Use of the boson-expansion theory for the description of collective nuclei

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A clear understanding of how to construct the boson expansion of a collective fermion pair operator is given. The criteria for the applicability of the procedure are also discussed. Following this prescription, the Pauli-principle violation is made negligible for the low-lying states of collective nuclei.

[NUCLEAR STRUCTURE Boson expansion; criteria for truncation and convergence; collective motions.]

I. INTRODUCTION

In the past several years, we have been using the Belyaev-Zelevinsky[1] type boson-expansion theory (BET) as a tool for describing states arising from quadrupole vibrations and/or deformations in even-even nuclei.[2-6] The first paper[2] and a part of the second paper[3] in this series dealt with the formal aspects of the problem along the lines developed earlier by Sorensen,[7] with a few key improvements. Succeeding papers were mostly of an application-minded nature. In Ref. 4, extension of BET to a higher order (sixth) was made to show the convergence *per se*. This convergence, i.e., the possibility of truncating the series expansion, was verified numerically and was seen to hold consistently in later applications.

Recently, Silvestre-Brac and Piepenbring[8] followed the prescription of Ref. 2, in treating the $K=0^+$ bands of deformed nuclei, and claimed that the boson expansion breaks down. Our most recent applications,[4-6] however, are based on a somewhat different understanding of the boson expansion[6] than in Ref. 2. The purpose of the present paper is to clarify, first, the difference in understanding between Refs. 2 and 6, and then show that the use of the latter is more correct for practical applications of BET. Discussion will also be presented on how the boson expansion should, in fact, be made and what are its limits. It will become clear why the problem, pointed out by Silvestre-Brac and Piepenbring, was not encountered in our applications,[4-6] and why it will probably disappear in their application as well, if they switch to the newer understanding of Ref. 6.

II. BRIEF SUMMARY OF THE BOSON EXPANSION METHOD

We begin by recapitulating a few formulas of Ref. 2. As done there, we first define the two-quasiparticle-pair operators which are needed:

$$B^\dagger_{\beta\lambda\mu}=\sum_{j_1\le j_2} D_{j_1j_2}^{-1}\,\psi^\beta_{j_1j_2\lambda}[\alpha^\dagger_{j_1}\alpha^\dagger_{j_2}]_{\lambda\mu}\,, \tag{1}$$

$$C^\dagger_{j_1j_22\mu}=[\alpha^\dagger_{j_1}\alpha_{\tilde{j}_2}]_{2\mu}\,, \tag{2}$$

where

$$D_{j_1j_2}=(1+\delta_{j_1j_2})^{1/2}\,. \tag{3}$$

Here $\alpha^\dagger_{jm}$ is a quasiparticle fermion creation operator and $\psi^\beta_{j_1j_2\lambda}$ is an element of some $N\times N$ unitary matrix, where N is the number of ways to couple two of the quasiparticle states to an angular momentum λ, as denoted by square brackets in Eqs. (1) and (2). In practice this matrix is chosen to be the result of a Tamm-Dancoff calculation, which results in a single collective mode and $N-1$ noncollective modes.[2,9] Using the abbreviated notation $a=\{\alpha\lambda\mu\}$ and $p=\{j_1j_2kq\}$, we may summarize the commutation relations between fermion operators as[2]

$$[B_a,B^\dagger_b]=\delta_{ab}-\sum_p P^p_{ab}C^\dagger_p\,, \tag{4a}$$

$$[C^\dagger_p,B^\dagger_a]=\sum_b P^p_{\tilde{a}b}B^\dagger_b\,, \tag{4b}$$

$$P^p_{ab}\equiv\hat{\lambda}_a\hat{\lambda}_b(\tilde{\lambda}_a\,\tilde{\mu}_a\lambda_b\mu_b\,|\,kq)\times\sum_j\psi^\alpha_{jj_2\lambda_a}\,\psi^\beta_{j_1j\lambda_b}W(j_2j_1\lambda_a\lambda_b;kj)D_{j_1j}D_{j_2j}\,. \tag{5}$$

See Ref. 2 for more details of notation.

In order to convert a fermion Hamiltonian, which may be written as products of the $B^\dagger$ and $C^\dagger$ operators, into boson expanded form, we begin by writing series expressions for the fermion pair operators as

$$B^\dagger_a=xA^\dagger_a+\sum_{bcd}X_3(abc\tilde{d})A^\dagger_bA^\dagger_cA_d+\sum_{bcdef}X_5(abcd\tilde{e}\tilde{f})A^\dagger_bA^\dagger_cA^\dagger_dA_eA_f+\cdots\,, \tag{6a}$$

$$C_p^\dagger = X_0(p) + \sum_{ab} X_2(p, a\tilde{b}) A_a^\dagger A_b + \sum_{abcd} X_4(p, ab\tilde{c}\tilde{d}) A_a^\dagger A_b^\dagger A_c A_d + \cdots , \quad (6b)$$

in terms of boson operators A and $A^\dagger$ that satisfy

$$[A_a, A_b^\dagger] = \delta_{ab} . \quad (7)$$

By substituting $B^\dagger$ and $C^\dagger$ of (6) into (4), the latter becomes a set of equations for the expansion coefficients X, which can be solved analytically.[2]

One nice property found[2,7] is that

$$X_0 = \tfrac{1}{2}\hat{j}_1 \delta_{j_1 j_2} \delta_{k0}(1-x^2), \quad X_2(p; ab) = P_{ba}^{p}, \quad X_4 = X_6 = \cdots = 0 , \quad (8)$$

i.e., that $C^\dagger$ has a finite expansion. The general forms for X_3 and X_5 are given as

$$X_3(abc\tilde{d}) = r(\delta_{ab}\delta_{cd} + \delta_{ac}\delta_{bd}) + sY(abcd) , \quad (9a)$$

$$X_5(abcd; \tilde{e}\tilde{f}) = u\Delta_{\delta\delta}(abcdef) + v\Delta_{\delta Y}(abcdef) + w\Delta_{YY}(abcdef) , \quad (9b)$$

where

$$\begin{aligned} Y(abcd) &= \sum_p P_{\tilde{a}b}^{p} P_{\tilde{c}d}^{p} , \\ \Delta_{\delta\delta}(abcdef) &= P_{bcd}(\delta_{ab}\delta_{ce}\delta_{df} + \delta_{ab}\delta_{cf}\delta_{de}) , \\ \Delta_{\delta Y}(abcdef) &= P\delta_{ab} Y(cefd) , \\ \Delta_{YY}(abcdef) &= P\sum_g Y(abge)Y(cfgd) , \end{aligned} \quad (10)$$

with

$$P = P_{bcd}P_{aef} \qquad P_{aef} = 1 + P_{ae} + P_{af} \quad P_{bcd} = 1 + P_{bc} + P_{bd} . \quad (11)$$

The operator P_{ab} exchanges the indices a and b.

The coefficients r, s, u, v, and w in (9) can be expressed[2] in terms of x. One can then substitute the boson expansion series, (6), into the Hamiltonian. This gives an infinite boson Hamiltonian defined on the boson space spanned by all states of the form

$$|B\rangle = (A_{a_1}^\dagger)^{n_1}(A_{a_2}^\dagger)^{n_2} \cdots (A_{a_K}^\dagger)^{n_K} |0\rangle_B ,$$

where K is the number of multipoles possible, and $a_1, \ldots, a_K$ distinguish between different modes of each multipole. The solution of such a problem would yield exactly the same answers as the original fermion problem, but obviously is even harder to solve. One realizes then that some truncation is necessary. If one begins truncation at this stage, however, then one has begun too late, and it is at this juncture that the prescription given in Ref. 2 could have been misleading.

III. TRUNCATION OF THE BOSON EXPANSION

In our applications[3-6] of BET, we intended to describe the properties of the positive parity low-lying states of even-even nuclei, which show collective quadrupole behavior. In practice, we may restrict ourselves to only a few modes of excitation, and describe many of the low-lying states of nuclei as superpositions of these modes. Whether or not this ansatz allows us to describe data, is shown *a posteriori* by comparing the obtained results with experiment.

Before continuing, we clarify why the fermion pairs must be expanded in a possibly infinite number of boson terms. The answer is the need to satisfy the Pauli principle and this becomes clear if one considers the following example. Let a given fermion state be denoted by $|F\rangle$. Suppose that this state definitely (with occupation probability of unity) contains two quasiparticles in the single-particle states $(j_1 m)$ and $(j_2 \text{-} m)$. Now consider a state $[\alpha_{j_1}^\dagger \alpha_{j_2}^\dagger]_{2\mu} |F\rangle$. By the Pauli principle, this expression contains some terms which vanish; e.g., for $\mu = 0$ and $j_1 \leq j_2$, one term out of $2j_1 + 1$ vanishes. Now the state $|F\rangle$ must have a counterpart (or image) in the boson space of the form $|B\rangle$, as given above. If we let only a single boson term represent the pure configuration $[\alpha_{j_1}^\dagger \alpha_{j_2}^\dagger]_{2\mu}$, i.e., consider only the first term of (6a), then when we construct $A^\dagger|B\rangle$, we find that the cancellation of Pauli-principle violating amplitudes does not take place. Thus, in some cases, the operation of $A^\dagger$ results in a state which has components violating the Pauli principle. It is the succeeding terms of Eq. (6a) which check the fermion content of $|B\rangle$ and cancel out any Pauli-principle violating terms. Thus the expansion is necessary to strictly satisfy the Pauli principle.

The above example hints at why it is inadvisable to boson expand pure fermion pair states such as $[\alpha_{j_1}^\dagger \alpha_{j_2}^\dagger]$. Things can go bad very quickly if one does not expand to very high order. The interested reader is referred to the work of Marshalek.[10]

We now return to the question of truncation which comes into our discussion in two ways. To discuss the first, we will begin with Eq. (6). We consider the $\lambda = 2$ collective solution of the Tamm-Dancoff problem. It defines a fermion operator $B_{\text{coll}}^\dagger$ of physical interest, the other $B^\dagger$ operators corresponding to excitations which lie at or above twice the energy gap.[9] In the summations in Eq. (6) over all different bosons, we will restrict ourselves to the above $\lambda = 2$ boson which has the collective nature. Thus the expressions to be substituted into Eq. (4) are those in Eq. (6), but with the indices $a, b, \ldots,$ subject to the restrictions that $\alpha = \beta = \cdots = \text{coll}$, and $\lambda_a = \lambda_b = \cdots = 2$. Thus the summations in fact disappear. The solutions, for the coefficients which define the X_n, are then easily found to be[4,6]

$$r = 0, \quad s \simeq -1/(4x), \quad u = v = 0, \quad w \simeq -s^2/(18x), \tag{12}$$

with the results for the coefficients of $C^\dagger$ unchanged from Eq. (8).

In (12), the relation $r = u = v = 0$ is exact, while the expressions for s and w are approximate. They can be used for practical calculations since they are obtained by neglecting terms which have been found to add corrections to these expressions of a few percent which subsequently have been seen to have virtually no effect on the final energies or wave functions in practical cases. The result that $r = 0$ eliminates large terms which appear in the Hamiltonian when the expression of Ref. 2 is used, i.e., when we set

$$r = [2(x^2 - 1)^{1/2} + (x^2 + 2)^{1/2} - 3x]/6 . \tag{13}$$

The danger of the r term is more evident if one notes the following. Instead of just retaining the collective mode with $\lambda = 2$, suppose we start picking up more modes, one by one, and repeatedly resolve the commutation relations for $B^\dagger$ and $C^\dagger$. One finds that $r = u = v = 0$ is exactly true continually, until one has decided to pick up all possible modes of every single multipole. Then, and only then, r changes discontinuously from 0 to that expression given in Eq. (13). Note that during this procedure, s and w are deviating a little bit from their simple form in Eq. (12), but that presents no problem or trouble in the calculations. At this final stage, the other problem that the expressions given in Ref. 2 for u, v, and w, demand $x^2 \geq 2$ and so on, also reappear.[2,8]

One may wonder what roles the terms in (9) play in the full general calculation. For this purpose we give a diagrammatic representation of the quadrupole collective operator $B^\dagger_{\text{coll}}$ in Fig. 1. The smooth lines represent single bosons while the dotted lines represent the quasiparticles. From Fig. 1 and Eq. (6), we see that the first diagram describes or creates the boson excitation of collective nature. The third diagram (s term) checks the fermion nature of all single bosons present in the basis state or sample boson state $|B\rangle$ and adds a correction (subtraction) according to the nature of the bosons in $|B\rangle$. Similarly, the sixth diagram (w term) checks the fermion nature of all possible boson pairs and makes corrections. The second diagram (r term) does not check anything as regards the fermion content of the bosons in the sample state. It picks out and counts all the bosons

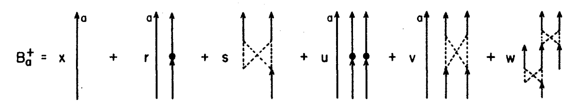

FIG. 1. First six terms of a diagrammatic expansion of the fermion pair operator $B_a^\dagger$ (i labels all quantum numbers). Smooth (dotted) lines represent bosons (quasiparticles). Permutation of indices in the r, u, v, and w terms and summations over all quasiparticle pair components of the bosons are omitted from the figure for clarity.

that are already present in the sample boson state and excites the collective boson onto that state. The purpose of this term in the most general case (of Ref. 2) is to effectively renormalize the coefficient of the linear boson operator, to account for higher order corrections to the Pauli principle, which because of indice permutations and contractions come in with large coefficients. If, by the physics of the problem, one knows that one does not desire to consider all possible multipoles of bosons as well as all possible modes of these multipoles, then it is incorrect to include these r, u, and v coefficients in a truncated calculation; they are necessary to preserve the Pauli principle only when all the fermion operators are to be handled. As an aside, we see that the vanishing of the r, u, and v coefficients in the truncated problem can be expressed, in the language of this diagrammatic representation, by saying that we ignore unconnected diagrams in Fig. 1.

Once we recognize that the unconnected diagrams are to be omitted in a realistic calculation, we may put the boson series in a more convenient form, and we begin to prepare for the second aspect of our truncation problem. We let ξ represent the diagram in the s term of Fig. 1. We will consider all boson lines to be collective bosons. Then we have

$$B^\dagger_{\text{coll}} = xA^\dagger - \frac{\xi}{4x} - \frac{\xi^2}{2\times 4^2 \times x^3} - \frac{\xi^3}{3\times 4^3\times x^5} - \frac{\xi^4}{4\times 4^4 \times x^7} - \cdots , \tag{14}$$

where $A^\dagger$ creates the collective boson. Permutation of indices which gave identical terms when the restriction to one collective boson was made, reduced the numbers in the denominators of the expressions for the w term, for instance. Before discussing convergence we digress to cover a few points.

The choice of x itself has invoked some controversy. Sorensen[7] had advocated both $x \geq 1$ and $x \leq 1$ on different occasions. Naively, from Eq. (14), one might suppose that large x improves convergence. However, when plugging the boson expansion for $B^\dagger$ into Eq. (4a), the leading term is $x^2\delta_{ab}$, to be compared to δ_{ab} on the right-hand side. The choice $x=1$ is naturally suggested and is in fact consistent with the derivation of Eq. (12). The only way x can be chosen larger is if all modes are being considered in $B^\dagger$. Then δ_{ab} terms can drop out of the commutators of the higher order terms to reduce $x^2\delta_{ab}$ from the left-hand side of Eq. (4a) to the δ_{ab} as required by the right-hand side. The choice of $x=1$ was used in all our previous applications. Nevertheless, the results are relatively insensitive to changes in x of at least 20%. As an aside, we note that if one were to take the boson expansion out to high order and include all modes, thus forcing the choice of x to be much greater than unity, the following happens.[2] The r coefficient is for large x a factor of x^2 smaller than s while u (v) is x^4 (x^2) smaller than w. Thus r, u, v, become more and more negligible as the full calculation is taken to higher and higher order. In addition, the exact expressions for s and w approach $-1/(4x)$ and $-s^2/(22.5x)$, respectively. These expressions are similar to Eq. (12), except in this case $x \gg 1$ while in Eq. (12), as pointed out above, only $x=1$ is consistent.

We now consider, under what conditions, the boson expansion can be useful in nuclear physics applications. Looking at Eq. (14), the only way the boson expansion can converge quickly is when it is applied for a collective mode (i.e., a fermion mode in which a large number of pairs of single-particle orbits are contributing coherently with individually small amplitudes). If all single-particle levels are degenerate, then the magnitude of the quantity ξ^n (which checks the fermion content of n boson configurations) is equal to $[1/\sum_j(2j+1)]^n$ which is very small even for $n=1$. Of course, in nuclear physics the single-particle levels are not degenerate; thus full collectivity is not reached. The quantity ξ is then figuratively $[1/\sum_j|a_j|(2j+1)]$, where a_j are coefficients less than unity, they are largest for states near the Fermi surfaces, and decrease to zero for states farther away. In practical applications,[4-6] where numerical convergence has been demonstrated, this quantity has a magnitude of about 0.2, making the net expansion coefficient of the series as small as 0.05. In particular in Ref. 4, it was pointed out and confirmed in later work that for nuclei which are mildly deformed, the fourth order results differed negligibly from the sixth order results. (In the present paper's terminology, e.g., fourth order means a calculation made by ignoring w terms in $B^\dagger_{\text{coll}}$ and s^2 terms in the product of $B^\dagger$ operators in the Hamiltonian.) Only when the nucleus is well deformed is there appreciable difference, but it can be safely said that the results (for low-lying states) have converged by sixth order, except for very fine details.

Thus, if one encounters a problem where one needs to treat the multiple excitations of a collective fermion mode, the boson expansion can work quite nicely. To put it another way, the spreading of the collective fermion operator over many single-particle orbits ensures that the Pauli-principle violating components are but a small fraction of the total boson state which is obtained when a truncated boson representation of a collective fermion operator operates on a boson state comprised of a finite number of purely collective bosons. It is possible to cut off the number of terms in Eqs. (6a) or (14), because the terms which are dropped add either very small or exactly zero contributions for the states of interest. However, if one envisions the boson expansion of several modes of basically pure quasiparticle pair nature, then Pauli-principle violations can become insurmountable if one tries to cut the order of the expansion at a calculationally reasonable point.[10]

IV. CONCLUSION

The correct procedure for using the boson expansion method has been set forth. Namely, that one represents the physical fermion operators by boson expanded expressions which do not involve boson excitations of nonphysical interest. One solves the commutation relations for the coefficients of this expansion and then converts the fermion Hamiltonian into boson expanded form. A second truncation may then be made as regards limiting the number of bosons in each boson product operator of the Hamiltonian.

From a graphical description, we were able to see that the r, u, and v terms do not check the fermion nature of the bosons and, in fact, violate the Pauli principle, if they are allowed to remain in a truncated calculation. The s, w, and higher order (connected diagram) terms do indeed take care of the Pauli principle and, for some problems, it may be possible to truncate this series and still describe the fermion nature accurately. Nuclear collective motion, wherein a large number of particle-hole excitations contribute coherently to produce low-lying energy states, is a good example of such a problem.

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