Some advances in pairing theory

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Two advances are reviewed in the application of pairing-force theory in the nuclear shell model. The first exploits a discovery that a wide range of two-nucleon interactions conserve seniority as a good quantum number. As a consequence, the eigenstates of a hamiltonian with such an interaction belong to irreducible representations of a compact unitary-symplectic group. This makes it possible to extend the simply-solvable models with \( J = 0 \) pairing forces to a much richer set of models and still obtain states uniquely classified by their seniority and angular momentum quantum numbers. Moreover, many of the low-lying energy levels of such models can be obtained algebraically; in technical terms, the models are in some cases completely solvable and in other cases partially solvable by algebraic methods. The second advance exploits the discovery that, in a coherent state representation, states of good nucleon number can be projected analytically from BCS vacuum and excited quasiparticle states. This makes it possible to perform calculations in a number-projected BCS basis without losing much of the advantage of working in a quasiparticle scheme.

Keywords: Nuclear shell model; pairing-force

Se presenta una revisión de dos avances en la aplicación de la teoría de apareamiento en el modelo de capas nuclear. El primero explota el descubrimiento de que una gran variedad de interacciones de dos nucleones conservan señorío (seniority) como si fuera un buen número cuántico. Como consecuencia, los eigenestados de un hamiltoniano con esa interacción pertenecen a representaciones irreducibles de un grupo simplectico unitario compacto. Esto hace posible extender los modelos de solución simple de fuerzas de apareamiento con \( J = 0 \) a un conjunto más rico de modelos, y aún obtener estados clasificados univocamente por sus números cuánticos de señorío y momento angular. Más aún, muchos de los estados de baja energía de esos modelos pueden ser obtenidos algebraicamente; en términos técnicos, los modelos son en algunos casos completamente solubles y en otros parcialmente solubles por métodos algebraicos. El segundo avance explota el descubrimiento de que, en una representación de estado coherente, los estados con buen número de nucleones pueden ser proyectados analíticamente a partir de estados del vacío BCS y de estados excitados de cuasipartícula. Esto hace posible hacer cálculos en una base BCS de número proyectado sin perder mucho de la ventaja de trabajar en un esquema de cuasipartículas.

Descriptores: Modelo de capas nuclear; fuerza de apareamiento

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1. Introduction

In reviewing the material on the superfluid effects that arise from the pairing interactions between nucleons for a chapter in the book “Fundamentals of Nuclear Models” I am writing with John Wood, I discovered a few things that appear not to be known.

Before describing them, I will start with a brief reminder of the seniority coupling scheme that results for a \( J = 0 \) pairing interaction. I will then show that this coupling scheme also occurs for a much wider class of seniority conserving interactions. Thus, one can construct rather realistic models of a single-closed shell nucleus with nucleons in a single \( j \)-shell. These models yield analytical expressions for some energy levels. Others are obtained with the help of a computer.

For a multishell nucleus, the concept of multi-shell seniority is well defined. However, it is not conserved by a realistic two-nucleon interaction. Apart from brute-force shell model calculations, one standard description of such nuclei is with BCS or Hartree-Fock-Bogolyubov quasi-particle approximations. These approximations give valuable insights into the mechanisms underlying superconductivity in systems for which the pairing interactions are important. However, for finite nuclei, they are not so realistic as a consequence of nucleon number non-conservation. Nucleon number can be restored as a good quantum number by number projection methods and, in appropriate situations, this can lead to remarkably good results. In fact, the results of number projection before variation from BCS states is essentially equivalent to Talmi’s generalized seniority coupling scheme [3] which is also known to be remarkably good for singly-closed shell nuclei. I plan to show that number projection can be carried out simply and analytically in a wide range of situations. Results will be given for a simple two-level model which exhibits the effects the finite particle number have on the BCS phase transition from a normal to a superconducting state. The substance of this talk is presented in more detail in two papers to be published shortly [1, 2]

2. The seniority coupling scheme

The seniority coupling scheme diagonalizes a hamiltonian for nucleons of a single type in a single \( j \)-shell with \( J = 0 \) pairing interactions. Evidence for the dominance of the \( J = 0 \) pairing interaction comes from consideration of closed-shell + two nucleons, shown for \( ^{210}\text{Po} \) in Fig. 1. Without two-body interactions all the levels would be degenerate. In fact the \( J = 0 \) level lies much below the others; this provides a
measure of the strength of the $J = 0$ interaction. However, one sees that the $J = 2$ and 4 interactions are also not zero. The problem is that inclusion of a completely general interaction would destroy the simplicity of the seniority coupling scheme and mean that one could only solve the many-body problem for such an interaction by unenlightening shell model methods.

The $J = 0$ pairing model is applied to the $N = 50$ isotones in Fig. 2. The observed spectra are shown on the left. A model with a closed neutron shell and valence-shell protons in a $g_{9/2}$ single-particle level interacting with simple $J = 0$ pairing forces gives the spectrum shown on the right. It is not so good. But it does give a zero-order caricature of the spectrum. What I will show, is that much better results can be obtained by inclusion of other $J \neq 0$ seniority-conserving two-body interactions.

In fact, there are many interactions that conserve seniority. The spectrum on the right shows one of them. Shortly I will show energy levels for the $N = 50$ isotones obtained with such an interaction.

3. Seniority-conserving interactions

Seniority is usually associated with the SU(2) quasi-spin algebra [4] spanned by the operators

\[
\hat{S}_+ \propto (a_j^\dagger \otimes a_j^\dagger)_0, \\
\hat{S}_- \propto (a_j \otimes a_j)_0, \\
\hat{S}_0 \propto (a_j^\dagger \otimes a_j)_0 + (a_j \otimes a_j^\dagger)_0. \tag{1}
\]

I denote the quasi-spin SU(2) algebra by SU(2)$_S$ to distinguish it from the SU(2)$_J$ angular momentum algebra.

In fact, seniority is a quantum number of a much larger spectrum generating algebra: the so-called unitary symplectic algebra USp($2j + 1$). The latter is a subalgebra of the U($2j + 1$) algebra of all one-body operators on the space [5, 6]. The USp($2j + 1$) algebra contains the angular momentum algebra SU($2j$) as a subalgebra

\[
U(2j + 1) \supset \text{USp}(2j + 1) \supset \text{SU}(2j) \nonumber \tag{2}
\]

The important fact is that the operators of the quasi-spin algebra SU(2)$_S$ commute with those of the unitary symplectic algebra USp($2j + 1$). Moreover, it is known [5] that the irreps of SU(2)$_S$ are associated with unique irreps of USp($2j + 1$). This means that a state labelled by quasi-spin quantum numbers, and belonging to an SU(2)$_S$ irrep, also has well-defined seniority and belongs to a USp($2j + 1$) irrep. The algebras SU(2)$_S$ and USp($2j + 1$) are said to be complementary or, equivalently, to form a dual pair. This duality relationship also means that the second-quantized operators that act on the Fock space of nucleons in a single $j$-shell can be classified by their quasi-spin tensorial properties.

Starting from the basic fermion creation and annihilation operators

\[
\{a^\dagger_{jm}, a_{jm}\}, \tag{3}
\]

which form a quasi-spin 1/2 tensor, one can form, for each $JM$ with $J$ even, the three components of a quasi-spin one tensor

\[
A_{JM} \propto (a_j^\dagger \otimes a_j^\dagger)_{JM}, \\
B_{JM} \propto (a_j \otimes a_j)_{JM}, \\
C_{JM} \propto (a_j^\dagger \otimes a_j)_{JM}. \tag{4}
\]
One also discovers that, for \( J \) odd, the operators
\[
C_{JM} \propto (a_j^\dagger \otimes a_j)_{JM} 
\]
are quasi-spin scalars. Moreover, the complete set of such scalar operators spans the \( \text{USp}(2j + 1) \) algebra. Finally, a general two-body interaction
\[
V = -\frac{1}{4} \sum_j V_j \sqrt{2J + 1} [A_J \otimes B_J]_0 
\]
is a mixture of quasi-spin scalars and components of \( S = 2 \) tensors.

Now, since any quasi-spin scalar interaction can only mix states of the same quasi-spin, it follows that a quasi-spin scalar interaction conserves seniority. In addition, a quasi-spin tensor made up from bilinear combinations of the quasi-spin operators \( \{ S_\pm, S_0 \} \) (which are quasi-spin vectors) also preserves quasi-spin and hence seniority.

We now discover a remarkable result. The set of scalar and tensor two-body interactions are expressible, to within terms linear in the nucleon number operator \( \hat{n} \), in the form
\[
X^0(J) = \sum_\gamma (M_{J\gamma} - 2\delta_{J\gamma}) [A_J \otimes B_J]_0 + (\hat{n}),
\]
\[
X^2(J) = \sum_\gamma (M_{J\gamma} + \delta_{J\gamma}) [A_J \otimes B_J]_0 + (\hat{n}),
\]
where \( M \) is the matrix with entries
\[
M_{J\gamma} = 2\sqrt{(2J + 1)(2\gamma + 1)} W(jjjj; \gamma J).
\]

It follows that the eigenvectors of the matrix \( M \) with eigenvalues equal to \(-1\) are all quasi-spin scalars and those with eigenvalues equal to \(+2\) are all quasi-spin tensors (to within terms linear in \( \hat{n} \)). Thus, it is easy to identify linearly-independent combinations of seniority-conserving and non-conserving interactions. The dimensions of the two subspaces are shown in Table I.

<table>
<thead>
<tr>
<th>( j )</th>
<th>Non-conserving</th>
<th>Conserving</th>
</tr>
</thead>
<tbody>
<tr>
<td>7/2</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>9/2</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>11/2</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>13/2</td>
<td>6</td>
<td>2</td>
</tr>
<tr>
<td>15/2</td>
<td>6</td>
<td>2</td>
</tr>
<tr>
<td>17/2</td>
<td>7</td>
<td>2</td>
</tr>
<tr>
<td>19/2</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>21/2</td>
<td>8</td>
<td>3</td>
</tr>
</tbody>
</table>

It can be seen from the table that, within a single \( j \) shell, the number of seniority conserving interactions greatly exceeds the number of seniority non-conserving interactions for the values of \( j \) that occur for real nuclei; for \( 9/2 < j < 13/2 \), all but one of a linearly-independent set of interactions conserves seniority. For example, if the \( N = 50 \) isotones are modeled by protons in a \( j = 9/2 \) shell and the most general seniority-conserving interaction is adjusted to give all the lowest states except for the \( J = 6 \) state at their observed energies, we get the spectra shown in Fig. 3.

It is worth remarking that the energy levels shown in the figure for a seniority-conserving interaction are all given by analytical expressions (derived by G. Rosensteel [1]). All levels of the model can be derived with the help of a computer.

### 4. Number-projected quasi-particle methods

For a single closed-shell nucleus with valence nucleons occupying many \( j \)-shells, a concept of multi-shell seniority is
well-defined. However, it is not conserved by a realistic interaction. For a realistic interaction, one can resort to general shell model methods, for relatively small nuclei. The problem with such calculations is that, even when they can be done, they provide little insight into the nature of the correlations. More insight can be obtained from BCS (or Hartree-Fock-Bogolyubov) quasi-particle methods. But, while invaluable in condensed matter physics, these approximations are not very realistic for a finite system. A better approach is to use the BCS formalism but restore particle number as a good quantum number by projection. If the projection is carried out before variation, this approach is equivalent to Talmi’s generalized seniority and has been considered by many authors; it is known, for example, as the broken pair approximation [7, 8].

It was shown a short while ago [9] that number projection could be carried out rather easily and analytically in a manner that makes it possible to retain the simplicity and insights of the BCS approximation. What is new is the recognition that by expressing the results of a quasi-particle calculation in an appropriate coherent state representation, the corresponding number projected results can be written down immediately. The techniques are discussed in some detail in a nuclear physics article to be published shortly [2]. Here I will simply outline a few special results and applications.

First, I remind you that a quasi-particle vacuum state can be expressed in the form

$$|x\rangle = e^{\hat{S}_{+}(x)}|0\rangle,$$

where \(\hat{S}_{+}(x)\) is the operator

$$\hat{S}_{+}(x) = \sum_j x_j \hat{S}_{+}^j,$$

$$\hat{S}_{+}^j \propto (a_j^\dagger \otimes a_j^\dagger)_0.$$  \(11\)

There are many vacuum states each characterized by a set of (generally) complex numbers \(x = \{x_j\}\). The BCS vacuum state is the one that minimizes the expectation of a given hamiltonian subject to the constraint that the mean nucleon number has a specified value.

The \(2n\)-particle component of such a vacuum state is seen to be given immediately by

$$|n(x)\rangle = [\hat{S}_{+}(x)]^n|0\rangle.$$  \(12\)

Of course it is easy to write down such a state. But, in this form, it is not so easy to use. For example, while it is simple to calculate the energy expectation of the state \(|x\rangle\) using the fact that it is a quasi-particle vacuum state, it is \(a\ priori\) less obvious how to evaluate the energy of its number projected components. In fact, it is easy in a coherent state representation.

The first observation to be made is that the set of quasi-particle vacuum states \(\{|x\rangle\}\), for different values of \(x\), are coherent states of a direct sum of SU(2) quasi-spin algebras. Thus, any multishell seniority-zero state \(|\psi\rangle\) can be represented by a coherent state wave function \(\psi\), which is a function of a set of complex variables \(z = \{z_j\}\) defined by

$$\psi(z) = \langle 0|e^{\hat{S}_{-}(z)}|\psi\rangle.$$  \(13\)

For example, any quasi-particle vacuum state \(|x\rangle\) has coherrent state wave function given by

$$\Phi(xz) = \langle 0|e^{\hat{S}_{-}(z)}|x\rangle = \prod_j (1 + z_j x_j)^{j+1/2}/.$$  \(14\)

What is more, the number-projected quasi-particle state \(|n(x)\rangle\) has wave function defined by

$$\Phi_n(xz) = \langle 0|e^{\hat{S}_{-}(z)}|n(x)\rangle = \langle 0|e^{\hat{S}_{-}(z)}[\hat{S}_{+}(x)]^n|0\rangle.$$  \(15\)

Thus, to within a constant factor \(n!\), \(\Phi_n\) is simply the component of \(\Phi\) of degree \(n\) in its argument. Furthermore, picking out this component is made extremely simple by the observation [9] that the set of such functions obey a simple recursion relation and are, in fact, standard orthogonal functions known as Schur functions. As shown in Refs. 7 and 8, they have the explicit form

$$\Phi_n(x) = \text{det}\begin{bmatrix} \phi_1 & 1 & 0 & 0 & \cdots & 0 \\ \phi_2 & \phi_1 & 2 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \phi_n & \phi_{n-1} & \phi_{n-2} & \phi_{n-3} & \cdots & \phi_1 \end{bmatrix},$$  \(16\)

where

$$\phi_n = \frac{1}{2} \sum_j (2j + 1) z_j^n.$$  \(17\)

Coherent state wave functions for excited quasi-particle states are almost as easy to derive. For example, a one quasi-particle state

$$a_j^\dagger m_k |x\rangle$$

has coherent state wave function

$$\psi_{x j a m_k}(z) = \xi_{x j a m_k} \phi_{(j)^a}(zx),$$  \(18\)

where \(\xi_{x j a m_k}\) is an intrinsic wave function representing the state of the odd particle and the cofactor

$$\phi_{(j)^a}(zx) = \prod_j (1 + z_j x_j)^{j+1/2-\delta_{ij}k}$$  \(19\)

is the wave function for the other pair-coupled particles. Observe that the function \(\phi_{(j)^a}\) has exactly the same form as the wave function \(\Phi\) for a vacuum state; the only difference is that the factor \((1 + z_j x_j)^{j+1/2}\) on the right hand side of Eq. (19) is reduced to \((1 + z_j x_j)^{j+1/2}\) to account for the blocking of one the \(j_k\)-shell substates by the odd particle. The important observation is that the \(2n + 1\) particle component

of the one quasi-particle state has coherent state wave function given immediately by
\[ \Psi_{n|G|J_k} = \xi_{J_k} \Phi_n^{(j_k)}(z), \]
where \( \Phi_n^{(j_k)} \) is again a standard Schur function.

Consider, for example, the energy expectation of a projected vacuum state \(|n(x)\rangle\). From standard BCS theory, the unprojected vacuum energy is given by
\[ \langle x | H | x \rangle = \sum_j (2j+1) \xi_j x_j^2 \Phi^{(j)}(x^2) - \frac{1}{2} G \sum_j (2j+1) x_j^4 \Phi^{(jj)}(x^2) - \frac{1}{4} G \sum_{ij} (2i+1)(2j+1) x_i x_j \Phi^{(ij)}(x^2), \]
where
\[ \Phi^{(j,j_k)}(x) = \prod_j (1 + x_j^{j+1/2} - \delta_{jj_k} - x_j^{j+1}). \]

It follows immediately that
\[ \langle n(x) | H | n(x) \rangle = \frac{n}{\Phi_n(x^2)} \times \sum_j \left[ (2j+1) \xi_j x_j^2 \Phi_n^{(j)}(x^2) - \frac{1}{2} G(n-1)(2j+1) x_j^4 \Phi_n^{(jj)}(x^2) - \frac{1}{4} G \sum_i (2i+1)(2j+1) x_i x_j \Phi_n^{(ij)}(x^2) \right]. \]

### 5. An example, a two-level model

Consider a model Hamiltonian
\[ H = \sum_j \xi_j \hat{n}_j - GS_+S_-, \]
for a system with just two levels with \( j_1 = j_2 = j \). The exact solutions of this model are easy to obtain and so can be used to test the number projection approximation. Figure 4 shows wave functions for the ground and first \( J = 0 \) excited states for \( j = 13/2 \) and 14 particles. The horizontal axis is the number of nucleon-pairs in the lower level. Thus, in the ground state, all particles are in the lower level when \( G = 0 \). However, as \( G \) is increased, the upper level starts to become populated. This Figure shows that the ground state is extremely close to being a number projected quasi-particle vacuum state for the full range of \( G \) values.

Figure 5 shows the occupancy ratio of the upper to lower level as a function of \( G \). It is seen that at a critical value of \( G \) (with units chosen so that \( G_{\text{crit}} = 1 \), the BCS solution undergoes a phase transition from an independent-particle state to a superconducting quasi-particle vacuum state. The exact results show the beginnings of such a phase transition which becomes sharp as \( j \to \infty \) but is smoothed out for finite \( j \). The number-projected results are seen to reflect the exact behaviour rather accurately.
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6. Where next?

I believe we now have rather good and simple models of singly-closed shell nuclei. For a single $j$ shell, seniority is a remarkably good quantum number and, for multiple $j$ shells, methods based on generalized seniority, which can be implemented by quasi-particle and number-projection methods, are capable of describing the underlying phenomena. The major challenge remaining is to construct realistic models of doubly-open shell nuclei which are known to exhibit rotational as well as superfluid properties. The conventional wisdom is that, with no interactions between them, the neutron and proton subsystems would separately form spherical states. However, the neutron-proton interactions result in a mutual polarization of the two subsystems which causes them to become deformed and exhibit rotational properties.

The challenge is an intriguing one. Without superfluid pairing correlations, it has a very elegant solution in the nuclear symplectic model [10]. Conversely, as we have been discussing, without rotational degrees of freedom, we have good model descriptions of the superfluid dynamics. It is the combination of the two that presents problems. The remarkable fact is that physical nuclei appear to be quite capable of exhibiting bands of states with superfluid rotational flows. Thus, it seems likely that there should be a relatively simple way to describe what they do so readily and which is superficially so easy to talk about. The best we have been able to come up with so far, to reconcile the seemingly incompatible symmetries associated with pairing and rotational correlations, is a concept of quasi-dynamical symmetry [11]. But that is another story.