Spurious states in quasiparticle theory

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0^+ spurious states arising due to the nonconservation of the number of particles, associated with the quasiparticle modified Tamm-Dancoff approximation method, up to the square of the number of particles operator are discussed. A procedure for eliminating the effects of these spurious states from the quasiparticle modified Tamm-Dancoff approximation basis states is prescribed and applied to structure studies of Ni isotopes employing the Kuo-Brown effective interaction, and the trends of the results thus obtained are compared with experiments and earlier calculations.

In recent works[1,2] by the authors of this Brief Report, an approach on the lines of Lipkin and Nogami and collaborators[3-7] to deal with the problem related to the nonconservation of the number of particles associated with the quasiparticle modified Tamm-Dancoff approximation (MTDA) method[8-11] for the description of low-lying states of spherical nuclei was developed and applied to the detailed structure studies of Ni isotopes. In this approach, a term $\lambda_2 N^2$ is added in the nuclear Hamiltonian in addition to the inclusion of the usual term $\lambda_1 N$ in the MTDA method. Here N represents the number of the particle operator. In literature, there exists another approach to tackle the above problem that makes use of the particle number projection method.[12,13]

Since the appearance of our papers,[1,2] where we carried out the calculations by eliminating the effects of the 0^+ spurious state arising only because of the N term (and not the N and N^2 terms) in the nuclear Hamiltonian from the MTDA basis states using the recipe of Refs. 10, 14 and 15, several requests have been privately received seeking information regarding the nature of the additional 0^+ spurious states that would arise because of the N^2 term in the nuclear Hamiltonian and the elimination of their effects from the MTDA basis states. It has now become possible for us to make available this information to a wider group of workers. A general discussion on the nature of the 0^+ spurious states arising because of the N and N^2 terms in the nuclear Hamiltonian and a procedure for eliminating their effects from the MTDA basis states is presented.

The zero-quasiparticle state is the quasiparticle vacuum $|0\rangle$ and the antisymmetric normalized two-quasiparticle state $\mathcal{A}^\dagger(abJM)|0\rangle$, in terms of the unnormalized pair creation operator $A^\dagger(abJM)$, is defined as

$$\mathcal{A}^\dagger(abJM)|0\rangle=(1+\delta_{ab})^{-1/2}A^\dagger(abJM)|0\rangle$$
$$=|abJM\rangle=\frac{1}{\sqrt{2}}[\,|a(1)b(2)JM\rangle-(-1)^{a+b-J}|b(1)a(2)JM\rangle\,]\,. \tag{1}$$

The two-quasiparticle, three-quasiparticle, and four-quasiparticle MTDA basis states containing the two-quasiparticle $J=0$ state of the type in Eq. (1) as one or more of the combinations in them require special treatment because the BCS ground state $|0\rangle$ is not an eigenstate of N and N^2. The states $N|0\rangle$ and $N^2|0\rangle$ are different from $|0\rangle$ and the spurious states thus arising are mixed with two-quasiparticle ($J=0$), three-quasiparticle ($J\neq 0$), and four-quasiparticle ($J=0$ and $J\neq 0$) MTDA basis states. One should therefore eliminate systematically and completely the effects of these spurious states from the two-, three-, and four-quasiparticle MTDA basis states before performing any actual numerical calculation. This task is achieved by first identifying the expressions for the spurious states and then constructing, by suitable linear combinations, the orthonormal set of states that are orthogonal to these spurious states using Schmidt orthogonalization procedure as described following.

One can obtain the following expressions for N and N^2 operating on $|0\rangle$ and $\mathcal{A}^\dagger(mnJM)|0\rangle$:

$$N|0\rangle=\left[\left[\sum_a [a]V_a^2\right]+A_a^\dagger\right]|0\rangle\,, \tag{2}$$

$$N^2|0\rangle=\left[\left[\sum_{ab}[ab]V_a^2V_b^2+2\sum_a[a]U_a^2V_a^2\right]+2\sum_b[b]V_b^2A_a^\dagger+2B_a^\dagger+A_a^\dagger A_b^\dagger\right]|0\rangle\,, \tag{3}$$

$$N\mathcal{A}^\dagger(mnJM)|0\rangle=\left[\left[\sum_a[a]V_a^2+U_m^2-V_m^2+U_n^2-V_n^2\right]+(A_a^\dagger+A_a)\right]\mathcal{A}^\dagger(mnJM)|0\rangle\,, \tag{4}$$

TABLE I. Calculated and experimental energy levels (MeV) of even Ni isotopes. The label LN/LN' refers to the results without/after eliminating the effects of the 0^+ spurious states arising because of the N^2 term in the nuclear Hamiltonian.

A/J^π		0^+	0_1^+	2_1^+	2_2^+	2_3^+	4_1^+	4_2^+
60	Expt.	0.0	2.29	1.33	2.16	3.12	2.50	
	LN	0.0	2.33	1.63	2.30	2.89	2.48	3.19
	LN'	0.0	2.31	1.59	2.22	2.98	2.49	3.23
62	Expt.	0.0	2.05	1.17	2.30		2.34	
	LN	0.0	2.55	1.67	2.33	2.95	2.61	3.18
	LN'	0.0	2.48	1.56	2.32	3.01	2.55	3.30
64	Expt.	0.0	2.28	1.34	2.89		2.62	
	LN	0.0	2.53	1.54	2.49	2.96	2.68	3.31
	LN'	0.0	2.50	1.48	2.60	3.14	2.66	3.40
66	Expt.	0.0						
	LN	0.0	2.41	1.40	2.69	2.82	2.70	3.29
	LN'	0.0	2.38	1.50	2.81	2.93	2.75	3.35

$$N^2\mathcal{A}^\dagger(mnJm)|0\rangle = \Big[\Big[\sum_{ab}[ab]V_a^2V_b^2+2\sum_a[a]U_a^2V_a^2-4(U_m^2V_m^2+U_n^2V_n^2)$$
$$+2\sum_a[a]V_a^2(U_m^2-V_m^2+U_n^2-V_n^2)+(U_m^2-V_m^2+U_n^2-V_n^2)^2\Big]$$
$$+2\sum_b[b]V_b^2(U_m^2-V_m^2+U_n^2-V_n^2)(A_a^\dagger+A_a)+(B_a^\dagger-B_a)$$
$$+(A_a^\dagger A_b^\dagger+A_aA_b)+2A_a^\dagger A_b\Big]\mathcal{A}^\dagger(mnJM)|0\rangle\ , \tag{5}$$

where U and V are the usual quasiparticle transformation coefficients and $[a]=(2a+1)$. The expressions in the large parentheses on the right-hand side of Eqs. (2)–(5) represent a constant multiplied by the same state that appears on the left-hand side. The operation of N (or/and N^2) should have given only the terms in the large parentheses, had there been a strict conservation of the number of particles in the quasiparticle theory. Because of nonconservation of number of particles, we get terms other than those in the large parentheses on the right-hand side of Eqs. (2)–(5) in which

$$A_a^\dagger=\sum_a[a]U_aV_a\,A^\dagger(aa00)=\sum_a C_a\mathcal{A}^\dagger(aa00)$$

and

$$B_a^\dagger=\sum_a[a]U_aV_a(U_a^2-V_a^2)A^\dagger(aa00)=\sum_a G_a\mathcal{A}^\dagger(aa00)\ ,$$

where

$$C_a=\sqrt{2[a]}U_aV_a \quad\text{and}\quad G_a=C_a(U_a^2-V_a^2)$$

create two-quasiparticle spurious states of zero angular momentum, and A_a and B_a are the corresponding destruction operators.

Case I. Elimination of the effects of spurious two-quasiparticle $J=0$ states from two-quasiparticle $J=0$ basis states. If there are n two-quasiparticle $J=0$ states $\mathcal{A}^\dagger(a_ia_i00)|0\rangle$, $i=1,2\ldots,n$, one can construct, by suitable linear combinations, a set of $(n-2)$ independent states $|\phi_1\rangle,|\phi_2\rangle,\ldots,|\phi_{n-2}\rangle$ that are orthogonal to the spurious states $A_a^\dagger|0\rangle$ and $B_a^\dagger|0\rangle$ using Schmidt orthogonalization procedure. The creation operators $Q_1^\dagger,Q_2^\dagger,\ldots,Q_{n-2}^\dagger$, which create $(n-2)$ new states $|\phi_1\rangle,|\phi_2\rangle,\ldots,|\phi_{n-2}\rangle$ and $A_s^\dagger$ and $B_a^\dagger$, are linear combinations of the original set of states $\mathcal{A}^\dagger(a_ia_i00)|0\rangle$, $i=1,2,\ldots,n$. These $(n-2)$ new nonspurious orthonormal states should be used in place of the original n states in any actual calculation.

TABLE II. $B(E2)$ values of even Ni isotopes in units of e^2F^4, where $F=10^{-13}$ cm and $e_{\text{eff}}=1.70e$ has been used.

$A/B(E2)$		2_1-0	2_2-0	2_2-2_1
60	Expt.[a]	190.0		
	LN	159.0	2.5	70.3
	LN'	170.2	1.1	97.7
62	Expt.[a]	150.0		
	LN	144.2	10.6	51.7
	LN'	146.4	6.5	76.3
64	Expt.			
	LN	142.4	1.02	27.8
	LN'	159.3	0.23	48.1
66	Expt.			
	LN	107.1	0.06	16.3
	LN'	132.6	0.01	29.2

[a]K.S. Krane, Phys. Rev. C **10**, 1197 (1974).

TABLE III. Calculated and experimental energy levels (MeV) of odd Ni isotopes.

A/J^π		$(\frac{1}{2})_1^-$	$(\frac{1}{2})_2^-$	$(\frac{3}{2})_1^-$	$(\frac{3}{2})_2^-$	$(\frac{3}{2})_3^-$	$\frac{5}{2}_1^-$	$(\frac{5}{2})_2^-$	$(\frac{7}{2})_1^-$
59	Expt.	0.47	1.30	0.0	0.89		0.34	1.19	1.34
	LN	0.64	1.69	0.0	1.63	1.80	0.52	1.86	2.10
	LN'	0.58	1.60	0.0	1.51	1.76	0.47	1.70	1.92
61	Expt.	0.28		0.0			0.07	0.91	
	LN	0.31	1.20	0.0	1.09	1.61	0.21	1.35	1.62
	LN'	0.30	1.23	0.0	1.20	1.72	0.18	1.27	1.71
63	Expt.	0.0	1.01	0.16	0.53		0.09		
	LN	0.0	1.17	0.17	0.52	1.55	0.10	1.28	1.39
	LN'	0.0	1.14	0.17	0.54	1.63	0.11	1.33	1.45
65	Expt.	0.6		0.32	0.70		0.0		
	LN	0.0	1.86	0.54	0.79	2.10	0.18	1.63	1.71
	LN'	0.0	1.91	0.43	0.78	2.13	0.10	1.68	1.80

Case II. Elimination of the effects of spurious four-quasiparticle states from the four-quasiparticle basis states. (i) For the case $J\neq 0$

$$A_a\mathcal{A}^\dagger(mnJM)|0\rangle=0$$

and

$$B_a\mathcal{A}^\dagger(mnJM)|0\rangle=0\ ,$$

and hence the four-quasiparticle states

$$A_a^\dagger\mathcal{A}^\dagger(mnJM)|0\rangle \text{ and } B_a^\dagger\mathcal{A}^\dagger(mnJM)|0\rangle$$

are entirely spurious. The nonspurious orthonormal states that are orthogonal to these spurious states may be constructed, by suitable linear combinations, using Schmidt orthogonalization procedure. (ii) For the case $J=0$, the use of nonspurious two-quasiparticle states $Q_i^\dagger|0\rangle$, $i=1,2,\ldots,n-2$, in place of $\mathcal{A}^\dagger(a_ia_i00)|0\rangle$, $i=1,2,\ldots,n$, will make $A_aQ_i^\dagger|0\rangle$ and $B_aQ_i^\dagger|0\rangle$ still zero, and hence $A_a^\dagger Q_i^\dagger|0\rangle$ and $B_a^\dagger Q_i^\dagger|0\rangle$ are entirely spurious. Besides these, there is one more $J=0$ four-quasiparticle spurious state $A_a^\dagger A_b^\dagger|0\rangle$. One can again construct, with little algebraic manipulation involving suitable linear combinations, the set of nonspurious orthonormal four-quasiparticle states of $J=0$ that are orthogonal to these spurious states (i.e., $A_a^\dagger Q_i^\dagger|0\rangle$, $B_a^\dagger Q_i^\dagger|0\rangle$, and $A_a^\dagger A_b^\dagger|0\rangle$). If the excitation is restricted to four-quasiparticles only (as is the case in the MTDA method), the effect of the spurious six-quasiparticle states $A_a^\dagger A_b^\dagger\mathcal{A}^\dagger(mnJM)|0\rangle$ may be ignored.

Case III. Elimination of the effects of spurious two-quasiparticle $J=0$ states from three-quasiparticle basis states. In this case, instead of using n three-quasiparticle states of the type $|a_i^20,b,JM\rangle$, $i=1,2,\ldots,n$, the use of $(n-2)$ nonspurious states of type $|\phi_i\rangle$, $i=1,2,\ldots,n-2$, introduced earlier, in place of $|a_i^20\rangle$, $i=1,2,\ldots,n$, eliminates the effects of the 0^+ spurious states from the three-quasiparticle basis states.

In this Brief Report we present our calculations on Ni isotopes employing the Kuo-Brown effective interaction assuming a Ni^{56} Core[16] by eliminating the effects of the 0^+ spurious states from the MTDA basis states using the prescription described above.

The quasiparticle treatment of the nuclear Hamiltonian and the essential details of the discussion regarding classification of the MTDA basis states and the calculation of the matrix elements of the quasiparticle interaction Hamiltonian (containing contributions due to the N and N^2 terms) connecting different quasiparticle MTDA basis states required for setting the energy matrix, are discussed in Refs. 1, 2, 10, and 14 and will not be repeated here. The diagonalization of the energy matrix so set for a given spin and parity in the MTDA basis space of zero-, two-, and four-quasiparticles for even Ni isotopes and in the MTDA basis space of one- and three-quasiparticles for odd Ni isotopes, gives eigenvalues and eigenfunctions.

The numerical calculations for Ni isotopes, as mentioned earlier, are carried out by using the effective matrix elements of Kuo and Brown[16] assuming Ni^{56} to be an inert core and distributing active neutrons among $2p_{3/2}$, $1f_{5/2}$, and $2p_{1/2}$ single-particle orbitals. Since the earlier calculations[1,2] using these matrix elements have already been made for Ni isotopes, we wish to therefore

TABLE IV. Magnetic moments of odd Ni isotopes in nuclear Bohr magneton μ_N.

	59		61		63		65	
J^π/A	*LN*	*LN'*	*LN*	*LN'*	*LN*	*LN'*	*LN*	*LN'*
$\frac{1}{2}^-$	0.69	0.70	0.69	0.70	0.68	0.69	0.67	0.68
$\frac{3}{2}^-$	−1.76	−1.73	−1.66	−1.62	−1.59	−1.56	−1.57	−1.53
$\frac{5}{2}^-$	1.36	1.35	1.38	1.40	1.40	1.42	1.40	1.42

TABLE V. Values of the reduced transition strength $B(M1)$ and $B(E2)$ for odd Ni isotopes. $B(M1)$ values are in units of μ_N^2 and $B(E2)$ values are in units of $e_{\text{eff}}^2/\alpha^2$, where e_{eff} is the effective charge of the neutron and $\alpha = M\omega/\hbar$ is the harmonic oscillator parameter.

Reduced transition strength	59		61		63		65	
	LN	LN'	LN	LN'	LN	LN'	LN	LN'
$B(M1\frac{1}{2}^- - \frac{3}{2}^-)$	1.90	2.95	1.83	2.90	1.81	2.86	1.97	3.01
$B(M1\frac{3}{2}^- - \frac{5}{2}^-)$	0.01	0.03	0.012	0.036	0.015	0.041	0.015	0.040
$B(E2\frac{1}{2}^- - \frac{3}{2}^-)$	0.52	0.90	0.042	0.081	0.92	2.01	3.60	7.72
$B(E2\frac{3}{2}^- - \frac{5}{2}^-)$	0.24	0.51	0.051	0.085	0.03	0.065	0.021	0.052

report here the results showing the effect of systematically and completely eliminating the effects of the 0^+ spurious states arising because of the term N^2 using the prescription described above and comparing the results thus obtained with the corresponding ones of Refs. 1 and 2, where these effects were not eliminated. The present results may therefore be analyzed/viewed with this underlying spirit in mind.

The results of the present calculations labeled as LN', are shown in Tables I–V along with the corresponding results of Refs. 1 and 2, labeled as LN, and the available experimental values for the purpose of comparison. it is clear from Tables I and III that the LN' results for the energy levels, on the whole, are much closer to the LN results, and the small shifts in the LN' results, in general, favor in bringing the agreement even closer to the experimental values, thereby indicating that the elimination of the effects of the 0^+ spurious states arising because of the N^2 term in the nuclear Hamiltonian does indeed play a positive role. It may not be unsuitable to comment that the LN' results may be looked upon as a calculation which in a sense is two steps ahead of the earlier MTDA results shown in Refs. 1 and 2 in improving the agreement with the experimental values. It is important to mention here that the total percentage admixture of the four-quasiparticle/three-quasiparticle states in the two wave functions LN' and LN is not much different and agrees in most of the cases within only a few percent, although the variations in the percentage composition of the individual components sometimes are quite appreciable. Such constituent differences in the wave functions are insensitive to the calculation of magnetic moments (Table IV) but are quite sensitive to the calculation of transition strengths (Tables II and V). It will therefore be desirable to compare Tables II and V (and also Table IV) with experiment as data become available.

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