A Deformed $Sp(4)$ Model for Studying Pairing Correlations in Atomic Nuclei

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Abstract

A fermion representation of the compact symplectic $sp(4)$ algebra introduces a theoretical framework for describing pairing correlations in atomic nuclei. The important non-deformed and deformed subalgebras of $sp_{(4)}$ and the corresponding reduction chains are explored for the multiple orbit problem. One realization of the $u(2)$ subalgebra is associated with the valence isospin; other reductions describe coupling between identical nucleons or proton-neutron pairs. Microscopic non-deformed and deformed Hamiltonians are expressed in terms of the generators of the $sp(4)$ and $sp_{(4)}$ algebras. In both cases eigenvalues of the isospin breaking Hamiltonian are fit to experimental ground state energies. The theory can be used to investigate the origin of the deformation and predict binding energies of nuclei in proton-rich regions. The $q$-deformation parameter changes the pairing strength and in so doing introduces a non-linear coupling into the collective degree of freedom.

1 Introduction

Nuclear models with a pairing term provide a better explanation of nuclear collective properties and a more detailed description of binding energies of nuclei and their low-lying vibrational spectra [1,2]. Along with many approximate mean field solutions, the pairing problem is solved exactly by the means of group theory, which considers the symmetries of nuclear structure based on $SU(2)$ [3, 4, 5], $SO(5)$ [6], $SO(8)$ [7] and the well known IBM [8]. The importance of isovector pairing [9] leads naturally to the $SO(5)$ seniority model [10,12], which is a generalization of the like-particle $SU(2)$ model, introducing a proton-neutron ($pn$) isovector pairing mode. The generalized seniority model is applicable to regions of light nuclei and exotic nuclei with proton excess or with $N \sim Z$. The studies of nuclear properties in these regions are of great recent interest.

Our aim is to investigate the properties of the pairing interaction by considering a fermion realization of the symplectic $sp(4)$ algebra (isomorphic to $so(5)$) and its deformation. The symplectic symmetry provides a classification scheme for the nuclei in a considered valence shell and allows for investigation of the experimentally observed odd-even mass staggering. The limiting cases of $sp(4)$ correspond to different reductions to $u(2)$ and reveal the properties of different coupling modes of the isovector pairing interaction. The concept of a dynamical symmetry leads to an isospin breaking phenomenological Hamiltonian constructed as a scalar product of the $Sp(4)$ group generators. Within the framework of the nuclear classification scheme, we use the phenomenological Hamiltonian to estimate the binding energy of atomic nuclei over a wide range of the isotope table.

The nature of the fermion realization introduces shell structure into the theory and allows for an investigation of the dependence of pairing correlations on the dimensionality of the model space.

To account for non-linear effects of the residual interaction we introduce a $q$-deformation parameter in the classical symplectic model. The deformation provides for novel algebraic structures with additional degree of freedom. The $q$-deformation parameter influences the pairing strength parameters and yields a better reproduction of pairing features in nuclei.

In both the deformed and non-deformed cases, an analysis of the results, obtained by fitting of the model parameters to experimental data, provides for a reliable prediction of the energies of low-lying excited $0^+$ states and the binding energies of nuclei, some of which are unknown and of contemporary interest.

2 Phenomenological Hamiltonian for the non-deformed and deformed cases

The deformed $sp_q(4)$ algebra [13] is realized in terms of $q$-deformed creation and annihilation operators $\alpha^+_{j,m,\sigma}$ and $\alpha_{j,m,\sigma}$, $(\alpha^+_{j,m,\sigma})^* = \alpha_{j,m,\sigma}$, $(\alpha^+_{j,m,\sigma})^* = \alpha_{j,m,\sigma}$, where $\alpha_{j,m,\sigma} \in \mathbb{C}$, $c_{j,m,\sigma}$, $j \leq m \leq j$, $\sigma = \pm 1$, create (annihilate) a particle of type $\sigma$ in a state of total angular momentum $j$, $j = 1/2, 3/2, 5/2, \ldots$, with projection $m$ on the $z$-axis. The deformed fermion operators satisfy the anticommutation relation $(\alpha_{j,m,\sigma}, \alpha^+_{j,m',\sigma}) = q^{m-m'}$ for a given $\sigma$,
the dimension of the fermion space is $2\Omega = \sum_{j_m=\frac{1}{2}}^{j_{m}} 2\Omega_{j_m} = \sum_{j_m} (2j_m + 1)$, and $N_{\pm l} = \sum_{j_m} j_{m,\pm l} \alpha_{j_m,\pm l}^{\dagger} \alpha_{j_m,\pm l}$ are non-deformed particle number operators. Based on different interpretations of the quantum number $\sigma$, the fermion operators have different physical meaning. When $\sigma$ distinguishes between protons ($\sigma = 1$) and neutrons ($\sigma = -1$), the Cartan generators of the $Sp(4)$ group $N_{\pm l}$ enter as the number of the valence protons and valence neutrons, respectively. The valence fermions are created (annihilated) by operator $a_{j_{m,\sigma}}^{\dagger} (a_{j_{m,\sigma}})$ above the pairing vacuum state of the nuclear system, which is a doubly magic core. A pair of $q$-deformed fermions can be created or destroyed by six of the generators of $Sp(4)$

\[
\begin{align*}
F_{(\sigma + \sigma')}/2 &\equiv F_{\sigma,\sigma'} \equiv \xi \sum_{j_m} (-1)^{j-m} \alpha_{j_m,\sigma}^{\dagger} \alpha_{j_m,-\sigma}^{\dagger} \\
G_{(\sigma + \sigma')}/2 &\equiv G_{\sigma,\sigma'} \equiv \xi \sum_{j_m} (-1)^{j-m} \alpha_{j_m,-\sigma} \alpha_{j_m,\sigma}
\end{align*}
\] (1)

where $\xi = 1/\sqrt{2(1+\delta_{\sigma,\sigma'})}$ and $F_{\sigma,\sigma'} = F_{\sigma',\sigma} = (G_{\sigma,\sigma'})^{\dagger}$. In the limit, the operators (1) coincide with the non-deformed ones $F_{(\sigma + \sigma')}/2 \rightarrow A_{(\sigma + \sigma')}/2$, $G_{(\sigma + \sigma')}/2 \rightarrow B_{(\sigma + \sigma')}/2$, where $A_{\sigma,\sigma'} = (B_{\sigma,\sigma'})^{\dagger}$. The operators $A_{0,\pm 1} (B_{0,\pm 1})$ create (annihilate) a pair of fermions coupled to a total angular momentum and parity $J^P = 0^+$ and constitute a boson-like objects. The rest of the group generators are the number preserving Weyl generators $T_{\pm 1} \equiv E_{\pm 1,0,1} = 1/2\sum_{j_m=\frac{1}{2}}^{j_{m}} \alpha_{j_m,1,\pm 1}^{\dagger} \alpha_{j_m,-1,\pm 1}$, $T_0 \equiv \tau_0 = N_1 - N_{-1} / 2$, $N = N_1 + N_{-1}$, which close on the $u'(2)$ subalgebra. The operators $T_{0,\pm 1}^{\pm 1}$, $T_{1,\pm 1}^{\pm 1}$, $T_{2,\pm 1}^{\pm 1}$, are associated with the isospin of the valence particles. The other three limits of the $Sp(4)$ group describe pairing between particles of different types ($SU^0(2) : pn$) and coupling between identical particles ($SU^\pm(2) : pp$ or $nn$). In the deformed and non-deformed cases, the basis states $|n_1 n_0 n_{-1}\rangle$, are labeled by the total number of pairs of each kind, $nn$, $pp$, $nn$, and describe the ground state of a nucleus with $N = 2n_1 + n_0$ valence protons (neutrons). The operators $N$ and $\tau_0$ are diagonal in the basis with eigenvalues $n = 2(n_1 + n_0 + n_{-1})$ and $i = n_1 - n_{-1}$, respectively. In this way, the symplectic symmetry provides a classification scheme with respect to $n$ and $i$ of the nuclei and their corresponding states. Such an example for the $1f7/2$ shell is shown in Table 1. The table is symmetric with respect to $i$, as well as to $n$, which is a consequence of the charge independence and a particle-hole symmetry [14], respectively.

In our approach, we use a phenomenological Hamiltonian of a system with symplectic symmetry, expressed through the generators of the $Sp(4)$ group [15]

\[
H = -\varepsilon N - GA_0 B_0 - F(A_1 B_1 + A_{-1} B_{-1}) - C \frac{N(N-1)}{4} - D \left( \tau_0^2 - \frac{N}{4} \right)
\] (2)

in the non-deformed case, which in the $q$-deformed case transforms to

\[
H_q = -\varepsilon N - G_q F_0 G_0 - F_0 (F_1 G_1 + F_{-1} G_{-1}) - C_q \frac{N(N-1)}{4} - D_q \left( \tau_0^2 - \frac{N}{4} \right)
\] (3)

where $\varepsilon$ is a Fermi energy, and $G(q)$, $F(q)$, $C(q)$ and $D(q)$ are constant interaction strength parameters ($G(q) \geq 0$, $F(q) \geq 0$). The $G$ and $F$ terms account for pairing between non-identical and identical particles, respectively.

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<td>2</td>
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<td>8</td>
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Table 1: $(N, \tau_0)$-classification scheme of nuclei in the $1f7/2$ level, $\Omega = 4$. 
and can be expressed in terms of the Casimir invariants of the corresponding subalgebras.

An important feature of the phenomenological Hamiltonian (2) is that it not only breaks the isospin symmetry \( (D \neq 0) \), but it also mixes states with definite isospin values \( (F \neq G) \). Indeed, in approximate solutions the isospin breaking is required in order to reproduce a non-zero proton pairing [16]. This is different from other applications of non-deformed and deformed \( sp(4) \) or \( o(5) \) algebras with isospin invariant Hamiltonian [11,12,17].

The last two terms \((C, D)\) arise naturally from the microscopic picture of the interaction Hamiltonian [4] and can be written through the other two diagonal operators \( N_{\pm 1} \). In that way, the energy operator (2) contains the quantity \( N_{+} N_{-} \) which is connected to the deformation of the nuclei [18], and therefore the Hamiltonian is applicable in the whole space \( \Omega \) including regions of deformed nuclei. As a consequence of the Pauli principle, the particle-hole description enters naturally in the pairing terms only and gives the decrease in energy with respect to a ground state with no pairing [14].

In each limit, when expanded in orders of \( \kappa \), the eigenvalue of the deformed pairing Hamiltonian can be expressed in terms of the non-deformed energies

\[
\varepsilon_{pm} = \frac{G}{\Omega} n_{0} \frac{2\Omega - N + n_{0} + 1}{2},
\]

\[
\varepsilon_{pp(nn)} = \frac{F}{\Omega} \frac{n_{\pm 1} (\Omega - n_{\pm 1} - n_{0} + 1)},
\]

which are the zeroth order approximation of the corresponding deformed pairing energies

\[
\varepsilon_{pair}^{2}_{SU(2)} = -G_{q} \varepsilon_{pm} \left\{ 1 + \frac{\kappa^{2}}{24\Omega^{2}} \left\{ (n_{0}^{2} - 4\Omega^{2} - 1) + \frac{2\Omega^{2}}{n_{0}} \varepsilon_{pp}^{2} \right\} + O(\kappa^{4}) \right\},
\]

\[
\varepsilon_{pair}^{2}_{SU^{+}(2)SU^{-}(2)} = -F_{q} \left\{ 1 + \frac{\kappa^{2}}{4\Omega} \left\{ \left( n_{1}^{2} - \frac{\Omega^{2}}{2} - \frac{5}{8} \right) + \frac{\Omega^{2}}{n_{1}^{2}} \varepsilon_{pp}^{2} \right\} + \frac{\kappa^{2}}{4\Omega} \left\{ \left( n_{2}^{2} - \frac{\Omega^{2}}{2} - \frac{5}{8} \right) + \frac{\Omega^{2}}{n_{2}^{2}} \varepsilon_{nn}^{2} \right\} \right\} + O(\kappa^{4}) \right\}.
\]

While the proton-neutron interaction is even with respect to the deformation parameter \( \kappa \), the identical particle pairing includes also odd terms as a consequence from the introduced coefficient \( \rho_{\pm} = \left( q^{\pm 1} + q^{\pm 2} \right) / 2 \).

3 Fitting procedure, results and discussion

Eigenvalue of Hamiltonians (2) and (3) gives a phenomenological formula for estimating of the ground state energy of nuclei in a \((N, \tau)\) classification scheme. Its positive value is defined as binding energy of the system, \(|BE|\), and can be fitted to the measured binding energy [19]. The latter needs to be corrected for the Coulomb energy since it is not accounted for by the model, \(|H| = |BE_{exp}| + V_{Coul}|. Where we use the Coulomb potential from [20]. In both the non-deformed and deformed cases, several groups of nuclei are considered: (I) \( \Omega = 2(1d3/2) \) with a \( 105\text{Sn} \) core; (II) \( \Omega = 4(1f7/2) \) with a \( 96\text{Ca} \) core; (III) \( \Omega = 11 (2p3/2, 1f5/2, 2p1/2, 1g9/2) \) with a \( 58\text{Ni} \) core; (IV) \( \Omega = 16(1g7/2, 2d5/2, 2d3/2, 1h1/2, 3s1/2) \) with a \( 100\text{Sn} \) core. The phenomenological formula for the maximum eigenvalue of the Hamiltonian (2) depends on the parameters, given in Table 2, for the non-deformed case.

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</tr>
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<td>( \chi, \text{MeV} )</td>
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</tbody>
</table>

Table 2: Parameters and statistics, \( q = 1 \)

The parameters are estimated by a non-linear least-squares fit to the experimental Coulomb corrected binding energies:

\[
|BE_{exp}|(N_{+}, N_{-}) = |BE_{exp}|(N_{+}, N_{-}) - |BE_{exp}|_{\text{core}} + V_{Coul}(N_{+}, N_{-}),
\]

where \( |BE_{exp}|_{\text{core}} \) is the binding energy of the core. The single-particle energies were considered fitting parameters in all cases but \( S_{n} \), for which the values were taken from theoretical calculations [21].

In Table 2, \( S = (|BE_{exp}^{th}|-|BE_{exp}|)^{2} \) is the residual sum of squares and the statistical factor \( \chi \equiv \sqrt{S/(N_{p} - n_{\rho})} \) defines the goodness of the fit, where \( N_{p} \) is the number of data in the statistics and \( n_{\rho} \) is the number of the fitting parameters. In all cases there is a good agreement with the experiment (small \( \chi \)), as it is seen in Table 2, as well as in Figure 1 for the case (II). In general, the pairing strength decreases as the nuclear mass increases. This fact is well known, but only for the identical particle case [2].
In both limits of the $Sp(4)$ group, the nuclear classification in $(n,i)$ yields a distinctive behavior of the respective different kinds of pairing energies (Figure 2). The theoretical model with the $sp(4)$ symmetry reproduces in a good agreement the properties of the identical nucleons pairing ($\epsilon_{pp} + \epsilon_{nn}$) [3,4,5,14], which has its maximum at half shell (Figure 2 (a)). The identical particle limit reveals an odd-even staggering as expected for the ground state pairing energy of odd-odd and even-even nuclei.

The proton-neutron coupling ($\epsilon_{pn}$) (Figure 2 (b)) has its maximum when $N_+ = N_-$ ($i = 0$) and sharply decreases as $|i|$ increases, which is consistent with $\alpha$-clustering theories [21] and the charge independence in the region of light nuclei when protons and neutrons fill up same shells [9,23]. In the region $N_+ = N_-$, the pairing energy due to the non-identical particle pairing ($H_{pp}$) is bigger than the identical particle one ($H_{pp} + H_{nn}$) for odd-odd nuclei and is of the same order for even-even nuclei (Figure 3), which is consistent with good isospin symmetry in even-even nuclei.

The fitting procedure for (3) was performed for all the cases, (I) to (IV), introducing the $q$-deformation (Table 3). The fit for nuclei in multiple orbits, (III)* and (IV)*, includes only isotopes with $N_+ = 0, 1$ and isotones with $N_- = 2\Omega - 1, 2\Omega$. The corresponding non-deformed limit is labeled by $q = 1$ and the deformation parameter is not a part of the fitting procedure in that case. The single-particle energies were kept fixed and their values taken from the non-deformed fit, or from theoretical calculations [21].

The fits with and without a deformation can be com-
pared by using the residual sum of squares ($S$), which is always smaller in the deformed case. Although the deformation does not change the parameters within the uncertainties in the case of a single level, for multiple orbits the role of the deformation parameter is significant when not all nuclei of a major shell are used in the fitting procedure. This turns out to be very important for fitting nuclei in a region where the binding energy of most of the proton-rich isotopes are not yet measured and therefore cannot be included in the fit. For these cases, the deformation varies the pairing strength parameters. This property of the $q$-deformation is consistent with the change of the pairing strength with respect to $q$ (Figure 4). The change of the $pn$ pairing strength $G_q$ with changes in the deformation parameter is relatively small for $q$-values around $q = 1$ but it always increases as $q \to 1$ (Figure 4) and (Table 3). The parameter $F_q$ decreases monotonically with $q$ only for nuclei without nn coupling and it increases for nuclei with a primary nn coupling. $F_q$ is always smaller than $F(q = 1)$ when both pp and nn coupling modes exist. Even though both SU$_q^\pm$(2) groups are complementary, the different behavior of the multiplication constants $\rho_q$ is responsible for different changes of $F_q$ in various isotopes, in difference with the like-particle SU$_q^\pm$(2) seniority model of [24].

The fitting procedure not only estimates the magnitude of the pairing strength and describes the type of the dominant coupling mode but also it can be used to predict binding energies of nuclei that have not been measured. From the fit for the case of 1$^f7/2$ the binding energy of the proton-rich nucleus of $^{54}_{36}$Ni is estimated to be 347.98 MeV. A much more interesting region includes the nuclei above the core of $^{58}_{36}$Ni. The neutron-rich isotopes are used in the fit in order to predict the ground state energy $E^{sp(4)}_q$ of the nuclei at the proton-rich side. Several of them (for which data was available) are compared to [25], with the percent difference 8.76% and the tendency the theoretically predicted binding en-

Table 3: Parameters and Statistics. The $q = 1$ case for (I) and (II) is same as in Table 2. Fits for (III)* and (IV)* include only isotopes with $N_+ = 0, 1$ and isotopes with $N_- = \{27 - 1, 2\}$.

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Figure 4: pn pairing strength $G_q$ (in MeV) and identical particle pairing strength $F_q$ (in MeV) for ($N_+, N_-$) nuclei vs. $q$. 
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Table 4: Overlap [%] of the ground state of \((N_+, N_-)\) nuclei and isospin states labeled by the isospin values \(\tau\) for the cases (I)–(III).

Energies \(E_g^{Sp(4)}\) to be smaller than the semi-empirical estimates.

The eigenvectors of the Hamiltonian (2) can have definite isospin values only if \(G = F\). The comparison to the ground state of real nuclei in the fitting procedure (Table 2) does not yield equality of both pairing strength parameters confirming the isospin invariance breaking and isospin mixing. The percent overlap of the ground state and the isospin eigenvectors \(|n, \tau, i, g.st.|\) is defined as

\[ |\langle n, \tau, i, g.st. \rangle|^2 \times 100\% \],

where \(|g.st.|\) is the normalized ground state vector for those nuclei having \(J^\pi = 0^+\) in their lowest state and it depends on the fit parameters \(G\) and \(F\).

The percent overlap (Table 4) shows that the isospin of the nuclear \(0^+\) ground state is primarily \(\tau = \tau_0\) for even-even nuclei, and \(\tau = \tau_0 + 1\) for odd-odd, with a mixture of the higher possible isospin values. For nuclei occupying a single-\(j\) shell, the mixing of the isospin states is less than 1%. It is even higher, more than 40%, when multiple shells are occupied. The mixing increases

![Figure 5: The predicted and measured energy (in MeV) of the low-lying 0^+ excited states of even-even isotopes in the 1f7/2 (\(\Omega = 4\)) level.](image-url)
toward the middle of the shell, with increasing of $j$ and around the region of $N_+ = N_-$. The low-lying excited $0^+$ states of even-even isotopes can be also described by the symplectic symmetry model and expressed as a linear combination of the pair-states $|n_1, n_0, n_{-1}\rangle$. The energy of these states is given by the second to the maximum eigenvalue of the Hamiltonian (2) (or (3) in the deformed case) and accounts for a decrease in the nuclear binding energy due to a different coupling between nucleons. The low-lying excited $0^+$ state energy is predicted using the parameters from Table 2 obtained in the fitting procedure for the binding energies. For six isotopes in the case (II), $^{48}$Ti, $^{44}$Ti, $^{44}$Cr, $^{44}$Ti, $^{42}$Cr and $^{42}$Fe (Figure 5), the root mean square of the difference between the predicted and experimentally measured values is 2.43 MeV, and for 30 isotopes in the case (III), it is 3.11 MeV. Introducing the $q$-deformation for the same even-even isotopes in the case (II), the energy of their second $0^+$ states can be fit only with respect the $q$-parameter. The $q$-deformed fitting procedure gives closer energies to the experimental ones and yields a smaller corresponding value of $\chi = 2.35$ MeV with $q = 0.63$. In this way, the $q$-deformation serves as additional characteristic for describing non-linearity in the nuclear spectra.

4 Conclusion

In order to describe pairing correlations in atomic nuclei, the symplectic $sp(4)$ algebra was investigated. Its $q$-deformation was obtained. Deformed subalgebras of $sp(4)$ were identified and the important reduction chains $Sp_q(4) \supset U(1) \otimes SU_q(2)$ constructed. The two Cartan generators of $Sp(4)$ were used to systemize the nuclei into a $(N,\tau_0)$-classification scheme. A phenomenological Hamiltonian was written in terms of the generators of $Sp(4)$ and related to the binding energy of nuclei and their low-lying excited $0^+$ state energy. The theory was tested by fitting calculated energies to experimental binding energies for single $j$ level as well as for multiple orbits. In general, the fitting procedure yielded results that were in good agreement with the experiment. The results did not call for isospin invariance and ground states with definite isospin values, which could be the case if the pairing parameters $F$ and $G$ turn out to be equal. The overlap of the ground states and isospin vectors also shows a non-negligible isospin mixing, especially in a multiple shell occupation space.

The theoretical framework of the $sp(4)$ dynamical symmetry algebra and its $q$-deformed version was used to investigate the properties of the pairing interaction. In both limits of $Sp(4)$, identical and non-identical particle pairing, the $(N,\tau_0)$-classification scheme were used to describe a distinctive behavior of the nuclear system. The identical-particle limit reveals an odd-even staggering in the pairing energy of the odd-odd and even-even nuclei. The proton-neutron interaction was found to be bigger than the identical particle interaction in odd-odd light nuclei and both interactions were found to be of the same order of magnitude in even-even nuclei.

The results indicate that the $q$-deformed case gives the best overall fit. It requires an increase in the coupling strength of the proton-neutron pairs. When $q > 1$, the neutron (proton) pairs are more strongly (weakly) bound and vice versa for $q < 1$. The binding energy of nuclei in the proton-rich region and the energy of the second $0^+$ states of even-even isotopes were predicted using a simple microscopic model based on a symplectic symmetry. In doing this we were able to suggest a reliable form for the pairing interaction.

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