+(b) \otimes a_+(a)]^J \otimes [\bar{a}_-(d) \otimes \bar{a}_-(c)]^J \right]_0^0 \quad (65) \end{aligned}$$

with (\hat{W} is the two-body part of \hat{H})

$$U_J^{(b)}(ab, cd) = (-1)^{l_a + l_a' + 1} \left[(1 + \delta_{ab})(1 + \delta_{cd}) \right]^{\frac{1}{2}} \hat{J} \langle abJM | \hat{W} | cdJM \rangle \quad (66)$$

For practical convenience, all the results are expressed in terms of quantities $U_{\alpha}^{(n)}(ab, cd; \underline{p})$ which i) are linear combinations of the quantities (66) and ii) depend upon the model parameters p_i . All these quantities are defined in Appendix together with their properties.

a) the case $|\alpha\rangle = |\alpha'\rangle \equiv |0\rangle$

$$\mathcal{H}^{(0)}(\alpha'; \underline{p}) = 0 \quad (67.a)$$

$$\mathcal{H}_{\alpha}^{(1)}(\alpha'; \underline{p}) = 2\Omega_{\alpha} \epsilon_{\alpha} + \frac{1}{2} \sum_{\beta} \epsilon_{\beta}^{l_{\alpha}+l_{\beta}+1} (\Omega_{\alpha} \Omega_{\beta})^{\frac{1}{2}} U_{\alpha}^{(0)}(\alpha, \beta; \underline{p}) \quad (67.b)$$

$$\mathcal{H}_{\alpha\beta}^{(2)}(\alpha'; \underline{p}) = \epsilon_{\beta}^{l_{\alpha}+l_{\beta}} (\Omega_{\alpha} \Omega_{\beta})^{\frac{1}{2}} U_{\alpha}^{(0)}(\alpha, \beta; \underline{p}) \quad (67.c)$$

b) the case $|\alpha\rangle = |am\rangle$, $|\alpha'\rangle = |bm\rangle$

$$\mathcal{H}^{(0)}(\alpha'; \underline{p}) = \delta_{\alpha\alpha'} \epsilon_{\alpha} \quad (68.a)$$

$$\begin{aligned} \mathcal{H}_{\alpha}^{(1)}(\alpha'; \underline{p}) &= \delta_{\alpha\alpha'} \left[2\Omega_{\alpha} \epsilon_{\alpha} + \frac{1}{2} \sum_{\beta} \epsilon_{\beta}^{l_{\alpha}+l_{\beta}+1} (\Omega_{\alpha} \Omega_{\beta})^{\frac{1}{2}} U_{\alpha}^{(0)}(\alpha, \beta; \underline{p}) \right] \\ &+ (p_b/p_a)^{\frac{1}{2}} (1/2\Omega_{\alpha}) \left[\delta_{\alpha\alpha'} \sum_{\beta} \epsilon_{\beta}^{l_{\alpha}+l_{\beta}} (\Omega_{\alpha} \Omega_{\beta})^{\frac{1}{2}} U_{\alpha}^{(0)}(b, \beta; \underline{p}) \right. \\ &\quad \left. + \epsilon_{\beta}^{l_{\alpha}+l_{\beta}} (\Omega_{\alpha} \Omega_{\beta})^{\frac{1}{2}} U_{\alpha}^{(0)}(\alpha, a, \beta; \underline{p}) \right] \quad (68.b) \end{aligned}$$

$$\begin{aligned} \mathcal{H}_{\alpha\beta}^{(2)}(\alpha'; \underline{p}) &= \delta_{\alpha\alpha'} \epsilon_{\beta}^{l_{\alpha}+l_{\beta}} (\Omega_{\alpha} \Omega_{\beta})^{\frac{1}{2}} U_{\alpha}^{(0)}(\alpha, \beta; \underline{p}) \\ &+ (p_b/p_a)^{\frac{1}{2}} (1+p_{\alpha\beta}) \left[\epsilon_{\alpha\beta} \epsilon_{\beta}^{l_{\alpha}+l_{\beta}+1} (\Omega_{\alpha} \Omega_{\beta})^{\frac{1}{2}} U_{\alpha}^{(0)}(\alpha, a, \beta; \underline{p}) \right] \quad (68.c) \end{aligned}$$

c) the case $|\alpha\rangle = |abJM\rangle$, $|\alpha'\rangle = |cdJM\rangle$

$$\mathcal{H}_0^{(0)}(\alpha'; \underline{p}) = \delta_{\alpha\alpha'} \sum_{\epsilon} v_{\epsilon}^{\alpha'} \epsilon_{\epsilon} + d_{\alpha'}^{\alpha} d_{\alpha}^{\alpha'} (1 + \sigma_{ab\tau})(1 + \sigma_{cd\tau}) \left[\frac{\epsilon^{\ell+\ell'+1}}{4\mathfrak{F}} U_{\tau}^{(0)}(cd, ab; \underline{p}) \right] \quad (69.a)$$

$$\begin{aligned} \mathcal{H}_0^{(1)}(\alpha'; \underline{p}) &= \delta_{\alpha\alpha'} \left[2\Omega_i^{\alpha} \epsilon_{\alpha} + \frac{1}{2} \sum_{\epsilon} \epsilon^{\ell+\ell'+1} (\Omega_i/\Omega_i)^{\frac{1}{2}} U_0^{(0)}(\epsilon\epsilon, \tau\tau; \underline{p}) \right] \\ &+ \frac{1}{2} (p_{\alpha} p_{\beta} / p_{\alpha} p_{\beta})^{\frac{1}{2}} d_{\alpha}^{\alpha'} d_{\alpha}^{\alpha'} (1 + \sigma_{ab\tau})(1 + \sigma_{cd\tau}) \\ &\times \left\{ \delta_{ac} \delta_{bd} \sum_{\epsilon} \epsilon^{\ell+\ell'} (\Omega_i/\Omega_i)^{\frac{1}{2}} U_0^{(0)}(dc, \tau\tau; \underline{p}) \right. \\ &\left. + \epsilon^{\ell+\ell'} \left[\delta_{bc} \mathfrak{F}^{-1} U_{\tau}^{(0)}(cd, ac; \underline{p}) + \delta_{bd} (\Omega_i/\Omega_i)^{\frac{1}{2}} U_0^{(0)}(\epsilon\epsilon, ac; \underline{p}) \right] \right\} \quad (69.b) \end{aligned}$$

$$\begin{aligned} \mathcal{H}_0^{(2)}(\alpha'; \underline{p}) &= \delta_{\alpha\alpha'} \epsilon^{\ell+\ell'} (\Omega_i/\Omega_i)^{\frac{1}{2}} U_0^{(0)}(\epsilon\epsilon, \tau\tau; \underline{p}) \\ &+ \frac{1}{2} (p_{\alpha} p_{\beta} / p_{\alpha} p_{\beta})^{\frac{1}{2}} d_{\alpha}^{\alpha'} d_{\alpha}^{\alpha'} (1 + \sigma_{ab\tau})(1 + \sigma_{cd\tau})(1 + \sigma_{ij}) \\ &\times \left[\delta_{ac} \delta_{bd} \epsilon^{\ell+\ell'+1} \mathfrak{F}^{-1} U_{\tau}^{(0)}(\epsilon\epsilon, cd; \underline{p}) \right. \\ &\left. + 2 \delta_{ad} \delta_{bc} \epsilon^{\ell+\ell'+1} (\Omega_i/\Omega_i)^{\frac{1}{2}} U_0^{(0)}(\epsilon\epsilon, \tau\tau; \underline{p}) \right] \quad (69.c) \end{aligned}$$

Note the extreme simplicity of the results which reflect nothing but the simplicity of the quasi-particle scheme.

4. Discussion and conclusion

As shown above, the properties of the "exponential procedure" are threefold :

i) it preserves the differential structure of BPM or, in other terms, the factorization of the model parameters in an exponential term $\exp(\sum_i \tilde{n}_i^* \ln p_i)$. This ensures that the effective operators acting in $\mathcal{E}(0)$ and $\bar{\mathcal{E}}(0)$ are the same (apart from the trivial coefficient $n!/n!$) -see eqs.(55) and (I.58)- ii) in practice, it enables to take advantage in a straightforward way of the existence of a vacuum (the q.p. one) iii) it gives simple expressions for the mean values $\tilde{n}_{i_1 i_2}^{(k)}(q; p)$ -see eq.(53)- so that the identification of the coefficients $O_{i_1 i_2}^{(k)}(q; k; p)$ is straightforward. We stress out that in many cases, because of the large amount of work done in the past with QPS, the only thing one has to do is to rewrite matrix elements of operators in the form (46) using results (53). Needless to say, number projection techniques ⁸⁾ would lead to the same result. However, from practical point of view, it appears simpler to use the "exponential procedure" than the various number-projection techniques. As a conclusion, it should be clear now that it is as easy to work with BPM as with QPS.

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Appendix

The symmetry properties of the quantities $U_{\mathcal{I}}^{(0)}(ab, cd)$ directly follow from their definition (56)

$$U_{\mathcal{I}}^{(0)}(ab, cd) = \epsilon^{\sum_i \ell_i + 1} \left[(1 + \delta_{ab})(1 + \delta_{cd}) \right]^{\frac{1}{2}} \mathcal{I} \langle abJM | \hat{W} | cdJM \rangle \quad (\text{A.1})$$

Then, from the antisymmetry of the two-particle states and the hermiticity of \hat{W} (with $\theta(ab\mathcal{I})_{\pm} = \epsilon^{\sum_i \ell_i - \mathcal{I} + 1}$)

$$U_{\mathcal{I}}^{(0)}(ab, cd) = \theta(ab\mathcal{I}) U_{\mathcal{I}}^{(0)}(ba, cd) \quad (\text{A.2a})$$

$$= \theta(cd\mathcal{I}) U_{\mathcal{I}}^{(0)}(ab, dc) \quad (\text{A.2b})$$

$$= \epsilon^{\sum_i \ell_i} U_{\mathcal{I}}^{(0)}(cd, ab)^* \quad (\text{A.2c})$$

In practice, the quantities $U_{\mathcal{I}}^{(0)}(ab, cd)$ are real quantities and \hat{W} commutes with the parity operator so that $\epsilon^{\sum_i \ell_i} = 1$. Quantities $U_{\mathcal{I}}^{(0)}(ab, cd; p)$ which depend upon the model parameters p_i are introduced by considering the parameter dependent operator

$$\hat{W}(p) = \hat{T}^{-1}(p) \hat{W} \hat{T}(p) \quad (\text{A.3})$$

with ⁹⁾

$$\hat{T}(p) = \exp \sum_i \hat{n}_i \ln p_i \quad (\text{A.4})$$

The definition of the quantities $U_{\mathcal{I}}^{(0)}(ab, cd; p)$

is simply obtained by replacing in eq. (A.1) the operator \hat{U} with the operator $\hat{U}(\underline{p})$

$$U_{\underline{J}}^{(0)}(ab, cd; \underline{p}) = (-1)^{l_c + l_d + 1} [(1 + \delta_{ab})(1 + \delta_{cd})]^{1/2} \hat{J} \langle abJM | W(\underline{p}) | cdJM \rangle \quad (A.5)$$

$$= (p_a p_d / p_b p_c)^{1/2} U_{\underline{J}}^{(0)}(ab, cd) \quad (A.6)$$

Obviously, symmetry relations similar to (A.2a) and (A.2b) are still valid when replacing $U_{\underline{J}}^{(0)}(ab, cd)$ with $U_{\underline{J}}^{(0)}(ab, cd; \underline{p})$ but relation (A.2c) has to be replaced with

$$U_{\underline{J}}^{(0)}(ab, cd; \underline{p}) = (p_c p_d / p_a p_b) U_{\underline{J}}^{(0)}(cd, ab; \underline{p}) \quad (A.7)$$

Quantities $U_{\underline{J}}^{(0)}(ab, cd; \underline{p})$ are then defined according to

$$U_{\underline{J}}^{(1)}(ab, cd; \underline{p}) = U_{\underline{J}}^{(0)}(ab, cd; \underline{p}) - (1 + \rho_{abJ}) R_{\underline{J}}(ab, cd; \underline{p}) \quad (A.8)$$

with

$$R_{\underline{J}}(ab, cd; \underline{p}) = \sum_{\underline{J}'} \begin{bmatrix} j_c & j_a & J' \\ j_d & j_b & J' \\ J & J & 0 \end{bmatrix} U_{\underline{J}'}^{(0)}(db, ca; \underline{p}) \quad (A.9)$$

where the square 9-j are related to the usual 9-j as

$$\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} = \varepsilon \hat{j} \hat{g} \hat{h} \begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix} \quad (A.10)$$

For these quantities $U_{\underline{J}}^{[0]}(ab, cd; \underline{p})$, only symmetry relation similar to (A.2a) is valid with, in addition

$$\sum_{\underline{J}} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \underline{J} \\ \frac{1}{2} & \frac{1}{2} & \underline{J} \\ \underline{J} & \underline{J} & 0 \end{bmatrix} U_{\underline{J}}^{[0]}(da, cb; \underline{p}) = -U_{\underline{J}}^{[0]}(ba, cd; \underline{p}) \quad (\text{A.11})$$

Replacing in eqs. (A.8) and (A.9), $U_{\underline{J}}^{[0]}(ab, cd; \underline{p})$ with the symmetrized quantities

$$U_{\underline{J}}^{[0]S}(ab, cd; \underline{p}) = \frac{1}{2} \left[U_{\underline{J}}^{[0]}(ab, cd; \underline{p}) + U_{\underline{J}}^{[0]}(cd, ab; \underline{p}) \right] \quad (\text{A.12})$$

one finally defines quantities $U_{\underline{J}}^{[0]}(ab, cd; \underline{p})$ for which symmetry relations similar to (A.2) and (A.11) are valid.

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