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Quantum algebraic description of the pairing correlations in a single-j nuclear shell

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Abstract. Pairing in a single-*j* shell is described in terms of two Q-oscillators, one describing the J = 0 fermion pairs and the other corresponding to the $J \neq 0$ pairs, the deformation parameter $T = \ln Q$ being related to the inverse of the size of the shell. Using these two oscillators an $SU_Q(2)$ algebra is constructed, while a pairing Hamiltonian giving the correct energy eigenvalues up to terms of first order in the small parameter can be written in terms of the Casimir operators of the algebras appearing in the $U_Q(2) \supset U_Q(1)$ chain, thus exhibiting a quantum algebraic dynamical symmetry. The additional terms introduced by the Q-oscillator are found to improve the agreement with the experimental data for the neutron pair separation energies of the Sn isotopes, with no extra parameter introduced.

Quantum algebras (also called quantum groups) [1-4] have recently attracted much attention in physics, especially after the introduction of the q-deformed harmonic oscillator [5, 6]. Applications in conformal field theory, quantum gravity, quantum optics, atomic physics, as well as in the description of spin chains have already been reported. In nuclear physics attention has been focused on the q-deformed rotator with $SU_q(2)$ symmetry and its use for the description of rotational spectra and B(E2) transition probabilities of deformed and superdeformed nuclei ([7, 8] and references therein), as well as on the construction of exactly solvable nuclear models with quantum algebraic dynamical symmetries [9, 10]. Similar efforts have been made for the description of rotational [11–13] and vibrational ([14, 15] and references therein) spectra of diatomic molecules. In many cases the deformation parameter q turns out to be related to some well defined physical quantity. In the case of the q-deformed rotator, for example, the deformation parameter has been related to the softness parameter of the variable moment of inertia (VMI) model [16].

For nuclear physics the description of correlated fermion pairs in terms of q-deformed bosons is of particular interest for several reasons. Correlated fermion pairs in a single-jnuclear shell or several non-degenerate j shells ([17] and references therein) are known to satisfy commutation relations which resemble boson commutation relations but contain corrections due to the presence of the Pauli principle. This fact has led to the development of boson mapping techniques for the description of many fermion systems (see [18] for an authoritative review). Boson mappings are of additional interest as a necessary tool in

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building a bridge between the phenomenologically successful algebraic models of nuclear collective motion, such as the interacting boson model (IBM) ([19], see also [20, 21] for recent overviews) and the shell model. Since q-bosons also satisfy commutation relations different from the usual ones, it is reasonable to check to what extent correlated fermion pairs can be described in terms of q-deformed bosons. For fermion pairs of J = 0 this question has been answered in [22], where an approximate mapping of these fermion pair operators onto Q-bosons [23-25] has been constructed, which correctly reproduces the commutation relations and the pairing energies up to first order corrections in the small parameter $T = \ln Q$, which is related to the inverse of the size of the single-*j* shell. The same problem has been solved exactly in [26] through the use of a generalized deformed oscillator [27]. The extension of this formalism to pairs of $J \neq 0$ is of obvious interest, since the $J \neq 0$ pairs are known to play an important role in the formation of nuclear properties.

In the present work a first step in this direction is taken. First, it is realized that for the description of pairing correlations in a single-j nuclear shell, it suffices to represent the $J \neq 0$ pairs by a Q-oscillator similar to the one used for the J = 0 pairs. The two oscillators are then used for building a quantum algebraic dynamical symmetry. Finally, the higher order terms introduced by the Q-oscillator are found to lead to improved agreement with the experimental data, without the introduction of any new parameter.

In the usual formulation of the theory of pairing in a single-*j* shell [28], fermion pairs of angular momentum J = 0 are created by the pair-creation operators

$$S^{+} = \frac{1}{\sqrt{\Omega}} \sum_{m>0} (-1)^{j+m} a^{+}_{jm} a^{+}_{j-m}$$
(1)

where a_{jm}^+ are fermion-creation operators and $2\Omega = 2j + 1$ is the degeneracy of the shell. In addition, pairs of non-zero angular momentum are created by the $\Omega - 1$ operators

$$B_{J}^{+} = \sum_{m>0} (-1)^{j+m} (jmj - m|J0) a_{jm}^{+} a_{j-m}^{+}$$
⁽²⁾

where (jmj - m|J0) are the usual Clebsch-Gordan coefficients. The fermion number operator is defined as

$$N_F = \sum_m a_{jm}^+ a_{jm} = \sum_{m>0} (a_{jm}^+ a_{jm} + a_{j-m}^+ a_{j-m}).$$
(3)

The J = 0 pair-creation and annihilation operators satisfy the commutation relation

$$[S, S^+] = 1 - \frac{N_F}{\Omega} \tag{4}$$

while the pairing Hamiltonian is

$$H = -G\Omega S^+ S. \tag{5}$$

The seniority V_F is defined as the number of fermions not coupled to J = 0. If only pairs of J = 0 are present (i.e. $V_F = 0$), the eigenvalues of the Hamiltonian are

$$E(N_F, V_F = 0) = -G\Omega\left(\frac{N_F}{2} + \frac{N_F}{2\Omega} - \frac{N_F^2}{4\Omega}\right).$$
(6)

For non-zero seniority, the eigenvalues of the Hamiltonian are

$$E(N_F, V_F) = -\frac{G}{4}(N_F - V_F)(2\Omega - N_F - V_F + 2).$$
(7)

For simplicity, we denote the operators N_F , V_F and their eigenvalues by the same symbol.

It has been proved [22] that the behaviour of the J = 0 pairs can be described, up to first-order corrections, in terms of Q bosons. Q bosons [23-25] are defined by the commutation relations

$$[N, b^+] = b^+ \qquad [N, b] = -b \qquad bb^+ - Qb^+b = 1 \tag{8}$$

where b^+ (b) are Q-boson creation (annihilation) operators and N is the relevant number operator. Q-numbers [23–25] are defined as

$$[x]_{Q} = \frac{Q^{x} - 1}{Q - 1}.$$
(9)

For $Q = e^T$ their Taylor expansion is

$$[x]_{\mathcal{Q}} = x + \frac{T}{2}(x^2 - x) + \frac{T^2}{12}(2N^3 - 3N^2 + 1) + \frac{T^3}{24}(N^4 - 2N^3 + N^2) + \dots$$
(10)

One can then easily see that

$$b^+b = [N]_Q$$
 $bb^+ = [N+1]_Q.$ (11)

Making the mapping

$$S^+ \to b^+ \qquad S \to b \qquad N_F \to 2N$$
 (12)

the Hamiltonian of equation (5) becomes

$$H(N, V=0) = -G\Omega b^+ b = -G\Omega[N]_Q.$$
⁽¹³⁾

Using equation (10) we see that it coincides with equation (6) up to first-order corrections in the small parameter, which is identified as $T = -2/\Omega$. Furthermore, the Q bosons satisfy the commutation relation

$$[b, b^+] = [N+1]_Q - [N]_Q = Q^N = 1 + TN + \frac{T^2 N^2}{2} + \frac{T^3 N^3}{6} + \dots$$
(14)

which coincides with equation (4) up to first-order corrections in the small parameter, which, consistently with the above finding, is identified as $T = -2/\Omega$. Therefore, the fermion pairs of J = 0 can be approximately described as Q bosons, which correctly reproduce both the pairing energies and the commutation relations up to first-order corrections in the small parameter.

For the case of non-zero seniority, one observes that equation (7) can be written as

$$E(N_F, V_F) = G\Omega\left(\frac{V_F}{2} + \frac{V_F}{2\Omega} - \frac{V_F^2}{4\Omega}\right) - G\Omega\left(\frac{N_F}{2} + \frac{N_F}{2\Omega} - \frac{N_F^2}{4\Omega}\right)$$
(15)

that is, it can be separated into two parts, formally identical to each other. Since the second part (which corresponds to the J = 0 pairs) can be adequately described by the Q bosons b, b^+ and their number operator N, as we have already seen, it is reasonable to assume that the first part can also be described in terms of some Q bosons d, d^+ and their number operator V (with $V_F \rightarrow 2V$) satisfying commutation relations similar to equation (8):

$$[V, d^+] = d^+ \qquad [V, d] = -d \qquad dd^+ - Qd^+d = 1. \tag{16}$$

From the physical point of view this description means that a set of Q bosons is used for the J = 0 pairs and another set for the $J \neq 0$ pairs. The latter is reasonable, since in the context of this theory the angular momentum value of the $J \neq 0$ pairs is not used explicitly. The $J \neq 0$ pairs are just counted separately from the J = 0 pairs. A Hamiltonian giving the same spectrum as in equation (15), up to first-order corrections in the small parameter, can then be written as

$$H(N, V) = G\Omega([V]_Q - [N]_Q).$$
⁽¹⁷⁾

Using equation (10), it is easy to see that this expression agrees with equation (15) up to first-order corrections in the small parameter $T = -2/\Omega$.

Two comments concerning equation (17) are in order:

(i) In the classical theory states of maximum seniority (i.e. states with N = V) have zero energy. This is also holding for the Hamiltonian of equation (17) to all orders in the deformation parameter.

(ii) A landmark of the classical theory is that E(N, V) - E(N, V = 0) is independent of N. This also holds for equation (17) to all orders in the deformation parameter.

Knowing the Schwinger realization of the $SU_q(2)$ algebra in terms of q bosons [5, 6], one may wonder if the operators used here close an algebra. It is easy to see that the operators b^+d , d^+b and N - V do not close an algebra. Considering, however, the operators [29]

$$J_{+} = b^{+}Q^{-V/2}d \qquad J_{-} = d^{+}Q^{-V/2}b \qquad J_{0} = \frac{1}{2}(N-V)$$
(18)

one can easily see that they satisfy the commutation relations [29, 30]

$$[J_0, J_{\pm}] = \pm J_{\pm} \qquad J_+ J_- - Q^{-1} J_- J_+ = [2J_0]_Q.$$
⁽¹⁹⁾

Using the transformation

$$J_0 = \tilde{J}_0 \qquad J_+ = Q^{(1/2)(J_0 - 1/2)} \tilde{J}_+ \qquad J_- = \tilde{J}_- Q^{(1/2)(J_0 - 1/2)}$$
(20)

one goes to the usual $SU_q(2)$ commutation relations

$$[\tilde{J}_0, \tilde{J}_{\pm}] = \pm \tilde{J}_{\pm} \qquad [\tilde{J}_+, \tilde{J}_-] = [2\tilde{J}_0]_q \tag{21}$$

where q-numbers are defined as

$$[x]_q = \frac{q^x - q^{-x}}{q - q^{-1}} \tag{22}$$

and $q^2 = Q$.

It is clear that N + V is the first-order Casimir operator of the $U_Q(2)$ algebra formed above (since it commutes with all the generators given in equation (18)), while N - V is the first-order Casimir operator of its $U_Q(1)$ subalgebra, which is generated by J_0 alone. Therefore the Hamiltonian of equation (17) can be expressed in terms of the Casimir operators of the algebras appearing in the chain $U_Q(2) \supset U_Q(1)$ as

$$E(N, V) = G\Omega\left(\left[\frac{C_1(U_Q(2)) - C_1(U_Q(1))}{2}\right]_Q - \left[\frac{C_1(U_Q(2)) + C_1(U_Q(1))}{2}\right]_Q\right)$$
(23)

that is, the Hamiltonian has a $U_Q(2) \supset U_Q(1)$ dynamical symmetry.

In [31] a q-deformed version of the pairing theory was assumed, with satisfactory results when compared to experimental data. The present construction offers some justification for this assumption, since in both cases the basic ingredient is the modification of equation (4). It should be noticed, however, that the deformed version of equation (4) considered in [31] is different from the one obtained here (equation (14)). A basic difference is that in [31] the deformed theory reduces to the classical theory for $q \rightarrow 1$, so that q-deformation is introduced in order to describe additional correlations, while in the present formalism the Qoscillators involved for $Q \rightarrow 1$ reduce to usual harmonic oscillators, so that Q-deformation is introduced in order to attach to the oscillators the anharmonicity needed by the energy expression (equation (6)).

In the construction given above we have shown that Q bosons can be used for the approximate description of correlated fermion pairs in a single-j shell. The results obtained in the Q-formalism agree to the classical (non-deformed) results up to first-order corrections in the small parameter. However, the Q-formalism contains in addition higher-order terms. The question then arises whether these additional terms are useful or not. To answer this question, the simplest comparison with experimental data which can be made concerns the classic example of the neutron pair separation energies of Sn isotopes used by Talmi [32, 33].

In Talmi's formulation of the pairing theory, the energy of the states with zero seniority is given by [32, 33]

$$E(N)_{cl} = NV_0 + \frac{N(N-1)}{2}\Delta$$
⁽²⁴⁾

where N is the number of fermion pairs and V_0 , Δ are constants. We remark that this expression is the same as the one in equation (6), with the identifications

$$\Delta/(2V_0) = -1/\Omega \qquad \Delta = 2G \qquad N_F = 2N. \tag{25}$$

The neutron pair separation energies are given by

$$\Delta E(N+1)_{cl} = E(N+1)_{cl} - E(N)_{cl} = V_0 \left(1 + \frac{\Delta}{V_0}N\right).$$
(26)

Thus the neutron pair separation energies are expected to decrease linearly with increasing N. (Note from equation (25) that $\Delta/V_0 < 0$, since $\Omega > 0$.)

In our formalism the neutron pair separation energies are given by

$$\Delta E(N+1)_{\mathcal{Q}} = -G\Omega([N+1]_{\mathcal{Q}} - [N]_{\mathcal{Q}}) = -G\Omega Q^{N} = -G\Omega e^{TN}.$$
 (27)

Table 1. Neutron pair separation energies ΔE (in keV) for the Sn isotopes. N is the number of valence neutron pairs. Experimental data (denoted by exp) are taken from [34]. The fits obtained with equation (27) are denoted by Q, while the fits obtained with equation (26) are denoted by cl. The parameter values obtained in each fit, as well as the quality measures of equations (28), (29) are also given.

Nucleus	N	ΔE exp	∆ <i>E</i> Q	∆ <i>E</i> cl	$\ln \Delta E$ exp	ln ∆ <i>E</i> Q	$\ln \Delta E$ cl
¹⁰⁴ Sn	2	22820	22778	22277	10.035	10.029	10.000
¹⁰⁶ Sn	3	21960	21767	21503	9.997	9.985	9.966
¹⁰⁸ Sn	4	20950	20801	20728	9.950	9.940	9.931
¹¹⁰ Sn	5	19900	19878	19954	9.898	9.895	9.894
¹¹² Sn	6	18967	18995	19179	9.850	9.851	9.856
¹¹⁴ Sn	7	18046	18152	18405	9.801	9.806	9.817
¹¹⁶ Sn	8	17109	17347	17630	9.747	9.761	9.776
¹¹⁸ Sn	9	16271	16577	16856	9.697	9.716	9.733
¹²⁰ Sn	10	15592	15841	16081	9.655	9.672	9.688
¹²² Sn	11	14987	15138	15307	9.615	9.627	9.641
¹²⁴ Sn	12	14443	14466	14532	9.578	9.582	9.592
¹²⁶ Sn	13	13926	13824	13757	9.542	9.538	9.541
¹²⁸ Sn	14	13560	13210	12983	9.515	9.493	9.486
¹³⁰ Sn	15	12900	12624	12208	9.465	9.448	9.429
Т			0.0454			-0.0447	
$-G\Omega$ (keV)			23836			23718	
Δ/V_0				-0.0336			-0.0324
V_0 (keV)				23052			22766
$10^6 \sigma (\text{keV})^2$			5.18	25.30			
$10^{-3}\sigma'$ (keV) ²						2.13	9.18

Since, as we have seen, T is expected to be $-2/\Omega$, that is, negative and small, the neutron pair separation energies are expected to fall exponentially with increasing N but the small value of T can bring this exponential fall very close to a linear one.

In table 1 the neutron pair separation energies of the even Sn isotopes from ¹⁰⁴Sn to ¹³⁰Sn (i.e. across the whole sdg neutron shell) are shown. We have performed a least-squares fitting of the energies using both theories. The quality of the fit was measured by

$$\sigma = \sum_{i=1}^{n} (\Delta E_i(\exp) - \Delta E_i(\operatorname{th}))^2$$
(28)

that is, by the sum of the squares of the differences between the experimental and theoretical values. Furthermore, we have performed a least-squares fit of the logarithms of the energies, since equation (27) predicts a linear decrease of the logarithm of the energies with increasing N. In this case the quality of the fit is measured by

$$\sigma' = \sum_{i=1}^{n} (\ln \Delta E_i(\exp) - \ln \Delta E_i(\operatorname{th}))^2.$$
⁽²⁹⁾

Both fits give almost identical results. Equation (27) (in which the free parameters are $G\Omega$ and T), gives a better result than equation (26) (in which the free parameters are V_0 and Δ/V_0) for every single isotope, without introducing any additional parameter; this is an indication that higher-order terms can be useful.

One should remark, however, that ¹¹⁶Sn lies in the middle of the sdg neutron shell. If we fit the isotopes in the lower half of the shell (¹⁰⁴Sn to ¹¹⁶Sn) and those in the upper half of the shell (¹¹⁸Sn to ¹³⁰Sn) separately, we find that both theories give indistinguishably good results in both regions. Therefore Q-deformation can be understood as expressing higher-order correlations which manifest themselves in the form of particle-hole asymmetry.

We have also attempted a fit of the neutron pair separation energies of the Pb isotopes from ¹⁸⁶Pb to ²⁰²Pb. In this case both theories give indistinguishably good fits. This result is in agreement with the Sn findings, since all of these Pb isotopes lie in the upper half of the pfh neutron shell. Unfortunately, no neutron pair separation energy data exist for Pb isotopes in the lower part of the pfh neutron shell.

Concerning the values of T obtained in the case of the Sn isotopes (T = -0.0454, = -0.0447), we observe that they are slightly smaller than the value (T = -0.0488) which would have been obtained by considering the neutrons up to the end of the sdg shell as lying in a single-*j* shell. This is, of course, a very gross approximation which should not be taken too seriously. However, in the case of the Pb isotopes mentioned above, the best fit was obtained with T = -0.0276, which is again slightly smaller than the value of $T^2 = -0.0317$ which corresponds to considering all the neutrons up to the end of the pfh shell as lying in a single-*j* shell.

In conclusion, we have shown that pairing in a single-*j* shell can be described, up to first-order corrections, by two Q-oscillators, one describing the J = 0 pairs and the other corresponding to the $J \neq 0$ pairs, the deformation parameter $T = \ln Q$ being related to the inverse of the size of the shell. These two oscillators can be used for forming an $SU_Q(2)$ algebra. A Hamiltonian giving the correct pairing energies up to first-order corrections in the small parameter can be written in terms of the Casimir operators of the algebras appearing in the $U_Q(2) \supset U_Q(1)$ chain, thus exhibiting a quantum algebraic dynamical symmetry. The additional terms introduced by the Q-oscillators serve in improving the description of the neutron pair separation energies of the Sn isotopes, with no extra parameter introduced.

In [26] a generalized deformed oscillator describing the correlated fermion pairs of J = 0 exactly has been introduced. This generalized deformed oscillator is the same as the one giving the same spectrum as the Morse potential [35], up to a shift in the energy spectrum. The use of two generalized deformed oscillators for the description of J = 0 pairs and $J \neq 0$ pairs in a way similar to the one of the present work is easy, while the construction out of them of a closed algebra analogous to the $SU_Q(2)$ obtained here is an open problem. The extension of the ideas presented here to the case of the BCS theory is under investigation.

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