Conservation of the Number of Particles in the Tamm-Dancoff Approximation for Spherical Superconductor Nuclei

P. L. OTTAVIANI
Centro di Calcolo del Comitato Nazionale per l'Energia Nucleare, Bologna, Italia
AND
M. SAVOIA
Istituto di Fisica dell'Università di Bologna, Bologna, Italia and
Istituto Nazionale di Fisica Nucleare, Sezione di Bologna, Bologna, Italia

(Received 16 September 1968)

A modified Tamm-Dancoff approximation for spherical superconductor nuclei is formulated. The approximation consists in diagonalizing the nuclear Hamiltonian in the space spanned by the components of zero- and two-quasiparticle excitations corresponding to a fixed particle number ("projected states"). Thus, spurious states arising from the Bogoliubov-Valatin canonical transformation, which are present in the usual Tamm-Dancoff approximation, are completely eliminated. Matrix elements between "projected states" are evaluated by the Bayman projection method of the generating functions. The model is applied to the calculation of the low-lying excited states of the tin isotope with $A=116$, and the results are compared with the corresponding ones obtained in the Tamm-Dancoff approximation. Our conclusion is that the effect of the particle-number nonconservation is important mainly for the energies of the highest levels. This becomes particularly clear for the $J=0$ case.

1. INTRODUCTION

IT is well known[1] that the Tamm-Dancoff approximation (TDA) for spherical superconductor (even-even) nuclei consists in diagonalizing exactly the Hamiltonian of the system in the space of the two-quasiparticle (qp) elementary excitations. The idea is that higher excitations (four- and more-qp) can be neglected, since to excite a single qp we need at least an amount of energy equal to the gap (which is of the order of 1 MeV for nuclei like tin isotopes). In spite of its simplicity, this model appears quite good for treating low-lying excited states of the so-called vibrational nuclei.[2,3] In fact, recent calculations,[3–5] which also take four-qp excitations into account, show that at least the lowest-lying vibrational states can be considered as almost pure linear combinations of two-qp excitations. Of course, this is untrue for higher energy states.

Formally, the standard TDA presents all the advantages resulting from the BCS theory of superconductivity, in which excited states of a N_0-nucleon system are treated as few-qp states. On the other hand, its main disadvantage is that the resulting states do not conserve the number of particles. This fact is more dangerous for excited states than for the ground state. In fact, for the excited states the nonconservation of the particle number introduces spurious components. Take, for instance, the state $\hat{N}\,|\,\Psi_0\rangle$, where $|\,\Psi_0\rangle$ is the BCS state. It is different from $N_0\,|\,\Psi_0\rangle$ (N_0 is the correct number of nucleons) and its component in the space of the excitations built up by two qp's coupled to an angular momentum $J=0$ is spurious. This well-known 0^+ state, which dramatically affects the physical properties, can be eliminated by simple methods before diagonalizing the Hamiltonian.[3–6] However, this is not the only spurious state; other spurious components arise from the successive powers of the particle number operator. Their complete elimination by standard methods is practically impossible, and their effects on the physical properties are unknown (for a complete description of the spurious states of higher order, see Ref. 7).

In order to eliminate the aforementioned difficulty it is important to formulate an approximation with the property of conserving the number of particles without losing the formal and physical advantages of a model built on the BCS theory of superconductivity. With this in mind, we propose a model, which we call the projected Tamm-Dancoff approximation (PTDA). In this model we shall diagonalize the Hamiltonian in the space spanned by the two-qp excitation components with a particle number equal to the effective valence-nucleon number. This is very similar to the procedure applied by Macfarlane[8] to the study of states of even Ni isotopes. Only the technique of picking out components with a fixed number of particles is completely different.

2. PROPOSED MODEL

Our starting point is to find "generating functions"[9] $|\,\psi(z)\,\rangle$ and $|\,\psi_{JM}(aa';z)\,\rangle$ defined as

$$|\,\psi(z)\,\rangle=\sum_p z^p\,|\,\psi_{2p}\rangle \qquad (1)$$

[1] M. Baranger, Phys. Rev. **120**, 957 (1960).
[2] R. Arvieu, E. Baranger, M. Baranger, M. Veneroni, and R. Gillet, Phys. Letters **4**, 119 (1963); R. Arvieu, E. Salusti, and M. Veneroni, *ibid.* **8**, 334 (1964).
[3] P. L. Ottaviani, M. Savoia, J. Sawicki, and A. Tomasini, Phys. Rev. **153**, 1138 (1967); P. L. Ottaviani, M. Savoia, and J. Sawicki, Phys. Letters **24B**, 353 (1967); Nuovo Cimento **56B**, 149 (1968).
[4] L. S. Hsu and J. B. French, Phys Letters **19**, 135 (1965); L. S. Hsu, Nucl. Phys. **A96**, 624 (1967).
[5] M. K. Pal, Y. K. Gambhir, and Ram Raj, Phys. Rev. **155**, 1144 (1967); **163**, 1004 (1967).
[6] T. T. S. Kuo, E. Baranger, and M. Baranger, Nucl. Phys. **79**, 513 (1966).
[7] M. Gmitro, A. Rimini, J. Sawicki, and T. Weber, International Atomic Energy Agency Report No. IC/68/29, Trieste (unpublished).
[8] M. H. Macfarlane, *Lectures in Theoretical Physics* (University of Colorado Press, Boulder, Colo., 1966), p. 583.
[9] B. F. Bayman, Nucl. Phys. **15**, 33 (1960); J. Högaasen-Feldman, Nuovo Cimento **29**, 428 (1963); K. Dietrich, H. J. Mang, and J. H. Pradal, Phys. Rev. **135**, 22 (1964).

TABLE I. Excitation energies (in MeV) for Sn^{116} calculated in TDA and PTDA. Numbers in parentheses denote percentage weights of components, with fixed nucleon number ($2p=16$), of states calculated in TDA.

$J=0^+$		$J=2^+$		$J=4^+$	
TDA	PTDA	TDA	PTDA	TDA	PTDA
0.0 (36)	0.0	1.61 (37)	1.54	2.45 (36)	2.63
1.63 (46)	1.51	2.30 (39)	2.41	2.89 (36)	3.17
2.35 (32)	2.92	2.42 (39)	2.54	3.23 (27)	3.64
2.89 (32)	3.55	3.03 (26)	3.56	3.39 (26)	3.80
4.83 (25)	5.77	3.28 (26)	3.89	3.45 (36)	4.04

and

$$|\psi_{JM}(aa';z)\rangle=\sum_p z^{p+1}|\psi_{2p,JM}(aa')\rangle, \quad (2)$$

respectively. Here, $|\psi_{2p}\rangle$ and $|\psi_{2p,JM}(aa')\rangle$ are components (not normalized), which correspond to a fixed number of particles equal to $2p$, of the BCS state and of two-qp excitations coupled to JM, respectively. We shall call these components "projected states" ("projected BCS state" and "projected two-qp states," respectively).

The functions (1) and (2) have the property that matrix elements between projected states of any operator O preserving the number of particles can be derived from the matrix elements between corresponding generating functions, apart from an identical constant factor, by using the equations

$$\langle\psi_{2p}|\hat{O}|\psi_{2p}\rangle=\oint dz\, z^{-2p-1}\langle\psi(z)|\hat{O}|\psi(z)\rangle, \quad (3)$$

$$\langle\psi_{2p}|\hat{O}|\psi_{2p,JM}(aa')\rangle=\oint dz\, z^{-2p-2}\langle\psi(z)|\hat{O}|\psi_{JM}(aa';z)\rangle, \quad (4)$$

$$\langle\psi_{2p,JM}(bb')|\hat{O}|\psi_{2p,J'M'}(aa')\rangle=\oint dz\, z^{-2p-3}\langle\psi_{JM}(bb';z)|\hat{O}|\psi_{J'M'}(aa';z)\rangle, \quad (5)$$

where the contour of integration includes the origin.

The generating functions can be constructed immediately in terms of creation and annihilation operators for nucleons ($c_\alpha^\dagger$ and c_α, respectively, where α designates all the quantum numbers which characterize a single-particle shell-model state, namely, $\alpha\equiv\tau_\alpha$, n_α, l_α, j_α, $m_\alpha=a$, m_α, where the meanings of the symbols are obvious). In fact, it is immediately seen that

$$|\psi(z)\rangle=\prod_{\alpha>0}(u_\alpha+s_\alpha z v_\alpha c_\alpha^\dagger c_{-\alpha}^\dagger)|0\rangle, \quad (6)$$

$$|\psi_{JM}(aa';z)\rangle=n_J(aa')\sum_{m_\alpha m_{\alpha'}}(j_\alpha j_{\alpha'};m_\alpha m_{\alpha'}|JM)\times(u_{\alpha'}zc_{\alpha'}^\dagger-s_{\alpha'}v_{\alpha'}c_{-\alpha'})(u_\alpha zc_\alpha^\dagger-s_\alpha v_\alpha c_{-\alpha})|\psi(z)\rangle. \quad (7)$$

Here $n_J(aa')=[1+(-)^J\delta_{aa'}]^{1/2}$, and u_a and v_a are the usual BCS coefficients with $u_a^2+v_a^2=1$; $s_\alpha=(-)^{j_\alpha-m_\alpha}$ and $-\alpha=a$, $-m_\alpha$. Matrix elements of the Hamiltonian between these functions can be constructed without any difficulty. We start by defining a new set of creation and annihilation operators through a z-dependent canonical transformation:

$$d_\alpha^\dagger=(u_\alpha c_\alpha^+-s_\alpha z v_\alpha c_{-\alpha})/(u_\alpha^2+z^2v_\alpha^2)^{1/2},$$
$$d_\alpha=(u_\alpha c_\alpha-s_\alpha z v_\alpha c_{-\alpha}^\dagger)/(u_\alpha^2+z^2v_\alpha^2)^{1/2}. \quad (8)$$

The generating function $|\psi(z)\rangle$ is the vacuum for these operators, and $|\psi_{JM}(aa';z)\rangle$ can be rewritten as

$$|\psi_{JM}(aa';z)\rangle=n_J(aa')\frac{z^2D_{JM}^\dagger(aa')-\delta_{J0}\hat{j}_a u_a v_a z(z^2-1)}{(u_a^2+z^2v_a^2)^{1/2}(u_{a'}^2+z^2v_{a'}^2)^{1/2}}|\psi(z)\rangle, \quad (9)$$

where

$$D_{JM}^\dagger(aa')=\sum_{m_\alpha m_{\alpha'}}(j_a j_{a'};m_\alpha m_{\alpha'}|JM)d_{\alpha'}^\dagger d_\alpha^\dagger \quad (10)$$

and $\hat{j}_a=(2j_a+1)^{1/2}$.

Transformation of the Hamiltonian in terms of $d_\alpha^\dagger$ and d_α operators is also very easy. All we have to do is to observe that the transformation (8) is perfectly equivalent to a Bogoliubov-Valatin canonical transformation if we change u_a into $u_a(u_a^2+z^2v_a^2)^{-1/2}$ and v_a into $zv_a(u_a^2+z^2v_a^2)^{-1/2}$. Obviously, $d_\alpha^\dagger$ and d_α operators reduce for $z=1$ to creation and annihilation operators for quasiparticles of the BCS theory. The trick consists in simply taking the Hamiltonian that one obtains after the Bogoliubov-Valatin transformation and before the "elimination of the dangerous terms" (with the chemical potential put equal to zero) and in changing u_a into $u_a(u_a^2+z^2v_a^2)^{-1/2}$ and v_a into $zv_a(u_a^2+z^2v_a^2)^{-1/2}$. Terms of the Hamiltonian transformed according to the Bogoliubov-Valatin transformation are given, for example, in Refs. 1 and 3.[10]

Using the Hamiltonian transformed according to Eqs. (8), the expression (9), and the property

$$d_\alpha|\psi(z)\rangle=0, \quad (11)$$

[10] Care must be taken in the different definitions of the antisymmetrized particle-particle and particle-hole matrix elements of the interaction used in Refs. 1 and 3; namely, we have $g_J(abcd)=-4G(abcdJ)$ and $f_J(abcd)=-4F(abcdJ)$.

it is very easy to construct matrix elements of the Hamiltonian between generating functions and from these, by Eqs. (3)–(5), to derive matrix elements between corresponding "projected states" through integrations in the complex plane.

Of course, for $J\neq 0$, "generating functions" (9) are orthogonal to each other; consequently, the corresponding "projected two-qp states" are also mutually orthogonal and can be taken directly as a good basis on which to diagonalize the Hamiltonian.

The situation is different for $J=0$. In this case, generating functions $|\psi(z)\rangle$ and $|\psi_{00}(aa;z)\rangle$, and hence projected states also, are no longer orthogonal to each other and we have to build an independent and orthonormal basis set from the projected states $|\psi_{2p}\rangle$ and $|\psi_{2p,00}(aa)\rangle$ through a Schmidt procedure. In principle, this is a simple procedure since, by Eqs. (3)–(5), we can express all scalar products between "projected states" in terms of calculable integrals in the complex plane. We have to make sure that, if there are n "projected two-qp states" corresponding to an n-subshell problem, only $n-1$ are independent of each other. In fact, it is immediately seen that

$$\sum_a \hat{j}_a u_a v_a \,|\,\psi_{2p,00}(aa)\rangle = 0. \tag{12}$$

After building the basis vectors as linear combinations of $|\psi_{2p}\rangle$ and of $n-1$ among the n "projected two states," we can construct, by Eqs. (3)–(5), matrix elements of the Hamiltonian in the space spanned by the vectors so obtained. Collective 0^+ states will be obtained in this model by diagonalization of this matrix.

3. NUMERICAL RESULTS AND CONCLUSIONS

Numerical applications have been performed for a tin isotope with $A=116$. This nucleus has a half-filled shell and hence the effects of nonconservation of the particle number must be particularly important. We have used a conventional finite-range residual force, namely, a Gaussian force:

$$V(1,2) = -V_0 \exp[-(r_{12}/r_0)^2](\hat{P}_s + t\hat{P}_t), \tag{13}$$

where $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$ and $\hat{P}_s$ and $\hat{P}_t$ are the singlet-even and triplet-odd projection operators. The parameters are fixed at $V_0=31.0$ MeV, $r_0=2.0$ fm and $t=-0.555$ (a Rosenfeld force). The five single-particle subshells we consider are $2d_{5/2}$, $1g_{7/2}$, $3s_{1/2}$, $2d_{3/2}$, $1h_{11/2}$. The neutrons and protons in subshells other than the above ones are considered as an inert core. We keep single-neutron energies as in Table (5a) of Ref. 6, $E_{5/2}{}^0=-2.45$, $E_{7/2}{}^0=-1.95$, $E_{1/2}{}^0=0.0$, $E_{3/2}{}^0=0.80$ and $E_{11/2}{}^0=1.25$ MeV. The unperturbed single-nucleon wave functions are of a harmonic-oscillator potential as given in Ref. 6. The assumed range parameter of the harmonic-oscillator wave functions is $\nu^{1/2}=(M\omega_0/\hbar)^{1/2}=0.454\ \text{fm}^{-1}$. The BCS solutions for the coefficients u_a and v_a of the Bogoliubov-Valatin transformation and the single-qp energies corrected by self-energy terms are determined consistently with the residual interaction used.

In Table I, we give results for the excitation energies (in MeV) of the 0^+, 2^+, and 4^+ lowest-lying levels. The first column refers to TDA calculations (with the 0^+ spurious state projected out) and the second one to the corresponding PTDA calculations. Numbers in parentheses denote percentage weights of components, with nucleon number equal to 16, of states calculated in TDA. For simplicity in both cases, we have taken the lowest 0^+ state at zero energy. Actually, the effect of nonconservation of the particle number lowers the ground-state energy in PTDA by an amount of 0.82 MeV with respect to the BCS energy. This seems in qualitative agreement with the results obtained by Dietrich *et al.*[9] and by Bang *et al.*[11] The difference between the ground-state energy in PTDA and the energy of the BCS component corresponding to $2p=16$ is very little and negligible (0.07 MeV in our case). Experimental values are not given since, for reproducing the experimental data, a better parametrization of the single-particle states and, in some cases, mixing of higher excitations are certainly necessary.[12] Through these results, we only want to compare TDA calculations with the corresponding ones of PTDA, in order to decide whether the effects on the energy spectrum arising from nonconservation of the number of particles are important or not. From Table I it can be seen that the effect of the spurious components is more important for higher stages. This general trend assumes relevance for the $J=0$ case, as we can expect, since we know that the spuriousness due to the particle number nonconservation affects especially 0^+ states.

ACKNOWLEDGMENT

We are greatly indebted to Professor J. Sawicki for illuminating discussions.

[11] J. Bang, J. Krumlinde, and S. G. Nilsson, Phys. Letters **15**, 55 (1965).

[12] Calculations taking into account these effects are in progress.