Lipkin-Nogami method using effective Yale interaction

T. S. Sandhu and M. L. Rustgi
Nuclear Physics Laboratory, Physics Department, State University of New York, Buffalo, New York 14260
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Using the effective Yale interaction the Lipkin-Nogami version of the spherical BCS method is applied to study the ground-state properties of Ni, Zn, and Ge isotopes. Calculations are performed using three different conditions to determine the parameter λ_2 of the Lipkin-Nogami method. Neutron-pair separation energies are compared with the experimental values.

[NUCLEAR STRUCTURE Lipkin-Nogami method applied to the Ni, Zn, and Ge isotopes. Effective Yale interaction.]

It is known that the Bardeen-Cooper-Schrieffer (BCS) theory[1] does not conserve the number of particles. Although Bogoliubov[2] has proved that the effect of this nonconservation on the physical properties of a system consisting of a large number (N) of particles is very small, the discrepancy is quite large for a system of finite number of particles as is the case in nuclear physics.[3]

Several attempts have been made[4,5] in the literature to improve the BCS calculations for nuclei. These attempts mostly made use of particle number projection. Following Lipkin,[6] a different approach has been suggested by Nogami[7-10] for calculating the energy of the projected ground state without actually having to perform the projection calculation. This method involves addition of a term $\lambda_2 N^2$ in the Hamiltonian together with the $\lambda_1 N$ term already present in the usual BCS approximation. Later on it was shown that the condition used by Nogami to calculate the parameter λ_2 is not unique and two more equally adequate conditions were suggested by Ng and Castel.[11] It was demonstrated in Ref. 11 that the conditions are model dependent. In all these studies by Nogami *et al.*[7-10] and Ng and Castel[11] the calculations were performed by using a phenomenological pairing interaction with constant matrix elements.

In the present paper we have extended the methods developed in Refs. 7 to 11 to incorporate the pairing interaction arising from the two-body matrix elements derived from realistic two-nucleon potentials. Furthermore, unlike in the previous applications, the formalism is applied to nuclei having both neutrons and protons outside the closed core. In the Lipkin-Nogami (LN) approach the modified Hamiltonian is written as

$$\mathcal{H} = H - \lambda_1 N - \lambda_2 N^2, \tag{1}$$

where H is the shell-model Hamiltonian describing the n particles outside the core, i.e.,

$$H = \sum_{\alpha} \epsilon_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V_A | \gamma\delta \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}, \tag{2}$$

ϵ_{α} bring the single-particle energy in a state $|\alpha\rangle \equiv |j_{\alpha} m_{\alpha} \tau_{\alpha}\rangle$ and $\langle \alpha\beta | V_A | \gamma\delta \rangle$ represents the antisymmetrized matrix elements between two-particle states. N represents the particle number operator. The Lagrange multiplier λ_1 is determined by the constraint

$$\langle N \rangle = n, \tag{3}$$

where n is the total number of nucleons outside the closed core. The expectation value $\langle N \rangle$ is calculated with respect to the BCS ground-state wave function which is approximated by the vacuum of quasiparticles ($C_{\alpha}^{\dagger}$) defined by

$$C_{\alpha}^{\dagger} = U_{\alpha} a_{\alpha}^{\dagger} + V_{\alpha} a_{\bar{\alpha}}, \tag{4}$$

where $|\bar{\alpha}\rangle = T|\alpha\rangle$ is the time reversed state. The parameter λ_2 was first determined[10] by requiring that

$$\langle \mathcal{H} N^2 \rangle = \langle \mathcal{H} \rangle \langle N^2 \rangle, \tag{5}$$

which gives the relation

$$\lambda_2 = \frac{\sum_4 \langle 0|H|4\rangle\langle 4|N^2|0\rangle}{\sum_4 \langle 0|N^2|4\rangle\langle 4|N^2|0\rangle} = -\frac{1}{4} \frac{\sum_{j_\alpha \neq j_\beta} (j_\alpha + \frac{1}{2})[(2j_\beta+1)/(2j_\alpha+1)]^{1/2} G(j_\alpha j_\alpha j_\beta j_\beta J=0\ T=1) U_\alpha V_\alpha{}^3 U_\beta{}^3 V_\beta}{\sum_{j_\alpha \neq j_\beta} (2j_\alpha+1)(2j_\beta+1) U_\alpha{}^2 V_\alpha{}^2 U_\beta{}^2 V_\beta{}^2}, \tag{6}$$

where

$$G(j_a j_b j_c j_d JT) = (1+\delta_{j_a j_b})^{1/2}(1+\delta_{j_c j_d})^{1/2}\langle j_a j_b JT | V_A | j_c j_d JT\rangle. \tag{7}$$

An alternate condition to determine λ_2 was suggested in Ref. 11 as

$$\langle \mathcal{H} H\rangle = \langle \mathcal{H}\rangle\langle H\rangle, \tag{8}$$

which leads to

$$\lambda_2 = \frac{\sum_4 \langle 0|H|4\rangle\langle 4|H|0\rangle}{\sum_4 \langle 0|H|4\rangle\langle 4|N^2|0\rangle} = \frac{\sum_{j_\alpha \neq j_\beta, J} (\langle j_\alpha j_\alpha JT=1|V_A|j_\beta j_\beta JT=1\rangle)^2 (V_\alpha{}^2 U_\beta{}^2)^2}{-2\sum_{j_\alpha \neq j_\beta}(2j_\alpha+1)^{1/2}(2j_\beta+1)^{1/2} G(j_\alpha j_\alpha j_\beta j_\beta J=0\ T=1) U_\alpha V_\alpha{}^3 U_\beta{}^3 V_\alpha}. \tag{9}$$

Another condition is obtained by combining (6) and (9), i.e.,

$$\lambda_2 = \frac{1}{4}\left(\frac{\sum_{j_\alpha \neq j_\beta, J} (\langle j_\alpha j_\alpha JT=1|V_A|j_\beta j_\beta JT=1\rangle)^2 (V_\alpha{}^2 U_\alpha{}^2)^2}{\sum_{j_\alpha \neq j_\beta}(2j_\alpha+1)(2j_\beta+1)(U_\alpha V_\alpha U_\beta V_\beta)^2}\right)^{1/2}. \tag{10}$$

The ground-state energy of a nucleus in this formalism is given by

$$E = \sum_{j_\alpha \tau}(2j_\alpha+1)\epsilon_\alpha (V^\tau_{j_\alpha})^2 + \sum_{j_\alpha \tau}(j_\alpha+\tfrac{1}{2})\Gamma^\tau_{j_\alpha}(V^\tau_{j_\alpha})^2 + \sum_{j_\alpha \tau}(j_\alpha+\tfrac{1}{2})\Delta^\tau_{j_\alpha} U^\tau_{j_\alpha} V^\tau_{j_\alpha} + 4\sum_\tau \lambda_2^\tau \sum_{j_\alpha}(j_\alpha+\tfrac{1}{2})(U^\tau_{j_\alpha} V^\tau_{j_\alpha})^2, \tag{11a}$$

where τ represents projection of isotopic spin,

$$\Gamma^\tau_{j_\alpha} = \frac{1}{(2j+1)}\sum_{j_\beta \tau'}\sum_J (2J+1) G(j_\alpha j_\beta j_\alpha j_\beta J)(V^{\tau'}_{j_\beta})^2, \tag{11b}$$

and

$$\Delta^\tau_{j_\alpha} = \frac{1}{2}\sum_{j_\beta}\left(\frac{2j_\beta+1}{2j_\alpha+1}\right)^{1/2} G(j_\alpha j_\alpha j_\beta j_\beta J=0 T=1) \times U^\tau_{j_\beta} V^\tau_{j_\beta}. \tag{11c}$$

$G(abcdJ)$ and $G(abcdJT)$ are related through the Clebsch-Gordan coefficients:

TABLE I. Comparison of the ground-state energies (E) and the pairing energies (E_{pair}) for Ni, Zn, and Ge isotopes obtained by solving the modified BCS equations using the three expressions (6), (9), and (11) for λ_2 labeled as I, II, and III, respectively, and the usual BCS equations. All the energies are given in MeV.

	E				E_{pair}			
	I	II	III	BCS	I	II	III	BCS
^{58}Ni	−22.124	−22.669	−22.578	−22.001	−2.030	−2.139	−2.126	−2.005
^{60}Ni	−43.357	−44.222	−44.032	−43.158	−2.728	−3.234	−3.165	−2.514
^{62}Ni	−63.206	−64.213	−63.977	−62.988	−2.891	−3.504	−3.391	−2.676
^{64}Ni	−81.180	−82.242	−81.942	−80.971	−2.797	−3.111	−3.034	−2.691
^{66}Ni	−97.215	−97.978	−97.749	−97.062	−1.941	−2.004	−1.980	−1.917
^{60}Zn	−46.769	−47.979	−47.729	−46.483	−3.550	−3.878	−3.817	−3.465
^{62}Zn	−70.723	a	−71.975	−70.379	−3.557		−4.321	−3.307
^{64}Zn	−93.520	−95.248	−94.704	−93.249	−2.863	−4.516	−4.173	−1.537
^{66}Zn	−113.451	−115.578	−114.920	−112.991	−3.479	−4.221	−3.998	−3.314
^{68}Zn	−131.117	−133.099	−132.452	−130.755	−3.049	−3.333	−3.245	−2.990
^{64}Ge	−97.727	a	−99.365	−97.320	−3.202		−4.216	−2.579
^{66}Ge	a	−126.638	−125.510	−123.682		−3.763	−3.792	−1.253
^{68}Ge	−145.374	−148.065	−147.338	−144.739	−3.155	−4.639	−3.938	−2.925
^{70}Ge	−164.476	−166.963	−166.292	−164.016	−2.906	−3.858	−3.477	−2.738

[a] No convergence was obtained for these entries.

TABLE II. Comparison of the parameter λ_2 obtained using different approximations. The superscripts n and p denote neutron and proton, respectively.

	λ_2^n			λ_2^p		
	I	II	III	I	II	III
^{58}Ni	0.041	0.211	0.183			
^{60}Ni	0.053	0.256	0.216			
^{62}Ni	0.057	0.288	0.237			
^{64}Ni	0.056	0.308	0.239			
^{66}Ni	0.052	0.315	0.233			
^{60}Zn	0.048	0.258	0.214	0.048	0.258	0.214
^{62}Zn	0.068		0.270	0.052		0.243
^{64}Zn	0.127	0.415	0.336	0.054	0.351	0.265
^{66}Zn	0.097	0.454	0.348	0.058	0.371	0.280
^{68}Zn	0.075	0.463	0.330	0.061	0.384	0.289
^{64}Ge	0.074		0.340	0.074		0.340
^{66}Ge		0.523	0.496		0.486	0.392
^{68}Ge	0.149	0.527	0.491	0.079	0.509	0.401
^{70}Ge	0.101	0.546	0.441	0.085	0.526	0.394

$$G(abcdJ)=\sum_T \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & T \\ \tau_z^a & \tau_z^b & T_z \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & T \\ \tau_z^c & \tau_z^d & T_z \end{pmatrix} \times G(abcdJT) . \tag{11d}$$

The transformation coefficients U and V and the parameters λ_1 and λ_2 are determined self-consistently by solving the gap equations

$$V_{j_\alpha}^\tau = \frac{1}{\sqrt{2}} \left(1+\frac{e_\alpha^\tau - \lambda^\tau}{E_\alpha^\tau}\right)^{1/2} , \tag{12a}$$

$$U_{j_\alpha}^\tau = (1-(V_{j_\alpha}^\tau)^2)^{1/2} , \tag{12b}$$

where

$$e_\alpha^\tau = \epsilon_{j_\alpha}^\tau + \Gamma_{j_\alpha}^\tau + 4\lambda_2^\tau (V_{j_\alpha}^\tau)^2 , \tag{12c}$$

$$\lambda^\tau = \lambda_1^\tau + 2\lambda_2^\tau (n_\tau + 1) , \tag{12d}$$

and

$$E_\alpha^\tau = [(e_\alpha^\tau - \lambda^\tau)^2 + (\Delta_{j_\alpha}^\tau)^2]^{1/2} . \tag{12e}$$

The above equations are solved for all the Ni, Zn, and Ge isotopes using renormalized matrix elements of the Yale potential.[12] A ^{56}Ni core has been assumed and the basis states are limited to $2p_{3/2}$, $2p_{1/2}$, and $1f_{5/2}$ harmonic oscillator states. The single-particle energies are taken to be -10.246, -9.466, and -9.166 MeV for the states $2p_{3/2}$, $1f_{5/2}$, and $2p_{1/2}$, respectively. The calculations have been performed using all the three expressions (6), (9), and (11) for λ_2 and the results in the tables are labeled I, II, and III respectively. The ordinary BCS solutions are also obtained self-consistently for all the isotopes by putting $\lambda_2 = 0$.

The results for the ground-state energies and the pairing energies are displayed in Table I. It is clear that there is little difference between the results of the usual BCS theory and the modified version using the expression (6) for λ_2 for the total energy, but there is a considerable change in the wave function as indicated by the differences in the pairing energies obtained from the modified equations and the usual BCS equations. This is different from the conclusion reached in Ref. 8 for Ni isotopes where constant two-body matrix elements were used for the pairing interaction. The trend remains the same for the Zn and Ge isotopes. The contribution to the energy due to the fluctuation of particle number is greatest for approximation II [Eq. (9)] and least in approximation I [Eq. (6)]. This is a direct consequence of the magnitude of

TABLE III. Comparison of neutron-pair separation energies obtained from different approximations and the corresponding experimental values. All the energies are given in MeV.

Nucleus	$-\Delta E_{NP}$ I	II	III	BCS	Experiment
^{58}Ni	22.124	22.669	22.578	22.001	22.452
^{60}Ni	21.233	21.553	21.454	21.157	20.386
^{62}Ni	19.849	19.991	19.945	19.830	18.421
^{64}Ni	17.974	18.029	17.965	17.983	16.500
^{66}Ni	16.035	15.736	15.807	16.091	15.093
^{62}Zn	23.954		24.246	23.896	
^{64}Zn	22.797		22.729	22.870	21.020
^{66}Zn	19.931	20.330	20.216	19.742	19.024
^{68}Zn	17.606	17.521	17.532	17.764	17.255
^{66}Ge			26.145	26.362	
^{68}Ge		21.427	21.828	21.057	21.980
^{70}Ge	19.102	18.898	18.954	19.277	20.130

the parameter λ_2. As is clear from Table II the value of λ_2 is largest in approximation II and smallest in approximation I. For a particular set of isotopes the values of λ_2^p increase when more neutrons are added. This suggests that the Hartree-type field for protons Γ^p changes as more neutrons are added.

To check the quality of the ground-state energies obtained by different approximations, neutron-pair separation energies are compared with the corresponding experimental values. The neutron-pair separation energy is defined as

$$\Delta E_{\mathrm{NP}}(N,Z) = E(N,Z) - E(N-2,Z). \tag{13}$$

The results are given in Table III. The experimental energies are those of Mattauch, Thiele, and Wapstra.[13] The agreement between the calculated values and the experimental values is surprisingly good even in the case of ordinary BCS solutions.

In general, there is no definite trend towards a better agreement when the modified version of the BCS method is used. However, for a definite conclusion the LN modification should be incorporated in a full Hartree-Fock-Bogoliubov calculation. Such calculations are in progress at present.

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