Ground-State Properties and Low-Lying States of the N^{14} Nucleus*

NAZAKAT ULLAH†
Brookhaven National Laboratory, Upton, New York

AND

R. K. NESBET
IBM Research Laboratory, San Jose, California

(Received 12 November 1963)

An approximate Hartree-Fock self-consistent-field calculation is carried out on the N^{14} nucleus using the concept of symmetry and equivalence restrictions. The configuration interaction matrices belonging to a definite value of J, Π, T are constructed using the jj coupled configurations arising from $(1p)^{-2}$ shell. The approximate Hartree-Fock binding energy turns out to be 38.5 MeV too small, while it was only 13 MeV too small for the O^{16}. This is attributed to an inadequate choice of the tensor interaction or to the omission of a two-body spin-orbit interaction. The static magnetic dipole moment is calculated to be 0.39 nuclear magneton and the rms radius is found to be 2.14 F. The results are compared with the earlier intermediate coupling calculations. A number of low-lying even-parity states are calculated and compared with the experimental values.

I. INTRODUCTION

IN the past a number of calculations have been done on $1p$-shell nuclei in intermediate coupling.[1] The Hamiltonian of these calculations has an *ad hoc* single-particle spin-orbit coupling term and a central nucleon-nucleon interaction and the single-particle wave functions are represented by the harmonic oscillator wave functions. Energy levels and various other quantities of interest like static magnetic dipole moment are then calculated as a function of intermediate coupling parameter, which is fixed by comparing the calculated quantities with their experimental values.

The strong spin-orbit coupling postulated in the shell model can be explained through tensor force.[2] Therefore, if one includes the tensor force in the Hamiltonian of the system, then it becomes unnecessary to include a separate spin-orbit term. This was first indicated by Elliott.[3]

In an earlier calculation[4] on O^{16} we had shown that the approximate Hartree-Fock self-consistent-field calculation gives an improved ground-state energy in zeroth order compared to the one obtained with harmonic oscillator wave functions. For the closed-shell nuclei like O^{16}, the contribution of the tensor force to the $^{1,1}S$ ground-state configuration is zero, but for the open-shell nuclei the tensor force can affect the ordering of the low-lying states and the ground-state properties quite a bit. For calculational purposes the nuclei which have either one or two holes in $1p$ shell or one or two nucleons outside the closed $1p$ shell are very suitable. It is of great interest to compare the results of these approximate Hartree-Fock calculations with the one in which an *ad hoc* single-particle spin-orbit term and simple-harmonic-oscillator wave functions are used.

We have carried out such a calculation on the N^{14} nucleus, using the matrix Hartree-Fock method.[5] In the intermediate coupling scheme, one may either work with a complete set of LS or jj basis functions. Because of the inclusion of tensor force in the Hamiltonian, the only good quantum numbers are J, the total angular momentum quantum number; Π, the parity; and T, the total isobaric spin quantum number. Therefore, if the states having a definite value of J, Π, T are constructed using the jj coupled orbitals, then because of the commutatibility of projection operator with the Hamiltonian, the configuration interaction matrix is easier to calculate.

Section II gives an analysis of the $1p$ shell for the N^{14} nucleus, the results of the approximate self-consistent-field calculation are given in Sec. III. Using these results the ground-state properties and the low-lying levels are calculated and compared with the earlier intermediate coupling calculations and the experimental values in Sec. IV.

II. ANALYSIS OF THE $1p$ SHELL FOR N^{14}

In this section we shall carry out the analysis of the jj coupled configurations $(p_{1/2})^{-2}$, $(p_{1/2})^{-1}(p_{3/2})^{-1}$, $(p_{3/2})^{-2}$. We shall use the following notation for the Slater determinant made up of the jj coupled orbitals

$$\Phi=(\ ,\ ;\ ,\ ),$$

where the normalization constant and the conventional antisymmetrizing operator are to be understood. The jj orbitals written to the left of the semicolon refer to the

* Research supported by the U. S. Atomic Energy Commission.

† Present address: Tata Institute of Fundamental Research, Bombay, India.

[1] D. R. Inglis, Phys. Rev. **87**, 915 (1952); Rev. Mod. Phys. **25**, 390 (1953); A. M. Lane, Proc. Phys. Soc. **A66**, 977 (1953); **A68**, 197 (1955); G. E. Tauber and Ta-You Wu, Phys. Rev. **93**, 295 (1954); D. Kurath, *ibid.* **101**, 216 (1956).

[2] A. M. Feingold, Phys. Rev. **101**, 258 (1956); **105**, 944 (1957); A. Arima and T. Terasawa, Progr. Theoret. Phys. (Kyoto) **23**, 115 (1960); P. Goldhammer, Phys. Rev. **122**, 207 (1961).

[3] J. P. Elliott, Proc. Roy. Soc. (London) **A218**, 345 (1953).

[4] Nazakat Ullah and R. K. Nesbet, Nucl. Phys. **39**, 239 (1962). See also Erratum, *ibid.* **46**, 254 (1963).

[5] R. K. Nesbet, Rev. Mod. Phys. **35**, 552 (1963).

neutrons (ν) and those to the right refer to the protons (π), the $p_{3/2}$ orbitals are written to the left of the comma and $p_{1/2}$ orbitals to the right. The eigenfunctions of the z component of angular momentum can be easily written down. The eigenfunctions of the square of the angular momentum are then constructed by taking a proper linear combination of these functions. The coefficients in the linear expansion are then obtained using the step-up operators.[6] We denote the eigenfunctions of J^2, T^2, J_z, T_z by $|JTJ_zT_z\rangle$. We shall now write down the states of definite J and T obtained from the various jj configurations of N^{14}.

Configuration $(p_{1/2})^{-2}$

$$|1010\rangle=(\ ,\tfrac{1}{2};\ ,\tfrac{1}{2}).$$

$$|0101\rangle=(\ ,\tfrac{1}{2}-\tfrac{1}{2};\ ,\ ).$$

Configuration $(p_{1/2})^{-1}(p_{3/2})^{-1}$

$$|2121\rangle=(\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2}-\tfrac{3}{2},\ \tfrac{1}{2}-\tfrac{1}{2};\ \tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2},\ \tfrac{1}{2}).$$

$$|2020\rangle=\frac{1}{\sqrt{2}}[(\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2}-\tfrac{3}{2},\ \tfrac{1}{2};\ \tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2},\ \tfrac{1}{2}-\tfrac{1}{2})$$
$$+(\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2},\ \tfrac{1}{2}-\tfrac{1}{2};\ \tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2}-\tfrac{3}{2},\ \tfrac{1}{2})].$$

$$|1111\rangle=\tfrac{1}{2}[(\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2}-\tfrac{3}{2},\ \tfrac{1}{2}-\tfrac{1}{2};\ \tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{3}{2},\ \tfrac{1}{2})$$
$$-\sqrt{3}(\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2}-\tfrac{3}{2},\ \tfrac{1}{2}-\tfrac{1}{2};\ \tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2},\ -\tfrac{1}{2})].$$

$$|1010\rangle=\frac{1}{\sqrt{8}}[\sqrt{3}(\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2}-\tfrac{3}{2},\ -\tfrac{1}{2};\ \tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2},\ \tfrac{1}{2}-\tfrac{1}{2})$$
$$-(\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2}-\tfrac{3}{2},\ \tfrac{1}{2};\ \tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{3}{2},\ \tfrac{1}{2}-\tfrac{1}{2})$$
$$+\sqrt{3}(\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2},\ \tfrac{1}{2}-\tfrac{1}{2};\ \tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2}-\tfrac{3}{2},\ -\tfrac{1}{2})$$
$$-(\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{3}{2},\ \tfrac{1}{2}-\tfrac{1}{2};\ \tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2}-\tfrac{3}{2},\ \tfrac{1}{2})].$$

Configuration $(p_{3/2})^{-2}$

$$|3030\rangle=(\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2},\ ;\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2},\ ).$$

$$|2121\rangle=(\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2}-\tfrac{3}{2},\ ;\tfrac{3}{2}\ \tfrac{1}{2},\ ).$$

$$|1010\rangle=\frac{1}{\sqrt{10}}[\sqrt{3}(\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2},\ ;\tfrac{3}{2}-\tfrac{1}{2}-\tfrac{3}{2},\ )$$
$$-2(\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{3}{2},\ ;\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{3}{2},\ )$$
$$+\sqrt{3}(\tfrac{3}{2}-\tfrac{1}{2}-\tfrac{3}{2},\ ;\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2},\ )].$$

$$|0101\rangle=\frac{1}{\sqrt{2}}[(\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2}-\tfrac{3}{2},\ ;\tfrac{3}{2}-\tfrac{3}{2},\ )$$
$$-(\tfrac{3}{2}\ \tfrac{1}{2}-\tfrac{1}{2}-\tfrac{3}{2},\ ;\tfrac{1}{2}-\tfrac{1}{2},\ )].$$

[6] R. K. Nesbet, J. Math. Phys. **2**, 701 (1961).

III. APPROXIMATE SELF-CONSISTENT-FIELD CALCULATIONS

To obtain the radial wave functions for the occupied $p_{3/2}$, $p_{1/2}$ orbitals an approximate Hartree-Fock self-consistent-field calculation is carried out using the determinant

$$(\ ,\tfrac{1}{2};\ ,\tfrac{1}{2}),$$

from the $(p_{1/2})^{-2}$ configuration.

The nucleon-nucleon interaction is the one obtained by Goldhammer[7] by fitting the data on light nuclei. It consists of a Serber potential with a repulsive core and a tensor-even component, and is given by

$$V_{12}=J_R\exp\left(-8\frac{r_{12}^2}{r_0^2}\right)+J_C(P_0+P_1)\exp\left(-\frac{r_{12}^2}{r_0^2}\right)$$
$$+\tfrac{1}{4}(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2)S_{12}\left(\frac{r_{12}}{r_0}\right)^2 J_S\exp\left(-\frac{r_{12}^2}{r_0^2}\right), \quad (1)$$

where

$$J_R=189.75\text{ MeV},\quad J_C=-58.65\text{ MeV},$$
$$J_S=-107.29\text{ MeV},$$
$$r_0=1.54\text{ F},\quad (1F=10^{-13}\text{ cm}).$$
$$P_0=\tfrac{1}{16}(1-\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)(3+\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2).$$
$$P_1=\tfrac{1}{16}(3+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)(1-\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2).$$
$$S_{12}=\frac{(\boldsymbol{\sigma}_1\cdot\mathbf{r}_{12})(\boldsymbol{\sigma}_2\cdot\mathbf{r}_{12})}{r_{12}^2}-\tfrac{1}{3}(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2).$$

The single-particle orbitals ϕ_a are expressed as a linear combination of a set of linearly independent basis orbitals η_i, which for jj coupled orbitals are chosen to be of the form

$$\eta_i=R_{il}(r)\chi_j{}^m\xi(m_\tau), \quad (2)$$

where $\xi(m_\tau)$ is an isospin function and $\chi_j{}^m$ is obtained by vector coupling the spherical harmonic $Y_l{}^m$ with the elementary spin function $v(m_s)$

$$\chi_j{}^m=\sum_{m_s=-1/2}^{1/2}(lm-m_s\tfrac{1}{2}m_s|l\tfrac{1}{2}jm)Y_l{}^{m-m_s}v_{1/2}{}^{m_s}. \quad (3)$$

The radial wave functions $R_{il}(r)$ are taken to be of the form

$$R_{il}(r)=N_{li}r^{2n_i+l_i}\exp(-\gamma_i r^2), \quad (4)$$

where N_{li} is the normalization constant, n_i a variable integer, and γ_i a variable parameter.

In our earlier calculation,[4] we had expanded the nucleon-nucleon potential in terms of Legendre polynomials to calculate the two-particle matrix elements. This is not very convenient since a definite form of $V(r)$

[7] P. Goldhammer, Phys. Rev. **116**, 676 (1959).

for the nuclear potential is not known at present. Talmi[8] has shown that if one uses the harmonic oscillator wave functions then the two-particle matrix element can be expanded in the form of a series. Talmi's analysis has been generalized by the second author[9] of this paper which enables one to express the two-particle matrix element of various operators in terms of linearly independent reduced matrix elements in a simple way. The two-particle matrix element for a scalar potential is given by

$$\langle\psi_a\psi_b|V|\psi_c\psi_d\rangle$$

$$=\int d\tau_1 d\tau_2 R_a(r_1)R_c(r_1)V(r)R_d(r_2)R_b(r_2)$$

$$\times Y_{l_a}^{m_{l_a}*}(1)Y_{l_b}^{m_{l_b}*}(2)Y_{l_c}^{m_{l_c}}(1)Y_{l_d}^{m_{l_d}}(2), \quad (5)$$

$$=\sum_k c^k(l_a m_{l_a}, l_c m_{l_c})c^k(l_d m_{l_d}, l_b m_{l_b})$$

$$\times F^k(ac|db)\delta[(m_{l_a}-m_{l_c}), (m_{l_d}-m_{l_b})], \quad (6)$$

where, greater of $|l_a-l_c|$, $|l_b-l_d| \leqslant k \leqslant$ lesser of (l_a+l_c), (l_b+l_d), $k+l_a+l_c=$ even, $k+l_b+l_d=$ even. The coefficients $c^k(lm,'lm')$ are the Gaunt coefficients, tabulated by Condon and Shortley.[10] The radial integral $F^k(ac|db)$ is given by

$$F^k(ac|db)=\tfrac{1}{2}(2k+1)\int_{r=0}^{\infty} r^2dr$$

$$\times\int_{R=0}^{\infty} R^2dR\int_{\alpha=0}^{\pi}\sin\alpha d\alpha P_k(\cos\omega)$$

$$\times V(r)R_a(r_1)R_c(r_1)R_b(r_2)R_d(r_2), \quad (7)$$

where $\mathbf{r}$ is the relative vector, $\mathbf{R}$ is the center of mass vector, α is the angle from $\mathbf{R}$ to $\mathbf{r}$, and ω is the angle from $\mathbf{r}_1$ to $\mathbf{r}_2$.

For the tensor operator $V(r)S_{12}$ the two-particle matrix element is given by

$$\langle\psi_a\psi_b|VS_{12}|\psi_c\psi_d\rangle$$

$$=(-1)^M(\tfrac{2}{3})^{1/2}\langle ab|s(2,-M)|cd\rangle$$

$$\times\sum_{k,k'} c^k(l_a m_{l_a}, l_c m_{l_c})c^{k'}(l_d m_{l_d}, l_b m_{l_b})$$

$$\times c^2(km_{l_a}-m_{l_c}, k'm_{l_d}-m_{l_b})I^{kk'}(ac|db), \quad (8)$$

where

$$|l_a-l_c| \leqslant k \leqslant (l_a+l_c), \quad |l_b-l_d| \leqslant k' \leqslant (l_b+l_d),$$

$l_a+l_c+k=$ even, $l_b+l_d+k'=$ even, the spin matrix $\langle ab|s(2,-M)|cd\rangle$ is tabulated in Ref. 9, $M=m_{l_a}+m_{l_b}-m_{l_c}-m_{l_d}$ and the radial integral $I^{kk'}(ac|db)$ is given by

$$I^{kk'}(ac|db)$$

$$=\int_0^{\infty} r^2dr\int_0^{\infty} R^2dR\int_0^{\pi}\sin\alpha d\alpha V(r)R_a(r_1)R_c(r_1)$$

$$\times R_b(r_2)R_d(r_2)\sum_s 2\pi\frac{\begin{pmatrix} k & 2 & k' \\ s & 0 & -s\end{pmatrix}}{\begin{pmatrix} k & 2 & k' \\ 0 & 0 & 0\end{pmatrix}}Y_k^s Y_{k'}^{-s}, \quad (9)$$

where Y_k^s are the spherical harmonics in a body-fixed reference frame.

A 709 computer program "SNUC" made by the second author of this paper is now available which calculates the values of the radial integrals given by (7) and (9) for an arbitrary nucleon-nucleon potential $V(r)$, which is integrable.

For LS coupling the coefficients which multiply the independent radial integrals in (6), (8) can easily be obtained from the tabulated values in Ref. 10. But when one uses the jj coupled orbitals given by (3), then a transformation is needed which gives the necessary coefficients for jj coupling. A 7090 FORTRAN program made by the first author[11] is available which calculates the coefficients multiplying the linearly independent radial integrals for jj coupled orbitals.

In the earlier self-consistent-field calculation[4] on O^{16}, the Coulomb operator was not included in the zeroth-order Hamiltonian. The Coulomb operator will cause the neutron and proton wave functions to be different and therefore will increase the number of parameters for s and p nucleons. Since the Coulomb contribution at least in the light nuclei is much smaller than the nuclear contribution, very small error will be introduced by taking the neutron and proton wave functions to be the same. Using the concept of symmetry and equivalence restrictions,[12] we shall average out the Coulomb contribution for the whole shell. The self-consistent-field

TABLE I. Parameters n_i, γ_i for the s and p radial wave functions R_{li}.

i	l_i	n_i	γ_i (F^{-2})
1	0	0	0.317
2	0	1	0.317
3	0	2	0.317
4	1	0	0.161
5	1	1	0.161
6	1	2	0.161

[8] I. Talmi, Helv. Phys. Acta **25**, 185 (1962).
[9] R. K. Nesbet, J. Math. Phys. **4**, 1262 (1963).
[10] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, London and New York, 1953), p. 178.
[11] Nazakat Ullah (to be published).
[12] R. K. Nesbet, Proc. Roy. Soc. (London) **A230**, 312 (1955).

TABLE II. One-nucleon energies ϵ_a and the coefficients $X_i{}^a$ for orthonormal self-consistent occupied orbitals ϕ_a of N^{14} expressed as linear combinations of normalized basis orbitals η_i.

ϕ_a	ϵ_a (MeV)	$X_1{}^a$	$X_2{}^a$	$X_3{}^a$
$1s_{1/2}$	−48.54	0.77231	0.30358	−0.04156
$1p_{3/2}$	−22.97	1.86491	−1.60331	0.69086
$1p_{1/2}$	−25.39	1.91327	−1.70577	0.73776

calculation will then give the average single nucleon energy. The single neutron or proton energy can then be calculated using the average value and the Coulomb contribution. The total isotopic spin will no longer remain a good quantum number. However, since we are dealing with light nuclei, in which Coulomb force is much weaker than nuclear force, we shall take the total isotopic spin as an approximately good quantum number.

The parameters for the radial wave functions R_{il} are shown in Table I. These are the parameters which give the lowest energy for the ground state of O^{16} in zeroth order when the Coulomb potential is averaged over the shells. Using these parameters the self-consistent-field calculation gives the values of one nucleon energies and the coefficients $X_i{}^a$ for the occupied $s_{1/2}$, $p_{3/2}$, $p_{1/2}$ orbitals for N^{14} shown in Table II.

In the calculation of the matrix elements of the matrices belonging to a particular value of J, II, and T we shall have to transform the two-particle matrix elements from the basis of η functions to that of ϕ functions. The number of independent two-particle matrix elements needed for this calculation can be greatly reduced if the radial wave functions for the occupied $p_{3/2}$ orbital is taken to be the same as $p_{1/2}$. The results of the approximate Hartree-Fock self-consistent-field calculation[13] on O^{15} and on N^{14} shown in Table II show that the $p_{3/2}$ and $p_{1/2}$ radial wave functions are only slightly different. By slightly extending the concept of equivalence restriction[12] these radial wave functions can be taken to be the same. The input data for the self-consistent-field calculation is now obtained by treating the p orbitals as a single shell, made up of the two jj coupling subshells. The best parameters for the s and p radial wave functions with this additional constraint are shown in Table III. The self-consistent-field results are shown in Table IV.

IV. GROUND-STATE PROPERTIES AND LOW-LYING STATES

The ground state of N^{14} has $J^{\Pi}=1^+$, $T=0$, its wave function Ψ can be approximated by

$$\Psi=X_a\Psi_a+X_b\Psi_b+X_c\Psi_c, \tag{10}$$

where Ψ_a, Ψ_b, Ψ_c denote the $|1010\rangle$ wave functions obtained from the configurations $(p_{1/2})^{-2}$, $(p_{3/2})^{-2}$, $(p_{1/2})^{-1}(p_{3/2})^{-1}$, respectively. The matrix elements of the 3×3 ground-state configuration have the following values

$$Haa=-55.481,\quad Hab=4.356,\quad Hac=-3.430,$$
$$Hbb=-60.313,\quad Hbc=4.251,\quad Hcc=-55.315.$$

The diagonalization of this matrix gives the eigenvalues

$$\epsilon_1=-65.702,\quad \epsilon_2=-53.439,\quad \epsilon_3=-51.967.$$

The eigenvectors belonging to the lowest eigenvalue are

$$X_a=0.47442,\quad X_b=-0.74866,\quad X_c=0.46304.$$

Thus the approximate Hartree-Fock binding energy of N^{14} is 65.70 MeV compared to an experimental value of 104.21 MeV. The rms radius $(\langle r^2\rangle)^{1/2}$ turns out to be 2.14 F compared to the experimental value of 2.45 F.

We shall now calculate the static magnetic dipole moment $\langle\mu\rangle$. It is given by[14]

$$\langle\mu\rangle=\int\Psi^*(M=J)(\mu_{\rm op})_z\Psi(M=J)d\tau, \tag{11}$$

where

$$\mu_{\rm op}=\tfrac{1}{2}\sum_{i=1}^{A}[(1-\tau_z{}^{(i)})(\mathbf{l}_i+g_p\mathbf{s}_i)+g_n(1+\tau_z{}^{(i)})], \tag{12}$$

in nuclear magnetons. The values of the gyromagnetic ratios g_p, g_n are 5.59 and −3.83, respectively.

To evaluate expression (11) we need the matrix elements of the z component of $\mathbf{l}$, $\mathbf{s}$ between jj coupled functions given by (3). The use of the reduced matrix

TABLE III. Parameters n_i, γ_i for the s and p radial wave functions R_{li} under equivalence restriction.

i	l_i	n_i	γ_i (F^{-2})
1	0	0	0.288
2	0	1	0.288
3	0	2	0.288
4	1	0	0.143
5	1	1	0.143
6	1	2	0.143

TABLE IV. One-nucleon energies ϵ_a and the coefficients $X_i{}^a$ for orthonormal self-consistent-field occupied orbitals ϕ_a of N^{14} under equivalence restriction.

ϕ_a	ϵ^a (MeV)	$X_1{}^a$	$X_2{}^2$	$X_3{}^a$
$1s$	−46.28	0.79594	0.29063	−0.06222
$1p$	−22.47	1.94555	−1.77764	0.77404

[13] Nazakat Ullah and R. K. Nesbet (unpublished).

[14] J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley & Sons, Inc., New York, 1958).

elements[15] gives the following expressions for these matrix elements

$$\langle j_a m_a | s_z | j_b m_b \rangle = (-1)^{-\frac{1}{2}-l_a-m_a+j_a+j_b}[\tfrac{3}{2}(2j_a+1)(2j_b+1)]^{1/2} \times \begin{pmatrix} j_a & j_b & 1 \\ m_a & -m_a & 0 \end{pmatrix} \begin{Bmatrix} j_a & j_b & 1 \\ \frac{1}{2} & \frac{1}{2} & l_a \end{Bmatrix} P^R \delta_{l_a,l_b} \delta_{m_a,m_b}, \quad (13)$$

$$\langle j_a m_a | l_z | j_b m_b \rangle = (-1)^{-\frac{1}{2}-l_a-m_a+j_a+j_b} \times [l_a(l_a+1)(2l_a+1)(2j_a+1)(2j_b+1)]^{1/2} \times \begin{pmatrix} j_a & j_b & 1 \\ -m_a & m_a & 0 \end{pmatrix} \begin{Bmatrix} j_a & j_b & 1 \\ l_a & l_a & \frac{1}{2} \end{Bmatrix} P^R \delta_{l_a,l_b} \delta_{m_a,m_b}, \quad (14)$$

where

$$P^R = \int_0^\infty R_{j_a} R_{j_b} r^2 dr.$$

With the help of these relations we can express the magnetic dipole moment as

$$\langle \mu \rangle = 0.373 X_a^2 + 0.627 X_b^2 + 0.690 X_c^2 - 0.253 X_a X_c + 0.401 X_b X_c. \quad (15)$$

Substituting the values of X_a, X_b, X_c we get the value of $\langle \mu \rangle$ to be 0.39 nuclear magneton. This is to be compared with the experimental value 0.40 and the value 0.36 obtained by Tauber and Wu in intermediate coupling.

The quadrupole moment $\langle Q \rangle$ of the nucleus is given by[14]

$$\langle Q \rangle = \int \Psi^*(M=J) Q_0^{(2)} \Psi(M=J) d\tau, \quad (16)$$

where the quadrupole moment operator $Q_0^{(2)}$ is given by

$$Q_0^{(2)} = e \sum_{i=1}^{z} (3z_i^2 - r_i^2). \quad (17)$$

As in the case of dipole moment, we calculate the matrix of $Q_0^{(2)}$, it is given by

$$\langle j_a m_a | Q_0^{(2)} | j_b m_b \rangle = (-1)^{l_a+l_b+j_a+j_b-m_a-\frac{1}{2}} 2eQ^R \begin{pmatrix} l_a & 2 & l_b \\ 0 & 0 & 0 \end{pmatrix} \times \begin{pmatrix} j_a & j_b & 2 \\ -m_a & m_a & 0 \end{pmatrix} \begin{Bmatrix} 2 & j_a & j_b \\ \frac{1}{2} & l_b & l_a \end{Bmatrix} \delta_{m_a,m_b}, \quad (18)$$

[15] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957).

TABLE V. Low-lying even-parity levels of N^{14}. The energies of the calculated levels are relative to the calculated ground state of N^{14}.

Excited levels J^Π	T	Calculated (MeV)	Experimental (MeV)
0^+	1	0.07	2.31
1^+	0	12.26	3.95
2^+	0	1.43	7.03
2^+	1	2.75	10.43
3^+	0	7.96	11.38
1^+	1	9.74	

where

$$Q^R = \int_0^\infty R_{j_a} R_{j_b} r^4 dr.$$

Because of the selection rules on j given by the second $3-j$ symbol in (18), the pure $(p_{1/2})^{-2}$ configuration gives a zero quadrupole moment. It can further be shown that the pure $(p_{3/2})^{-2}$ configuration gives a negative quadrupole moment. The quadrupole moment $\langle Q \rangle$ using the approximate ground-state wave function can be expressed as

$$\langle Q \rangle = [-0.160 X_b^2 + 0.100 X_c^2 + 0.400 X_a X_c + 0.126 X_b X_c] eQ^R. \quad (19)$$

Its value turns out to be $-0.12e-\mathrm{F}^2$. Thus the calculation gives the wrong sign to the quadrupole moment.

N^{14} has a number of low-lying states. These states can be calculated by constructing the appropriate matrices belonging to a given J^Π and T and then diagonalizing them. The calculated results for even parity states are shown in Table V along with their experimental values.[16] As can be seen from Table V most of the calculated states lie much lower than they should.

V. DISCUSSION

We shall now discuss the results of this calculation and the possible ways to improve them. As we have seen, the approximate Hartree-Fock binding energy for N^{14} turns out to be about 38.5 MeV too small, while it was only 13 MeV too small for O^{16}. This can either be attributed to an inadequate choice of tensor interaction or to the omission of a two-body spin-orbit interaction. An incorrect choice of tensor interaction can also give the wrong sign to the quadrupole moment. However, the magnetic moment is not very sensitive to the choice of the nucleon interaction potential but is affected by the mode of coupling, as has been pointed out by Lane.[1] Thus our magnetic moment is in good agreement with the experimental value.

One way to improve the results of this calculation is to include more configurations in the calculation and see the effect of the higher configurations on the ground

[16] F. Ajzenberg-Selove and T. Lauritsen, Nucl. Phys. **11**, 1 (1959); Ann. Rev. Nucl. Sci. **10**, 409 (1960).

state and the low-lying states. But since the most strongly interacting configurations are the ones which we have considered here, we feel that this may not make any big improvement in the results and will rather make this calculation more complicated. Probably the best way will be to use a different two-body potential. The nucleon-nucleon potential which we are using here has been fitted by the bound state properties of the very light nuclei, $2 \leqslant A \leqslant 4$. It may be that these parameters are not as good for the nuclear levels which we are considering here. A new set of parameters can be chosen by a least-square fit of the ground-state properties and low-lying states of one of the nuclei in which the closed $1p$ shell is either missing one or two nucleons or has one or two additional nucleons outside. Once these parameters are fixed they can be used for other nuclei and by comparing the results with the known experimental values we can check the accuracy of this type of calculation. Since in the Hamiltonian of this calculation we have not included a two-body spin-orbit interaction, therefore, another possibility which must be considered is that the nuclear Hamiltonian should contain an explicit two-body spin-orbit interaction.

ACKNOWLEDGMENT

One of the authors (N. U.) would like to thank Dr. C. E. Porter for a number of helpful discussions.

PHYSICAL REVIEW VOLUME 134, NUMBER 2B 27 APRIL 1964

Improved Superconductivity Approximation for the Pairing Interaction in Nuclei

YUKIHISA NOGAMI*

Division of Pure Physics, National Research Council, Ottawa, Canada and Department of Physics, Battersea College of Technology, London, England

(Received 23 December 1963)

The pairing interaction in nuclei is investigated by using a model Hamiltonian $H-\lambda_1 N-\lambda_2 N^2$, where H is the original Hamiltonian and N is the nucleon-number operator. The introduction of the term $\lambda_2 N^2$ enables one to suppress the effect of the nucleon-number fluctuation, which is inherent in the Bardeen-Cooper-Schrieffer (BCS) approximation and is a main source of its inaccuracy. A prescription is given to determine the parameters λ_1 and λ_2. The method is first illustrated in the case where all levels are degenerate, and then applied to realistic cases with nondegenerate levels. Quadrupole and other interactions are not considered. Excited states with seniority zero as well as those with nonzero seniority are discussed. The results obtained by this method are compared with those of Kisslinger and Sorenson and of Kerman, Lawson, and Macfarlane. For the ground-state energy an excellent accuracy is attained easily. It is observed that the BCS states obtained by Kisslinger and Sorenson are much better approximations to eigenstates of our model Hamiltonian rather than to those of their Hamiltonian. A new light is shed on the problem as to why the projected and renormalized BCS states are very good approximations to the true eigenstates.

1. INTRODUCTION

THE physical ideas and mathematical techniques developed in the theory of superconductivity[1] have been applied to the problem of the pairing interaction in nuclei to explain low-lying energy levels of heavy nuclei.[2] According to this theory, a system of nucleons which have pairing correlations between them can approximately be described as an assembly of free quasiparticles which are connected to the original nucleons by means of the Bogoliubov-Valatin transformation. It is characteristic of this method that the Bogoliubov-Valatin transformation is not commutable with the nucleon-number operator, and consequently the wave function which results does not correspond to a system having a definite number of nucleons. Energies and other quantities which are calculated with this wave function are then interpreted as averages of the corresponding quantities over a set of neighboring nuclei.

Once the Bogoliubov-Valatin transformation is exercised, it seems difficult, if not impossible, to remove the nucleon number fluctuation from the wave function without losing the essential merit of the theory, the energy gap. Lipkin[3] has suggested, however, that it would be possible to eliminate this effect from energy eigenvalues. He has proposed to use the model Hamiltonian

$$\mathcal{H}=H-f(N) \tag{1.1}$$

where H is the original Hamiltonian, N is the nucleon

* Present address: Department of Physics, Battersea College of Technology, London, England.

[1] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957); N. N. Bogoliubov, Zh. Eksperim. i Teor. Fiz. **34**, 58 (1958) [English transl.: Soviet Phys.—JETP **7**, 41 (1958)]; J. G. Valatin, Nuovo Cimento **7**, 843 (1958). This theory will be referred to as the BCS theory.

[2] A. Bohr, B. R. Mottelson, and D. Pines, Phys. Rev. **110**, 936 (1958); S. T. Belyaev, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **31**, No. 11 (1959); L. S. Kisslinger and R. A. Sorenson, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **32**, No. 9 (1960). KS will hereafter mean the last paper or its authors.

[3] H. J. Lipkin, Ann. Phys. (N. Y.) **9**, 272 (1960).