The one nucleon transfer operator in the microscopic IBM without NOA

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A B S T R A C T
The mapping of the single fermion creation operator \( \langle \psi \rangle \) onto the Interacting Boson–Fermion space (IBM) is revisited within the Generalized Seniority scheme. In the original work the Number Operator Approximation (NOA) was used. Here the exact evaluation of the relevant terms using exact values for the fermion matrix elements in the Generalized Seniority scheme is worked out. This provides a new, improved, single particle transfer operator to be used in IBM.

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1. Introduction

The Interacting Boson Model (IBM) [1,2] was first introduced in a phenomenological way as a boson model for describing low-lying collective states in medium mass even–even nuclei. The model is based on a scalar s-boson plus five quadrupolar d-bosons and the 36 bilinear products of the corresponding creation and annihilation operators close under the u(6) algebra [1,3]. On one hand, the group structure of the model was soon completely studied and calculations for different chains of isotopes were extensively done [1]. On the other hand, the microscopic foundation of the model was established by introducing the neutron–proton degree of freedom in the Interacting Boson Model 2 (IBM2) and considering the bosons as the counterparts of fermion pairs [4]. The next step was to add fermionic degrees of freedom in the Interacting Boson Fermion Model (IBFM) so as to be able to treat odd–even nuclei [5,6]. In general, in the IBM one has too many parameters in the Hamiltonian to account for the boson–fermion interactions. The crucial point for the development of the IBM was to derive the different terms in the boson–fermion interaction on a microscopic basis [6–8], to reduce the number of free parameters to just three, corresponding to monopole, quadrupole and exchange interactions. This was accomplished within the Generalized Seniority (GS) scheme [9] using the Number Operator Approximation (NOA) [10] by obtaining the image of the shell model nucleon (proton or neutron) creation operator in the boson–fermion IBM space. This was a major achievement that allowed to study entire chains of odd–even nuclei in many regions of the nuclear mass table [6]. In addition, the calculated IBM image of the nucleon creation operator is needed for the study of one-nucleon transfer in IBM and IBM and also for the study of \( \beta \)-decay in nuclei [11], since this process can be simulated in IBM as the combination of a neutron pick-up and a proton stripping reactions. Also, some time ago, the use of the IBM to provide detailed nuclear wavefunctions for the study of dark matter detection limits was suggested [12]. Since the IBM Hamiltonian is based on the IBM image of the one nucleon transfer operator, improvements in this fundamental operator will provide a better nuclear model to evaluate the matrix elements relevant for WIMP scattering on heavy nuclear targets in dark matter detectors. Consequently, any improvement in the IBM one nucleon transfer operator will be important. It is worth noting that, apart from the original derivation, other alternatives, based on the Nuclear Field theory [13] or the Holstein–Primakoff mapping [14] have been proposed with limited impact. Here we would like to point out that the NOA approximation is a weak point in the original derivation as it gets worse when one goes apart from closed shells. Consequently, a rederivation of the one nucleon transfer operator in IBM without this approximation is needed. In this work, such operator is obtained.

The manuscript is structured as follows. In Section 2, the NOA approximation is briefly revised and examples of its failure when going apart from closed shells are shown. In Section 3, the image of the single fermion creation operator in the IBM space, without using NOA, is presented. The detailed derivation is worked out in Appendix A. In Section 4, simple examples of application of the new operator for one nucleon transfer reactions in the Sm–Pm–Gd region are presented and confronted with the original one. Finally, in Section 5, the conclusions and future developments of this work are briefly commented.

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2. NOA approximation and its failure

In this section, the so-called Number Operator Approximation (NOA) is revisited and examples of its failure far from closed shells are shown. First we define correlated pair creation operators as

\[
S^+ = \sum_{i=1}^{k} \alpha_i^{\dagger} \frac{\gamma_i}{2} A_{ij}^{(00)}, \quad D_{\mu} = \sum_{i, i' \in F} \beta_{ii'} A_{ii'}^{(2\mu)},
\]

(1)

where \(\gamma_i = \sqrt{2j_i + 1}\), \(A_{ii'}^{(JM)} = (c_i^J \times c_i'^J)^M\) and the \(\alpha_i's\) and \(\beta_i's\) are the structure coefficients for the \(S\) and \(D\) pairs, respectively.

When several nondegenerate single particle orbits are available the NOA approximation \([10]\) consists in making

\[
\hat{N} = \sum_j \hat{N}_j \approx \sum_j \alpha_j^2 \hat{N}_j,
\]

(2)

where \(\hat{N}_j = c_j^\dagger \cdot c_j\) is the number operator for a particular \(j\)-orbit and \(\hat{N}\) is the number operator for the full set of single particle orbits in the shell. For degenerate orbits all \(|\alpha_j|\) are equal to one and the above equation is exact. However, for nondegenerate orbits the \(|\alpha_j|\) are no longer equal to one and Eq. (2) is only approximately valid. The NOA is assumed to recover the quasispin algebra for the \(S^+\) and \(S^- = (S^+)^\dagger\) operators of the Generalized Seniority (\(V\)) scheme.

Since the occupation probability of orbit \(j\) is defined as \(v_j^2 = \frac{n_j}{\Omega_j}\), where \(\Omega_j = j + 1/2\) and \(n_j\) is the expectation value of the number operator \(\hat{N}_j\), under the NOA approximation it is obtained that

\[
n_j \approx n \alpha_j^2 \frac{\Omega_j}{\Omega_e} \quad \Rightarrow \quad v_j^2 \approx \alpha_j^2 \frac{n}{2\Omega_e}
\]

(3)

for states with \(n\) particles and \(\hat{v} = 0\). Here \(\Omega_e\) is given by

\[
\Omega_e = \sum_j \alpha_j^2 \Omega_j.
\]

(4)

This value of \(n_j\) (or \(v_j^2\)) implies a linear dependence in \(n\) when the \(\alpha_j\) quantities are independent of \(n\), which is the case of the semi-magic nuclei where \(\hat{v}\) is approximately a good quantum number. However the filling of the single particle levels is not linear in \(n\) when the subshell effects are important, where the lower single particle level first fills quickly, then the next single particle level and so on (quoted in \([17, p. 175]\)). Even worse, unphysical results can be obtained in some cases if NOA is used. For instance, in Ref. \([17]\) the \(S\) and \(D\) correlated pair-creation operators are obtained by assuming a residual Surface Delta Interaction (SDI). Taking the \(\alpha_j's\) of \([17]\), given under column labeled MSSP (mid-shell single particle) in Table 2 for neutrons in the major shell 82–126 and in Table 7 for protons in the major shell 50–82, NOA provides for \(v_j^2\) the results given in Table 1 for \(Z = 64\) and \(N = 102\).

We can observe in Table 1 (column 4 under NOA) that the predicted values for \(v_{3/2}^2\) are greater than 1 in both cases, which is unphysical, showing clearly the failure of the NOA approximation.

It should be noted that this problem arises when one calculates microscopically the structure of the \(S\) pair getting its structure constants \(\alpha_j's\) and, then using NOA (3) for obtaining the occupation probabilities \(v_j^2\). Obviously, one could forget about microscopic and calculate first the occupation probabilities with BCS or other appropriate method and then using NOA through (3) to get the \(\alpha_j's\) if needed.

| Level | Energy (MeV) | \(\alpha_j\) | \(v_j^2\) (NOA) | \(v_j^2\) |
|-------|-------------|-------------|----------------|--------|
| 1g_{7/2} | 0.00 | -1.717 | 1.290 | 0.827 |
| 2d_{5/2} | 1.00 | -0.814 | 0.290 | 0.490 |
| 1h_{11/2} | 2.06 | 0.523 | 0.120 | 0.269 |
| 2d_{3/2} | 2.52 | -0.453 | 0.090 | 0.213 |
| 3s_{1/2} | 2.85 | -0.413 | 0.075 | 0.182 |

The exact value for \(n_j\), without using NOA can be obtained using Eq. (22) in Ref. \([18]\), from which the exact value for the occupation probability reads

\[
v_j^2 = -\sum_{i=1}^{n/2} (-1)^i \left( \frac{j}{2} \right)^i n_{h_{i-1}} - 2s_{0.0} 0.0(\eta_e)^2 \left( \frac{1}{2} - s_j^v n_{h_{i+1}}.0.0 \right),
\]

(5)

where \(n_{h,i,j}\) is the normalization constant of states with \(n\) particles, generalizied seniority \(v\) and total angular momentum \(j\). We quote in column 5 of Table 1 the values obtained using this expression.

3. The one-nucleon transfer operator without NOA

The one nucleon transfer operator is the one nucleon (proton or neutron) creation operator in the \(i\) shell specified by the standard single particle level quantum numbers \(n_i, l_i, j_i, m_i\) and \(m_i\). We will replace them by just one label for convenience and denote this operator by \(c_i^\dagger\). When necessary we will make explicit \(j_i\) and \(m_i\). The annihilation operator with good tensor character is given by \(c_i m_i = (-1)^j m_i c_i m_i\), where \(c_i = (c_i^\dagger)^i\).

The first few terms in the boson expansion of \(c_i^\dagger\) which change generalized seniority in one unit are

\[
c_i^\dagger \mapsto A_i q_i^\dagger + B_i (s_i^T + \vec{a}_i)(j_i)
\]

\[
+ \sum_{i' = 1}^{k} C_{ii'} (d_i^T + \vec{a}_{i'})(j_{i'})
\]

\[
+ \sum_{i' = 1}^{k} D_{ii'} s_i^T (\vec{a} + a_{i'}^T)(j_{mi})
\]

\[
+ \ldots
\]

(6)

where \(k\) is the number of single particle orbits considered and \(a_i^T\) is the fermion creation operator in the IBFM space. The coefficients \(A_i, B_i, C_{ii'}\) and \(D_{ii'}\) are obtained following the OAI method \([15]\), in which the matrix elements of \(c_i^\dagger\) between states with different generalized seniority are made equal to the matrix elements of the boson expansion between the corresponding boson states. The correspondence between the states is

\[
|S^N⟩ \mapsto |s^N⟩,
\]

(7)

\[
|S^N; j⟩ \mapsto |s^N; j⟩,
\]

(8)

\[
|S^{N-1} D; 2μ⟩ \mapsto |s^{N-1} d; 2μ⟩.
\]

(9)
where
\[ |S_N^i\rangle = \gamma^{-1}_{2N,0,0} (S^+)^N |0\rangle \] (10)
\[ |S_N^i; 0\rangle = \gamma^{-1}_{2N+1,1} (S^+) N c_j^i |0\rangle \] (11)
\[ |S_N^{-1} D_2; 2\mu\rangle = \gamma^{-1}_{2N+2,2} (S^-)^N D_\mu^i |0\rangle \] (12)
\[ |S_N^i = (N^1)^{-1/2} (S^i)^N |0\rangle \] (13)
\[ |S_N^i; \hat{i} = (N^1)^{-1/2} (s^i)^a_0^i |0\rangle \] (14)
\[ |S_N^{-1} d_2; 2\mu\rangle = [(N - 1)^1]^2 (s^i)^N d_\mu^i |0\rangle \] (15)

and the different \( \eta \)'s are the norms of the states.

In Appendix A the detailed derivation of the one-nucleon transfer operator in the boson–fermion space without the use of NOA is worked out. The result is
\[ c_i^\dagger \rightarrow \frac{\eta_{2N,1,i}}{\eta_{2N,0,0}} a_i^\dagger + \sqrt{N} \alpha_i \eta_{2N-1,0,i} (s^i \times \tilde{a})_{ij} m_i \]
\[ + \sum_{i'=1}^k \frac{\sqrt{5} \beta_{i'i}}{\eta_{2N,2,2,i}} \eta_{2N,N-1,i'} (d^i \times \tilde{a})_{im} \]
\[ - \sum_{i'=1}^k \frac{\sqrt{N} \alpha_{i'i} \beta_{i'i}}{\eta_{2N,2,2,i}} \eta_{2N-1,i'i} (\hat{d}^i \times \tilde{a})_{im} \]
\[ + \frac{\eta^2_{2N,2,2}(ii')}{\eta^2_{2N,2,2}2N,1,i'} s^i \hat{d}^i a_i^\dagger (j_i) m_i \] (16)

Some of the \( \eta \)'s were already calculated in Refs. [16–18]:
\[ \eta^2_{n=0,0} = \left( \frac{n}{2} \right)^2 \sum_{m=0}^{n} (-1)^m \left( \begin{array}{c} n \vspace{0.1cm} \end{array} \right) \eta_{m}^2 \] (17)
\[ \eta^2_{n=2,2} = \sum_{i',i=1}^k \frac{\eta^2_{n=2,2}(ii')}{\sqrt{6}} \] (18)
\[ \eta^2_{n=2,2}(ii') = \sum_{p=0}^{n/2} \left( \frac{(2n-1)!}{p!} \right)^2 (-1)^{n-1-p} \]
\[ \times \eta^2_{2p,0,0} \sum_{q=0}^{n-2-p} \left( \frac{2q-2p-2q}{2} \right)^2 \] (19)

The missing \( \eta \) in (16), \( \eta_{2N,1,i} \), is calculated in Appendix A, Eq. (28), to be
\[ \eta^2_{2N,1,i} = \sum_{m=1}^{N} \left( -m^2 \alpha^2_i \right) + \sum_{m=0}^{N} \eta^2_{2m,0,0} \left( \frac{N}{m+1} \right) \] (20)

The procedure to obtain the one-nucleon transfer operator is: i) first calculate the structure coefficients \( \alpha_i \) and \( \beta_{i'i} \) of the \( S \) and \( D \) pairs by assuming an appropriate nucleon–nucleon residual interaction; ii) then, with the above equations, the norms \( \eta \)'s are obtained; iii) finally, with these results, Eq. (16) provides the approximate image of the one-nucleon transfer operator in the boson–fermion space.

Once the one-nucleon transfer operator in the boson–fermion space is obtained, the complete program should start by comparing some results from this and the previous operator based in NOA. This will be done in the next section by using realistic wavefunctions already obtained in Ref. [19] for Nd, Sm and Pm isotopes.

### Table 2

| Final state | \(^{147}\text{Pm}\) | \(^{149}\text{Pm}\) |
|-------------|----------------|----------------|
| \(7/2 + (1)\) | 3.441 | 1.564 |
| \(7/2 + (2)\) | 0.002 | 0.035 |
| \(7/2 + (3)\) | 0.001 | 0.358 |
| \(7/2 + (4)\) | 0.000 | 0.001 |
| \(7/2 + (5)\) | 0.000 | 0.010 |
| \(5/2 + (1)\) | 1.768 | 3.018 |
| \(5/2 + (2)\) | 0.000 | 0.327 |
| \(5/2 + (3)\) | 0.021 | 0.027 |
| \(5/2 + (4)\) | 0.000 | 0.011 |
| \(5/2 + (5)\) | 0.000 | 0.000 |

However, a consistent approach will require the microscopic rederivation of the boson–fermion interaction in the IBFM starting with this one-nucleon creation operator. This will be done in a forthcoming publication. The use of the derived operator for the study of \( \beta \)-decay will be also analyzed elsewhere.

### 4. Applications

In order to check the obtained one-nucleon transfer operator, stripping and pick-up reactions to odd-Pm isotopes are studied here using wavefunctions already obtained in Ref. [19] within the IBFM. There, details on the IBFM parameters and the full calculation for the even–even \( ^{60}\text{Nd} \) core isotopes and the odd–even \( ^{61}\text{Pm} \) isotopes are given. The main idea is to show a realistic calculation with the new operator and the differences with the one used up to now, based on NOA.

We present results for spectroscopic intensities of one-proton stripping reactions \(^{60}\text{Nd} \rightarrow ^{61}\text{Pm}\), in Table 2, and one-proton pick-up reactions \(^{151}\text{Sm} \rightarrow ^{152}\text{Pm}\), in Table 3. The intensities are calculated to the lowest states with spin \( 7/2^+ \) and \( 5/2^+ \) for both the operator with NOA and the operator obtained without NOA in this work. The spectroscopic intensities are defined as the square reduced matrix elements of the transfer operator between the ground state of the even–even initial nucleus and the final state in the odd–even one. The results obtained with each operator were normalized to fulfill the Macfarlane–French sum rules [20]. Regarding the negative parity states \( 11/2^- \) no results for transfer to them are shown since, as this is a one-orbit calculation, NOA and the present transfer operator provide the same results.

It can be observed in Tables 2 and 3 that differences are small for spherical \(^{147}\text{Pm}\) and larger for the more deformed \(^{153}\text{Pm}\), where fragmentation is stronger and consequently the values of the spectroscopic intensities are more sensitive to the transfer operator. Unfortunately, the scarce experimental information for these transfers and the large error bars do not allow a conclusive statement on the improvement of the new operator with respect to the old one. In any case, Tables 2 and 3 show that there are measurable differences between the results obtained with the
traditional (with NOA) and the new (without NOA) transfer operators. These differences are expected to increase for well deformed nuclei and when more single particle orbits are active.

5. Summary and conclusions

A rederivation of the IBFM image of the one-fermion creation operator within the Generalized Seniority scheme but without the NOA approximation has been obtained. A comparison with previous results of spectroscopic factors for stripping and pick-up of one proton involving $^{61}$Pm isotopes has been presented and sizeable differences have been found.

The consistent applicability and limitations of the use of the derived operator need to be done by using it in the derivation of the IBFM boson–fermion interaction. This will be accomplished by including it in the standard IBFM-2 code ODDPAR [21]. Then, another important application of the derived operator, apart from the study of the one nucleon transfer reactions, is the study of single $\beta$-decay between odd-even nuclei, which is simulated in the IBFM through the combination of a one-neutron pick-up and a one-proton stripping transfer reactions. We are working along these lines and results will be reported elsewhere. Finally, the expected improvement in the wavefunctions of heavy odd-A nuclei through the use of the new boson–fermion interaction can have deep impact in the study of other quantities, such as the matrix elements of the magnetic moment operator or those present in the cross section of WIMP-nucleus scattering.

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Appendix A

In this appendix, the derivation of the one-nucleon transfer operator in IBFM without the use of NOA is worked out completely.

We start from Eq. (6) and calculate here the coefficients $A_i$, $B_i$, $C_{iv}$ and $D_{iv}$. They can be obtained from

$$A_i = \langle S^N_i | c_{jm}^\dagger | S^N \rangle$$

(21)

$$B_i = \langle S^N_i | c_{jm}^\dagger | S^{N-1} \rangle$$

(22)

$$C_{iv} = \langle S^{N-1}_D; 2 | c_{jm}^\dagger | S^{N-1}_i \rangle$$

(23)

$$D_{iv} = \langle S^{N}_i | c_{jm}^\dagger | S^{N-1}_D; 2 \rangle$$

(24)

First of all we calculate the norm of the $v = 1$ states, $\eta_{2N,1,i}^2$:

$$\langle 0 | \left( S^N_i \right) c_{jm,0}^\dagger \left( S^N_i \right) c_{jm,1} | 0 \rangle = -N^2 \alpha_i^2 \left\langle 0 \right| \left( S^N_i \right) \left( S^N_i \right)^\dagger \delta_{iv,2N,0,0} + \delta_{iv,2N,0,0}$$

(26)

where we have used

$$\left[ c_{jm,0} \left( S^N_i \right) \right] = -(-1)^{j+m} N \alpha_i \left[ c_{jm,1} \left( S^N_i \right) \right]^{N-1}.$$

Hence the norm $\eta_{2N,1,i}^2$ can be calculated from the recurrence relation

$$\eta_{2N,1,i}^2 = \eta_{2N,0,0}^2 - N^2 \alpha_i^2 \eta_{2N-1,1,i}^2$$

(27)

which can be solved to

$$\eta_{2N,1,i}^2 = N \prod_{m=1}^N \left( -m^2 \alpha_i^2 \right) + \sum_{m=1}^N \eta_{2m,0,0}^2 \prod_{n=m+1}^N \left( -n^2 \alpha_i^2 \right).$$

(28)

Using the Wigner–Eckart theorem we calculate the following matrix elements:

$$\langle S^N_i | c_{jm}^\dagger | S^N \rangle = -j_i \eta_{2N,1,i} \quad \eta_{2N,0,0}$$

(29)

$$\langle S^N_i | c_{jm,1}^\dagger | S^{N-1}_i \rangle = N \alpha_i \eta_{2N-1,1,i} \quad \eta_{2N,0,0}$$

(30)

$$\langle S^{N-1}_D; 2 | c_{jm}^\dagger | S^{N-1}_D \rangle = \sqrt{5} \eta_{2N,2,2}^2 \left[ \eta_{2N-1,1,i}^2 \right]^{1/2} \left[ \eta_{2N-1,1,i}^2 \right]^{1/2}$$

(31)

$$\langle S^N_i | c_{jm}^\dagger | S^{N-1}_D; 2 \rangle = \sqrt{5} \eta_{2N,2,2}^2 \left[ \eta_{2N-1,1,i}^2 \right]^{1/2} \left[ \eta_{2N-1,1,i}^2 \right]^{1/2}$$

(32)

where we used Eq. (3.7) from [16].

The boson matrix elements can be calculated straightforward

$$\langle s^N_i | a_{jm}^\dagger | s_N \rangle = -j_i,$$

(33)

$$\langle s^N_i | s \times \tilde{a}_j | s^N_i \rangle = j_i \sqrt{N},$$

(34)

$$\langle s^N_i | a_{jm}^\dagger | s^N_i \rangle = j_i \sqrt{N},$$

(35)

$$\langle s^N_i | s \times \tilde{a}_j | s^N_i \rangle = j_i \sqrt{N},$$

(36)

Then, the coefficients in the boson expansion of the one-nucleon transfer operator read

| Final state | $^{147}$Pm | $^{151}$Pm |
| --- | --- | --- |
| NOA | This work | NOA | This work |
| $9/2^+ (1)$ | 2.000 | 0.000 | 2.000 | 0.000 |
| $9/2^+ (2)$ | 0.090 | 0.036 | 0.090 | 0.036 |
| $11/2^+ (1)$ | 0.030 | 0.001 | 0.030 | 0.001 |
| $11/2^+ (2)$ | 0.050 | 0.001 | 0.050 | 0.001 |
| $13/2^+ (1)$ | 0.030 | 0.001 | 0.030 | 0.001 |
| $13/2^+ (2)$ | 0.050 | 0.001 | 0.050 | 0.001 |

Table 3 Spectroscopic intensities for one-proton pick-up reactions $^{63}$Sm $\rightarrow ^{61}$Pm.
\[ A_i = \frac{\eta_{2N,1,i}}{\eta_{2N,0,0}}, \]
\[ B_i = \sqrt{N} \eta_{i} \frac{\eta_{2(N-1),1,i}}{\eta_{2N,0,0}}, \]
\[ C_{ii'} = \frac{\sqrt{5}}{j_i} \frac{\eta_{2N,2,2}(ii')}{\eta_{2N,2,2}(ii')} \frac{\beta_{ii'}}{\sqrt{1 + \delta_{ii'}}}, \]
\[ D_{ii'} = -\frac{\sqrt{5}}{j_i} \frac{\eta_{2N,2,2}(ii')}{\eta_{2N,2,2}(ii')} \frac{\sqrt{N}\alpha_{ii'}\sqrt{1 + \delta_{ii'}}}{\beta_{ii'}}, \]

(37) (38) (39) (40)

to obtain finally the expression of Eq. (16), which complete the derivation of the single fermion creation operator in IBFM to the lowest order without using NOA.

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