Pair-vibrational states in the presence of neutron-proton pairing

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Abstract

Pair vibrations are studied for a Hamiltonian with neutron-neutron, proton-proton and neutron-proton pairing. The spectrum is found to be rich in strongly correlated, low-lying excited states. Changing the ratio of diagonal to off-diagonal pairing matrix elements is found to have a large impact on the excited-state spectrum. The variational configuration interaction (VCI) method, used to calculate the excitation spectrum, is found to be in very good agreement with exact solutions for systems with large degeneracies having equal $T = 0$ and $T = 1$ pairing strengths.

Key words: N-P Pairing, Excited States, Variational Configuration Interaction Method
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1. Introduction

The collective features of many quantum systems are driven by the tendency of the constituent particles to form pairs which translates into the existence of a strong attractive pairing interaction. In atomic nuclei the correlations between pairs of nucleons give rise to pair-vibrational states which occur when nucleons are collectively excited across a gap in the single-particle spectrum [1]. The conditions for the existence of such states are level degeneracies just above and below the gap and an appropriate value for the pairing interaction strength. Given these conditions, there exist excited (pair-vibrational) states with energies substantially less than the energy required to promote a pair of nucleons across the gap. In such cases the correlation energy in the excited state is comparable to or larger than it is in the ground state.

The problem of pair vibrations has been previously studied for a Hamiltonian with like-particle pairing [1, 2]. However in systems such as nuclei with two different kinds of particles, the pairing interaction has both isoscalar ($T = 0$) and isovector ($T = 1$) components. The interaction between identical nucleons is of pure isovector character while the neutron-proton interaction has both an isoscalar and an isovector compo-

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nent. Since there is no *a priori* reason for the isoscalar pairing to vanish—empirically it is found to be of the same order as isovector pairing—both modes are present in nuclei, rendering the problem of pair vibrations in nuclei considerably more complex but also richer.

In this Letter we investigate the nature of pair-vibrational states in the presence of isoscalar and isovector pairing. Using a variational configuration-interaction (VCI) [3] method, we solve a many-body problem for neutrons and protons distributed over levels interacting through the two types of pairing with adjustable strengths. This method is tested by comparing to solvable cases and is found to be excellent for the lowest eigenstates. We then present results for more realistic choices of the strengths and parameters of the model Hamiltonian, and study the influence of these modifications on the character of the pair vibrations.

2. Model, Calculations and Results

Our Hamiltonian is [4, 5]

$$\begin{aligned} H = & \sum_{i>0} \epsilon_i \left(a_i^\dagger a_i + a_{-i}^\dagger a_{-i} + b_i^\dagger b_i + b_{-i}^\dagger b_{-i} \right) \\ & - \sum_{i,j} G_{i,j}^{T=1} \left[A_i^\dagger A_j + B_i^\dagger B_j + C_i^\dagger C_j \right] \\ & - \sum_{i,j} G_{i,j}^{T=0} \left[(M_i^\dagger M_j + N_i^\dagger N_j) \delta_{\Omega_i \Omega_j} \right] \\ & - \sum_{i,j} G_{i,j}^{T=0} \left[D_i^\dagger D_j \right], \end{aligned} \tag{1}$$

where, in the spherical limit, i denotes a single-particle state with spin projection $j_z = \pm\Omega_i$ and energy ϵ_i. In the deformed limit, i denotes a Nilsson orbital whose projection on the nuclear symmetry axis is $\pm\Omega_i$. In either case, each level i accommodates at most two neutrons and two protons. The operators $a_i^\dagger$ and $b_i^\dagger$ create a neutron (n) and a proton (p), respectively. Furthermore, the n-n and p-p pair creation operators are $A_i^\dagger = (a_i^\dagger a_{-i}^\dagger)$ and ${B_i}^\dagger = (b_i^\dagger b_{-i}^\dagger)$. The $T = 1$ n-p pair creation operator is ${C_i}^\dagger = \frac{1}{\sqrt{2}}(a_i^\dagger b_{-i}^\dagger + a_{-i}^\dagger b_i^\dagger)$ and the $T = 0$ n-p pair creation operator is ${D_i}^\dagger = \frac{i}{\sqrt{2}}(a_i^\dagger b_{-i}^\dagger - a_{-i}^\dagger b_i^\dagger)$. Also, $M_i^\dagger = (a_i^\dagger b_i^\dagger)$ and $N_i^\dagger = (a_{-i}^\dagger b_{-i}^\dagger)$. We choose the proton wave function with $j_z = 1/2$ as the negative of the equivalent neutron wave function.

In the model system that we use to elucidate the properties of pair vibrations, we take eight levels at $\epsilon = 0$ MeV and eight levels at $\epsilon = 1$ MeV. Each levels has an angular momentum $J = 1/2$ and accomodates two neutrons and two protons. Because all levels have $J = 1/2$, the $T = 0$ $M_i^\dagger$ and $N_i^\dagger$ modes play an important role in determining correlations in the wave functions and are in fact equivalent to the $A_i^\dagger$ and $B_i^\dagger$ $T = 1$ modes. We consider 16 neutrons and 16 protons here so that for zero pairing strengths the ground state has all levels filled up to the gap and the lowest pair excitations are at 2 MeV. We carry out calculations for several (off-diagonal) interaction strengths $G^{T=1} = 0.05$, 0.10, 0.15, 0.20 and 0.30 MeV. We consider three cases.

Case 1. We set $G^{T=0} = G^{T=1}$ and take equal diagonal and off-diagonal matrix elements; diagonal matrix elements refer to $i = j$ in Eq. (1) while off-diagonal ones involve $i \neq j$ interactions. It is known from the work of Flowers and Szpikowski [6] that a system of neutrons and protons, interacting through pairing with equal $T = 0$ and $T = 1$ strengths and occupying degenerate orbits, is analytically solvable because of an underlying dynamical symmetry associated with the SU(4) algebra which occurs as a subalgebra of the total n-p pair-

ing algebra SO(8). If we group the single-particle levels into two sets at different energies, we obtain a two-level SO(8) problem which is no longer analytically but still numerically solvable through the diagonalization of matrices of modest size [7, 8]. This is true for the lowest eigenstates of the pairing Hamiltonian which are of low seniority (provided the pairing force is attractive) and for which the necessary coupling coefficients [for SO(8) $\supset$ SU(4) and SU(4) $\supset$ SU$_S$(2) $\otimes$ SU$_T$(2)] are known [7]. The current problem of eight-plus-eight $J = 1/2$ levels is equivalent to a two-level SO(8) description in which each level has a spatial degeneracy of eight, *i.e.*, each level can accommodate 16 neutrons and 16 protons. Exact energies can also be obtained with the Richardson-Gaudin method for the higher-rank algebra SO(8) for non-degenerate levels with equal $T = 0$ and $T = 1$ pairing strengths [9]. These exact solutions provide a very valuable test for the approximate solutions described below.

Case 2. We again set $G^{T=0} = G^{T=1}$ but diagonal matrix elements are now 2.4 times the off-diagonal ones. Our motivation is that the increased value of the diagonal matrix elements explains the Wigner energy anomaly [5] and also the discrepancy between 'observed' single-particle gaps and those obtained from Woods-Saxon potentials in $N = Z$ nuclei [10]. In the SO(8) model of Refs. [7, 8] it is also possible to take unequal diagonal and off-diagonal pairing strengths, if only two levels are considered. However, in the current application we have 16 levels. In this case, the unequal diagonal and off-diagonal pairing strengths suggested by physical arguments, no longer permit the same solution technique as in Refs. [7, 8].

Cases 3 and 3'. We set diagonal matrix elements to be 2.4 times the off-diagonal ones and we change the relative strengths of $T = 0$ and $T = 1$ pairing, *i.e.*, in case 3 we set $G^{T=0} = 0.9 \times G^{T=1}$ and in case 3' we interchange the pairing strengths. Case 3 suggests the sorts of differences to be expected in heavier nuclei where odd-odd $N = Z$ nuclei have a 0^+ ground and a 1^+ excited state. Case 3' suggests light nuclei where the 0^+ state is not the ground state in odd-odd $N = Z$ nuclei. The energies are the same in cases 3 and 3' but the (J, T) labels of the states are interchanged.

For the even-even systems considered here, we use a variational wave function of the form

$$\Theta_i = \mathcal{P} \prod^{k} \psi^\dagger_{i,k} |0\rangle, \tag{2}$$

where $|0\rangle$ is the physical vacuum and $\psi^\dagger_{i,k}$ is a creation operator of the form

$$\begin{aligned} \psi^\dagger_{i,k} \;=\; & \Big[1 + U_i(1,k)A^\dagger_k + U_i(2,k)B^\dagger_k \\ & + U_i(3,k)C^\dagger_k + U_i(4,k)D^\dagger_k \\ & + U_i(5,k)M^\dagger_k + U_i(6,k)N^\dagger_k \\ & + U_i(7,k)W^\dagger_k\Big], \end{aligned} \tag{3}$$

with $W^\dagger_k = A^\dagger_k B^\dagger_k$. This is an extended version of the variational wavefunction used in previous studies [3, 5, 10] by virtue of the addition of the $M^\dagger_k$ and $N^\dagger_k$ terms which are needed because all j_z values are the same and these modes are collective. The operator $\mathcal{P}$ projects definite neutron number, proton number, number parity of $T = 0$ n-p pairs [5] and now also J_z. We project before carrying out the variational procedure.

The variational trial wave function, Ξ^{n+1}_m, is [3]

$$\Xi^{n+1}_m = \Phi^n_m + \Theta_{n+1}, \tag{4}$$

where Φ^n_m, the starting wave function, is

$$\Phi^n_m = \sum_{i=1}^{n} t^n_{i,m} \Theta_i, \tag{5}$$

with n the number of VCI basis states, and m the specific state (ground or excited state) that we are approximating. All Θ_i have exactly the same structure differing only in the numerical values of the amplitudes $U_i(j,k)$. Each of the fully projected states Θ_i consists of 1.108×10^{12} Slater determinants.

For case 1, we have exact results for comparison. In Table 1 we list the exact energies for case 1. The exact solutions provide valuable tests for future approximate methods. Our approximation is in extremely good agreement with the exact results over the entire range of interaction strengths. The ground state and first four excited states for even isospin T are obtained accurately for 150–200 VCI basis states. For odd isospin T, we consider only the lowest solution as it is the only one in the energy range of the four low-lying T-even excited states. The even-T ground state and the lowest T-odd state are approximated to a few keV accuracy. This seems to be a general feature of our approximate method - the lowest eigenstate for a given set of quantum numbers can be obtained more accurately than excited states having those quantum numbers. The first three even-T excited states are accurate to 10–20 keV and the fourth state to 40–50 keV for the largest values of the interaction strength and somewhat better for weaker interaction strengths. The agreement in energy is quite satisfactory and can be further improved by increasing the number of VCI configurations.

In Fig. 1 we show the spectra calculated for the four cases 1-3'. For cases 1 and 2 the four lowest excited states are degenerate, one has odd isospin and the other three have even isospin. The (J,T) assignments of these four states are (0,0), (1,1), (2,0), and (0,2). The fifth excited state is (0,0). Although the excited-state degeneracy pattern is the same for cases 1 and 2, the excitation energies of the states in the quadruplet differ substantially. This has important implications for the relation between relative $T = 0$ and $T = 1$ pairing strengths and moments of inertia. The only difference between the two cases is in the ratio of off-diagonal to diagonal matrix elements. Yet the moment of inertia, as determined by the energy difference of the first 2^+ state and the 0^+ ground state, changes by 30–40% between the two cases.

In case 3 a 10% reduction of the $T = 0$ strength from the values in case 2 leads to large changes in the excited-state spectrum and in the moment of inertia. As there are no exact solutions for guidance in this case, we can get some sense of the quality of the VCI method for excited states by comparing the energy of the $J_z = 0$ member of the J=2 multiplet with the $J_z = 2$ member of the same multiplet. The $J_z = 2$ member of the multiplet is the lowest $J_z = 2$ state and can be calculated more accurately. The $J_z = 2$ state is calculated to be roughly 10 keV below the states labelled (2,0), giving us further confidence in the VCI method for excited states. We have calculated the lowest $J_z = 2$ state for both cases 3 and 3'.

The similarity of the energies of the lowest $J = 2^+$ in case 3' and case 1 should make one cautious about inferring anything about relative $T = 0$ and $T = 1$ interaction strengths from moments of inertia as the 2^+ excitation energies depend strongly on both the relative interaction strengths and diagonal matrix element strengths. The effects of large diagonal matrix elements, when properly taken into account by including $W^\dagger$ terms, should persist to higher spins.

Not only are excitation spectra affected by these differences, ground-state correla-

Table 1: Exact energies (in MeV) for case 1.

$G^{T=0,1}$	$E_0^{T=\mathrm{e}}$	$E_0^{T=\mathrm{o}}$	$E_1^{T=\mathrm{e}}$	$E_2^{T=\mathrm{e}}$	$E_3^{T=\mathrm{e}}$	$E_4^{T=\mathrm{e}}$
0.05	−3.0146	−1.5206	−1.5206	−1.5206	−1.5206	−1.4482
0.10	−7.7112	−6.6071	−6.6071	−6.6071	−6.6071	−6.4395
0.15	−14.401	−13.299	−13.299	−13.299	−13.299	−12.526
0.20	−22.181	−20.852	−20.852	−20.852	−20.852	−19.327
0.30	−38.780	−36.902	−36.902	−36.902	−36.902	−34.189

The superscripts $T = \mathrm{e}$ and $T = \mathrm{o}$ denote T-even and T-odd states.

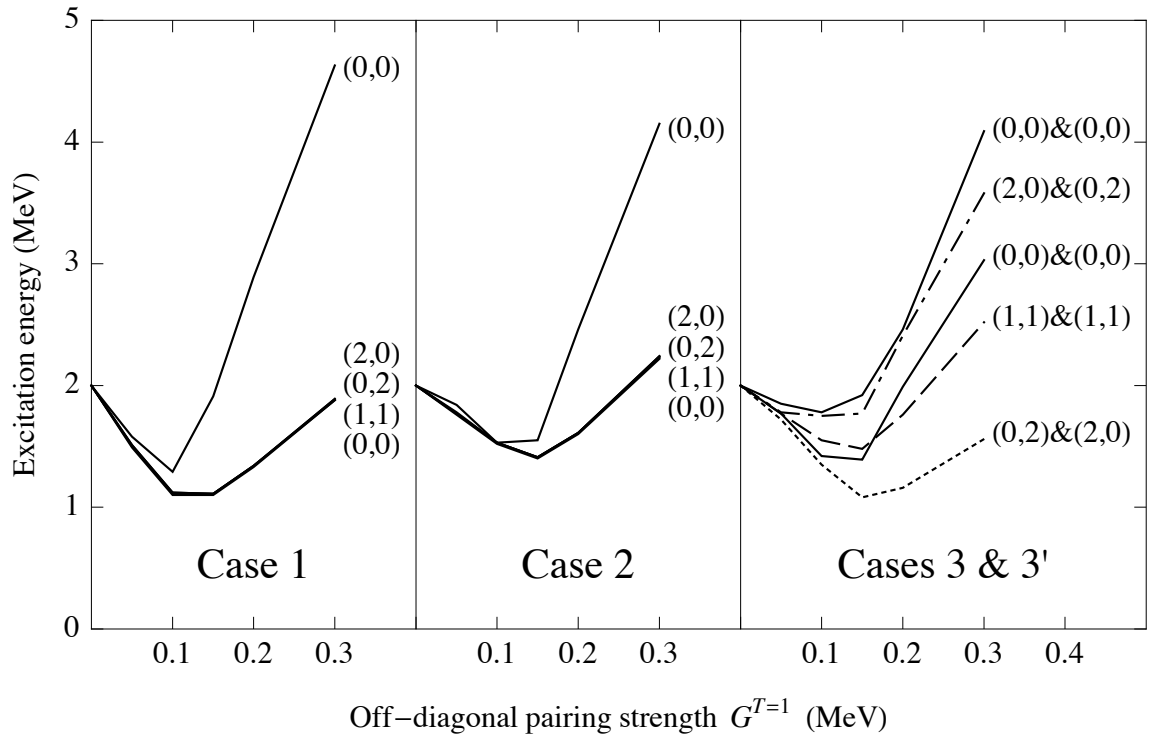

Figure 1: Excitation spectra as a function of the off-diagonal pairing strength $G^{T=1}$. The leftmost spectrum is obtained for the parameters of case 1, described in the text, the center spectrum is for case 2, and the rightmost for cases 3 and 3'. Levels are labelled with the quantum numbers (J, T).

Table 2: Off-diagonal ground-state correlation energies (in MeV).

	$A^\dagger A$	$B^\dagger B$	$C^\dagger C$	$D^\dagger D$	$M^\dagger M$	$N^\dagger N$
Case 1	1.21	1.21	1.20	1.20	1.21	1.21
Case 2	0.92	0.92	0.91	0.91	0.92	0.92
Case 3	1.07	1.07	1.06	0.61	0.62	0.62
Case 3'	0.62	0.62	0.61	1.06	1.07	1.07

Table 3: Off-diagonal correlation sums (dimensionless).

	G.S.	1∗	2∗	3∗	4∗	5∗	6∗	7∗
Case 1e	1.05	1.01	1.01	1.01	0.91	0.95	0.95	0.95
Case 1o	1.01	0.95	0.95	0.95	—	—	—	—
Case 2e	1.01	0.98	0.98	0.97	0.85	0.85	0.92	0.91
Case 2o	0.98	0.92	0.92	0.92	—	—	—	—
Case 3e	0.98	0.92	0.91	0.90	0.83	0.91	0.85	0.83
Case 3o	0.93	0.89	0.86	0.85	—	—	—	—
Case 4e	0.95	0.82	0.82	0.72	0.72	—	—	—

An asterisk denotes an excited state.

tion energies also change noticeably in going from case 1 to case 2 and differ substantially in cases 3 and 3'. In Table 2 we compare the ground-state off-diagonal correlation energies in the three cases for an off-diagonal strength $G^{T=1} = 0.1$ MeV. For example, a value of 1.21 MeV for $A^\dagger A$ means $\langle \sum_{i\neq j} G^{T=1}_{i,j} A^\dagger_i A_j \rangle = 1.21$ MeV. It is the off-diagonal correlation energy that measures the collectivity of a state. Diagonal correlation energies are typically large, whether or not a state is collective. For a Slater determinant configuration, there is no collectivity and the off-diagonal correlation energy vanishes. In our model system, the diagonal correlation energy is $24 \times (G^{T=1}_{i,i} + G^{T=0}_{i,i})$ for the Slater determinant configuration. A 10% reduction in $T = 0$ matrix elements reduces the off-diagonal $T = 0$ correlation energy in the ground state by roughly 40%. Small changes in the relative strengths are greatly amplified in the wavefunctions. If the wave functions were exact, the values for the first three entries in each line would be identical, as would be the last three.

In Table 3 we compare the sum of all off-diagonal correlation energies for the first eight T-even approximate states and the first four T-odd states for $G^{T=1} = 0.3$ for all three cases. In addition, we have included results for a system with only like-particle pairing, labeled case 4. Although we have not carried out any minimizations of the T-even states 6-8 or for T-odd states 2-4, the energies are in moderately good agreement with the exact results calculated for case 1. We choose $G^{T=1} = 0.3$ because this is the largest value for which we have carried out calculations. Collectivity persists in all of the excited states. In a system with only n-n and p-p pairing, the ground state off-diagonal correlation energy is $2G \times P(L-P)$ in the degenerate limit, where $P(= 8)$ is the number of like-particle pairs and $L(= 16)$ is the number of levels; so we have divided all correlation energy sums by $128G^{T=1}$. The correlation energy of excited states drops off somewhat faster in case 4 than in the cases with n-p pairing. This suggests that many excited states will show collective features in nuclides near the $N = Z$ line.

3. Summary

In summary, we have applied the VCI method to the pair-vibrational excited states of a Hamiltonian with $T = 0$ and $T = 1$ pairing. We find that there are at least five excited states with energies below the two-nucleon excitation energy (ı.e., pair

vibrations) over much of the range of vibrational interaction strengths. This contrasts with systems having only n-n and p-p pairing where only two low-lying pair-vibration states [2] exist. The large off-diagonal correlation energies (indicative of collectivity) of these excited states suggests that many collective states should be seen in nuclei near the $N = Z$ line. We find that the moment of inertia is very sensitive to the ratio of diagonal to off-diagonal matrix elements, as well as expectedly sensitive to the ratio of $T = 0$ to $T = 1$ interaction strengths. Comparing VCI results with exact calculations shows that the VCI method gives accurate energies for both ground and excited states, in systems with large single-particle energy level degeneracies. In a previous study [3] the method was successfully applied to systems with non-degenerate levels. The VCI method is quite general in that it does not impose any restrictions on energies or matrix elements.

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