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Application of Linear Response Theory to Light Odd – A Nuclei in s-d Shell

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Microscopic calculations have been performed for light s-d shell nuclei using the linear Response Theory (LRT), in which the odd-A nuclear wave function is built on the even even (A-I) Hartree-Fock-Bogoliubov solution. The variational pararneters are obtained by solving the linearized equations. The pairing plus quadrupole force has been used as residual interaction. Calculated BE, Q_J and $B(E2)$ values agree fairly well with available experimental data.

Cálculos microscópicos foram realizados para núcleos leves de camadas s-d, usando-se a teoria da resposta linear, em que a função de onda nuclear para A ímpar é construida sobre a solução de Hartree-Fock-Bogoliubov para par-par (A-I). Os parâmetros variacionais são obtidos resolvendo-se as equações linearizadas. A força de "pairing" mais quadrupolo foi usada como interação residual. Os valores calculados para energia de ligação Q_J é B(E~) estão em bom acordo com a experiência.

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1. INTRODUCTION

Satisfactory microscopic calculation for odd nuclei is a difficult problem. This is evident from the fact that there exist relatively few odd-A calculations in contrast to vast abundance of calculations for even-even nuclei. Hartree-Fock-Bogoliubov (HFB) method is one of the microscopic methods which is widely used in the calculations of even-even nucleus. But satisfactory adoptation of HFB method for odd nuclei is both difficult and rare. Only a few HFB calculation for odd nuclei has been done so far[1-4]. In the earlier attempts[1], the mixing of one and three quasiparticle states were suppressed for numerical simplicity. As a result, the blocking effect in the core is neglected and there is a loss of correct expectation value of particle number for the one quasiparticle state. Hence a method which is free from theore ical encumbrances and numerically simple is desirable.

In this paper we investigate the ground state properties of some light odd nuclei within the framework of Linear Response Theory (LRT)[5]. In this method the wave function of the odd-A nucleus is written as an "ansatz" built on the ground state wave function of the neighbouring even-even nucleus such that the extra particle may induce a general reshuffling of the Bogoliubov transformation of theeven-even core nucleus. We selected HFB ground state for even system as our starting point for LRT calculation. In ref(5) LRT method was applied to the pseudo nuclear but exactly soluble Lipkin model with spectacular success, however an application to the realistic nuclear problem has not been made so far.

'2. THEORY

We start with the HFB ground state wavefunction of the neighbouring even-even (A-1) nucleus and add one extra particle to it. The extra particle may go to one of the unoccupied levels or may even reshuffle the active particles of the (A-1) even-even core. The Thouless Theorem[6] states that the most general quasiparticle vacuum $|\phi'>$ which is not orthogonal to $|\phi_0>$ can be written in the form

(1)

Thus this is a convenient way to introduce new quasiparticle operators (which is assumed to be the result of addition of the extra particle) for which $|\phi_-'>$ is the new quasiparticle vacuum. We write the trial wavefunction for the odd system as

$$|\psi_\alpha> = \exp(s_\alpha)\beta_\alpha^\dagger|\phi_0> \tag{2}$$

where

$$S_\alpha = 1/2 \sum_{\mu\nu} C_{\mu\nu}^{(\alpha)}\beta_\mu^\dagger\beta_\nu^\dagger - \text{h.c.} \tag{3}$$

, and β_μ^+ are the quasiparticle creation operators corresponding to even--even core. The state a is then blocked. $|\phi_0>$ is the HFB ground state of the neighbouring (A-1) even-even nucleus which also happens to be the vacuum for β_μ. $C_{\mu\nu}^{(\alpha)}$ are variational parameters. The exponential factor in equation (2) incorporates the possibility that the quasiparticles of the even-even core may themselves be modified due to the addition of another particle. $C_{\mu\nu}^{(\alpha)}$'s are expected to be small since addition of the last particle is unlikely to reshuffle the core drastically. With $C_{\mu\nu}^{(\alpha)} = 0$ one recovers the one quasiparticle state built on the even-even HFB ground state. The Hamiltonian of the many body system is written as

$$H = \sum_{ij} \varepsilon_{ij} a_i^\dagger a_j + 1/4 \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k \tag{4}$$

where $a_i^\dagger$ is the particle creation operator. The variation pararneters $C_{\mu\nu}^{(\alpha)}$ are deterrnined by the minization of $<\hat{H}>$ subjects to the restriction that $<\hat{N}>$ has the correct value. This is done by minimizing $<\hat{H}''> =$ $= <\hat{H}-\lambda_{N+1}\hat{N}>$ with respect to $C_{\mu\nu}^{(\alpha)}$. Lagrange multiplier λ_{N+1} (chemical potential) is determined from

$$<\psi_\alpha|\hat{N}|\psi_\alpha> = A \text{ (odd number)} \tag{5}$$

We follow the notations of ref. (5)

The equation for $C_{\mu\nu}^{(\alpha)}$ are

$$\sum_{\mu'\nu'} \left(X^{(\alpha)}_{\mu\nu\mu'\nu'} C^{(\alpha)}_{\mu'\nu'} + Y^{(\alpha)}_{\mu\nu\mu'\nu'} C^{(\alpha)*}_{\mu'\nu'} \right) = -Z^{(\alpha)} - V^{(\alpha)} (C^{(\alpha)} \cdot C^{(\alpha)*}) \quad (6)$$

where

$$X^{(\alpha)}_{\mu\nu\mu'\nu'} = 1/2 \langle \phi_\alpha | H'' \beta_\nu \beta_\mu \beta^\dagger_{\mu'} \beta^\dagger_{\nu'} | \phi_\alpha \rangle + 1/2 \langle \phi_\alpha | \beta_\nu \beta_\mu \beta^\dagger_{\mu'} \beta^\dagger_{\nu'} H'' | \phi_\alpha \rangle -$$

$$- \langle \phi_\alpha | \beta_\nu \beta_\mu H'' \beta^\dagger_{\mu'} \beta^\dagger_{\nu'} | \phi_\alpha \rangle \quad (7)$$

$$Y^{(\alpha)}_{\mu\nu\mu'\nu'} = -1/2 \langle \phi_\alpha | \beta_\nu \beta_\mu \beta_{\nu'} \beta_{\mu'} H'' | \phi_\alpha \rangle \quad (8)$$

$$Z^{(\alpha)}_{\mu\nu} = \langle \phi_\alpha | \beta_\mu \beta_\nu \hat{H}'' | \phi_\alpha \rangle \quad (9)$$

where $|\phi_\alpha\rangle = \beta^\dagger_\alpha |\phi_0\rangle$

Since $C^{(\alpha)}_{\mu\nu}$ is expected to be small, this equation is then linearized by writing

$$C^{(\alpha)}_{\mu\nu} = C^{(\alpha,1)}_{\mu\nu} + C^{(\alpha,2)}_{\mu\nu} + \ldots \quad (10)$$

sucessive terms on right side being of successive order.

To the lowest order in C, one obtains

$$\begin{pmatrix} X^{(\alpha)}_{\mu\nu\mu'\nu'} & Y^{(\alpha)}_{\mu\nu\mu'\nu'} \\ Y^{(\alpha)*}_{\mu\nu\mu'\nu'} & X^{(\alpha)*}_{\mu\nu\mu'\nu'} \end{pmatrix} \begin{pmatrix} C^{(\alpha,1)}_{\mu'\nu'} \\ C^{(\alpha,1)*}_{\mu'\nu'} \end{pmatrix} = - \begin{pmatrix} Z^{(\alpha)}_{\mu\nu} \\ Z^{(\alpha)*}_{\mu\nu} \end{pmatrix} \quad (11)$$

This process can be generalized to higher orders for which only the right side changes, left side remaining the same. The energy of the system is given by

$$E_{LRT} = \frac{\langle \psi_\alpha | H | \psi_\alpha \rangle}{\langle \psi_\alpha | \psi_\alpha \rangle} = H_0 + (H_{11})_{\alpha\alpha} - 1/2 \sum_{\mu\nu} (Z^{(\alpha)}_{\mu\nu} C^{(\alpha)*}_{\mu\nu} + Z^{(\alpha)*}_{\mu\nu} C^{(\alpha)}_{\mu\nu}) \quad (12)$$

where H_0 and H_{11} are the matrix part of $\hat{H}_0$ and $\hat{H}_{11}$ of H (when expressed in terms of quasiparticle operators of the even even Core .

The quadrupole moment (Q_0) and the expectation value of number operator (@ can be written in a similar way as follows.

$$Q_0 = Q_0 + (Q_{11})_{\alpha\alpha} + \sum_{\substack{\mu\nu \\ (\neq\alpha)}} (Q_{20})_{\mu\nu} C^{(\alpha)}_{\mu\nu} + \text{c.c.} \tag{13}$$

$$N = N_0 + (N_{11})_{\alpha\alpha} + \sum_{\substack{\mu\nu \\ (\neq\alpha)}} (N_{20})_{\mu\nu} C^{(\alpha)}_{\mu\nu} + \text{c.c.} \tag{14}$$

3. RESULTS

The numerical calculations have been perforined for some odd mass nuclei in the *s-d* shell. We restricted our model space tothe complete Is, Ip and 2s-Id shells open to all nucleons in the nucleus chosen. The single particle energies are chosen to coincide with those of Nilsson[7] for zero deformation. The residual interaction has been chosen to be the pairing plus quadrupole force of Baranger and Kumar[8]. Although it is not customary to use this interaction in the s-d shell nuclei, we havechosen itfor itssimplicity. Furthermore HFB calculations for C^{12} and Si^{28} using this residual force has yielded reasonable results as compared with experiment[9,10]. This has encouraged us to use this simple interaction more exhaustively. Fair agreement between calculations in the present work and experimental result further underlines the usefulness of this simple interaction beyond its usually accepted domain. Because of the known importance of the neutron-proton pairing in the light nuclei, we include such term also in the usual form of pairing plus quadrupole force, although customarily these are dropped in the rare-earth region. The total Hamiltonian is thus

$$H = \sum_i \varepsilon_i a_i^\dagger a_i + 1/2 \sum_{\tau_3\tau_3'} Q_{\tau_3\tau_3'} \sum_{\substack{u=-2 \\ ijkl}}^{+2} Y^{2\mu}_{ij} a_l^\dagger a_i^\dagger a_j a_k$$
$$+ 1/4 \sum_{\tau_3\tau_3'} G_{\tau_3\tau_3'} \sum_{ij>0} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j \tag{15}$$

The parameters $Q_{\tau_3\tau_3'}$ and $G_{\tau_3\tau_3'}$ are fixed in the following fashion. We perform a cranked HFB (CHFB) calculation for Ne^{20} and choose the values of $Q_{\tau_3\tau_3'}$ and $G_{\tau_3\tau_3'}$ so as to get the best overall agreement of the calculated members of the ground state rotational band with the experimental ones. This set of parameters are kept fixed for all the nuclei investigated. The values adopted for these parameters are

$$Q_{pp} = Q_{nn} = Q_{np} = Q_{pn} = -0.550 \text{ MeV}$$

$$G_{nn} = G_{pp} = -0.325 \text{ MeV}, \quad G_{np} = G_{pn} = -0.17 \text{ MeV}$$

For each odd nucleus we perform a CHFB calculations for the ground state of the even-even (A-l) nucleus. The Bogoliubov transformation is restricted to mix particles and holes of a given kind and parity only. Effect of neutron proton pairing in the Hamiltonian is taken by surnming appropriate terms over both parity states of neutron and proton in the pairing potential A. Since the HFB equations are solved iteratively for each parity state of proton and neutron separately, the sum in the pairing potential is obtained from the solutions or the previous iteration (for other isospin-parity states). This will lead to the correct treatrnent when self-consistency is achieved. The energy scale $\hbar\omega$ is ajusted to fit the first 2^+ states of the even-even nucleus. With the energy scale $\hbar\omega$ and with no other free parameters, we calculate the matrices $X^{(\alpha)}$, $Y^{(\alpha)}$ and $Z^{(\alpha)}$ and solve the LRT equations for $C^{(\alpha)}$. The calculations are repeated for various blocked state a . The particular one resulting in the lowest value of energy is chosen as the ground state. Both energy and intrinsic quadrupole moment (Q_0) of the ground state have been calculated.

For calculation of binding energy *(BE)* we need a constant single particle well depth (V_0) which is determined from the HFB calculation for a neighbouring even-even nucleus and kept fixed for several neighbouring nuclei. The result of our calculation are presented in Table 1. Since the Hamiltonian chosen does not involve the Coulomb interaction between the protons we compare the calculated *BE* with the experimental *BE* corrected for Coulomb repulsion:

$$B.E.(N,Z)_{\text{no Coulomb}} = BE(N,Z) + E_{\text{Coul}}(N,Z) \qquad (16)$$

Where $BE(N,Z)_{\text{no Coulomb}}$ is the quantity to be compared with our calculation. The Coulomb energy E_{coul} is estimated for nuclei in the s-d Shell from ref. 11 as follows

$$E_{\text{Coul}}(N,Z) = CZ' + 1/2aZ'(Z'-1) + b[Z'/2] + E_{\text{Coul}}(O^{16}) \tag{17}$$

where $Z' = Z-8$, C = 3.557 MeV, a = .376 MeV, b = .194 MeV $[Z'/2]$ is the largest integer $\leqslant Z'/2$. Fourth column of Table 1 lists the calculated BE of the odd nuclei. Fifth column lists the experimental value of $(BE)_{\text{no Coulomb}}$ estimated from equation (16) and (17). The agreement is quite encouraging. In the seventh and eight column of table 1 we presented calculated and experimental values of quadrupole moment of the ground state. The agreement is quite good especially for Ne^{21}, Na^{23}, Al^{27}. Finally we calculated reduced electric quadrupole transition rates (from first excited state to G.S. of the ground State rotational band) using the rotational model formula

$$B(E2,\ J_iK \rightarrow J_fK) = 5/16\pi\ (2J_f + 1)Q_0^2 \begin{pmatrix} J_i & 2 & J_f \\ K & 0 & -K \end{pmatrix}^2 \tag{18}$$

The last two columns of table 1 list the calculated and experimental $B(E2)$ values. Except for Ne^{21} the agreement with experiment is not so good. However we should note that $B(E2)$ has been calculated with rotational model formula (equation (18)) and not by direct calculation of the transition matrix element.

CONCLUSION

In this work the LRT method has been applied to some odd-A nuclei in the s-d Shell. The motivation is to investigate how this method fares in the description of the ground states of odd nuclei. We have chosen the pairing plus quadrupole-quadrupole residual force of Kumar and Paranger with n-p pairing included. Since one has only to solve a system of linear inhomogenous equations (eq. (11)), the computer time for this calculation is substantially reduced, compared to the usual HFB method adopted for odd nuclei. The fair overall agreement of

Table 1 - Results of LRT Calculations.

Nucleus	G.S. $\bar{J}^{\pi}$	K	$B.E.$ no Coulomb (MeV) Calc.	$B.E.$ no Coulomb (MeV) Expt.	Calc. Q_0 (e fm^2)	Q_J (e. fm^2) Calc.	Q_J (e. fm^2) Expt.	$B(E2, J_i \to J_f)$ (e^2 fm^4) $J_i \to J_f$	$B(E2, J_i \to J_f)$ (e^2 fm^4) Calc.	$B(E2, J_i \to J_f)$ (e^2 fm^4) Expt.
C^{13}	$1/2^-$	1/2	108.38[f)]	109.15	43.33	0	0	$1/2^- \to 3/2^-$	74.70	22.4 a)
N^{13}	$1/2^-$	1/2	108.38[f)]	109.04	40.86	0	0	$1/2^- \to 3/2^-$	66.43	20 b)
C^{15}	$1/2^+$	1/2	121.34[f)]	118.54	46.31	0	0	$1/2^+ \to 3/2^+$	85.32	
O^{15}	$1/2^-$	1/2	120.26[f)]	130.16	46.27	0	0	$1/2^- \to 3/2^-$	84.78	
N^{15}	$1/2^-$	1/2	120.26[f)]	130.43	46.15	0	0	$1/2^- \to 3/2^-$	84.34	14.2[c)]
Na^{21}	$3/2^+$	3/2	199.19[g)]	193.28	45.62	9.12		$3/2^+ \to 5/2^+$	106.503	
Ne^{21}	$3/2^+$	3/2	202.37[g)]	193.38	47.93	9.59	10.3±.8[e)]	$3/2^+ \to 5/2^+$	117.562	107±5[d)]
Na^{23}	$3/2^+$	3/2	211.25[g)]	216.77	43.24	8.65	10.8±.8[e)]	$3/2^+ \to 5/2^+$	95.66	157±12[d)]
Mg^{25}	$5/2^+$	5/2	230.05[g)]	240.07	38.07	13.59	22[e)]	$5/2^+ \to 7/2^+$	68.62	142±5[d)]
Mg^{27}	$1/2^+$	1/2	232.11[g)]	258.20	38.58	0	0	$1/2^+ \to 3/2^+$	59.24	
Al^{27}	$5/2^+$	5/2	239.17[g)]	265.1	31.92	11.4	14.0±02[e)]	$5/2^+ \to 7/2^+$	48.26	90±10[d)]
P^{29}	$1/2^+$	1/2	244.69[g)]	290.87	26.95	0	0	$1/2^+ \to 3/2^+$	28.9	
P^{31}	$1/2^+$	1/2	267.44[h)]	314.50	19.32	0	0	$1/2^+ \to 3/2^+$	14.86	60±10[d)]
Si^{31}	$3/2^+$	3/2	271.70[h)]	307.99	18.96	3.79		$3/2^+ \to 5/2^+$	18.39	

a) Ref. (14)

b) Ref. (16)

c) Ref. (15)

d) Ref. (12)

e) Ref. (13)

f) V_0 and $\hbar\omega$ are calculated from Ne^{18} nucleus.

g) V_0 and $\hbar\omega$ are calculated from Si^{28} nucleus.

h) V_0 and $\hbar\omega$ are calculated from Si^{39} nucleus.

the calculated quantities with experiment indicate that the LRT method is suitable for a microscopic description of odd nuclei.

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