Toward a New Theory of Spherical Nuclei. II*

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A study is carried out of one of several possible mechanisms contributing to the quadrupole moment of the first excited (2^+) state of spherical nuclei. The possibility of a deformed solution is investigated for a set of Hartree-Bogoliubov equations describing the 2^+ state in an angular-momentum-conserving approximation. In the pairing–plus–quadrupole-quadrupole model, a sharp transition from spherical to deformed density distribution is shown to occur just beyond the value of the quadrupole coupling strength necessary to yield the 2^+ excitation energy.

I. INTRODUCTION

IN this paper we continue our exploration of mechanisms not contained in current microscopic theories of spherical nuclei, which may help explain the fact that the so-called one-phonon state exhibits an appreciable quadrupole moment.[1] One such mechanism has been suggested by Tamura and Udagawa,[2] namely the mixing of one- and two- phonon states. A more detailed discussion of the consequences of previous theories can be found in the same reference. In the preceding paper,[3] a second mechanism, referred to as the self-consistent blocking effect, which contributes to the enhancement of the quadrupole moment, is discussed in detail.

Here we shall discuss a third mechanism, which can be characterized as a Hartree-Bogoliubov calculation for the excited state. Again we find a self-consistent deviation from a spherical density distribution for this state, which indicates the relevance of this mechanism. But again the calculation is too severely restricted in scope to stand on its own feet and to be compared seriously with experiment. It seems clear that a complete and adequate theory will require an appropriate simultaneous consideration of all three mechanisms, but we feel that a separate discussion will give us some insight into the more general problem.

Our approach follows the methods developed in previous papers[4] on the generalized Hartree-Fock approximation. The observables of an even A-nucleon system corresponding to one-body operators can be expressed (in second quantization) in terms of amplitudes

$$\Psi_{J\mu\nu}(\alpha,IMS)=\langle J\bar{\mu}\nu(A-1)|a_\alpha|IMS(A)\rangle, \quad (1.1)$$

which connect the states of the A-nucleon system with those of the neighboring $(A-1)$-nucleon system. They thus correspond to parentage coefficients. In Sec. II we shall set up coupled equations of motion for the amplitudes (1.1) and additionally the amplitudes

$$\phi_{J\bar{\mu}\nu}{}^*(\bar{\alpha},\mathrm{IMS})=\langle J\bar{\mu}\nu(A-1)|a_{-\alpha}{}^\dagger|\mathrm{IMS}(A-2)\rangle, \quad (1.2)$$

which also enter in a natural way using the pairing-plus-quadrupole force model.[5] Section III gives a discussion of the approximations necessary to obtain the Hartree-Bogoliubov equations for the first excited state of "vibrational nuclei" and their relation to previous microscopic theories. In Sec. IV, the solution of these equations is discussed in detail. Results for the nuclei Ni^{62} and Cd^{114} are presented in Sec. V.

II. EQUATIONS OF MOTION

We consider as before a Hamiltonian[6] representing shell-model particles interacting via pairing and quadrupole forces,

$$H=\sum_{\alpha i} h_{\alpha i}a_{\alpha i}{}^\dagger a_{\alpha i}-\tfrac{1}{4}\sum_{i\alpha\beta} G_i(s_\alpha a_{\alpha i}{}^\dagger a_{-\alpha i}{}^\dagger)(s_\beta a_{-\beta i}a_{\beta i})-\tfrac{1}{2}\sum_{ij}\chi_{ij}\sum_{\alpha\beta\gamma\delta}\langle\alpha i|r^2Y_{2q}(\hat{r})|\gamma i\rangle\langle\delta j|r^2Y_{2q}(\hat{r})|\beta j\rangle a_{\alpha i}{}^\dagger a_{\beta j}{}^\dagger a_{\delta j}a_{\gamma i}, \quad (2.1)$$

where i and j are indices for the species of nucleon, proton, and neutron, $\alpha=(n_a,l_a,j_a,m_\alpha)$, and $\bar{\alpha}=-\alpha=(n_a,l_a,j_a,-m_\alpha)$. G and χ are the pairing and quadrupole force constants. With this Hamiltonian, the Heisenberg equations of motion

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[6] The quadrupole part of this Hamiltonian differs from the form given in Paper I by single-particle operators. Though Paper I follows Kisslinger and Sorensen, Ref. 5, only the definition of this paper allows the $h_{\alpha i}$ to be interpreted as shell-model energies. This difference does not affect any of our qualitative conclusions.

are[6] $[a=(n_a,l_a,j_a)]$

$$[a_{\alpha i},H]=(h_{\alpha i}+2F_{ai})a_{\alpha i}-\tfrac{1}{2}G_i s_\alpha a_{-\alpha i}{}^\dagger(\sum_\beta s_\beta a_{\beta i}a_{-\beta i})-X_i\sum_{\beta q}F_i(a,b)s_\beta(j_a j_b m_\alpha \bar{m}_\beta|2q)a_{\beta i}\Lambda_q{}^i, \tag{2.2}$$

$$[a_{-\alpha i}{}^\dagger,H]=-(h_{-\alpha i}-G_i)a_{-\alpha i}{}^\dagger-\tfrac{1}{2}G_i s_\alpha a_{\alpha i}(\sum_\beta s_\beta a_{\beta i}{}^\dagger a_{-\beta i}{}^\dagger)+X_i\sum_{\beta q}F_i(a,b)s_\alpha(j_a j_b m_\alpha \bar{m}_\beta|2q)a_{-\beta i}{}^\dagger\Lambda_q{}^i, \tag{2.3}$$

where all quantities are defined in I (2.3)–(2.7). The coupling constants χ_{ij} and X_{ij} are connected by the equation

$$X_{ij}=(5/4\pi)[N_i+\tfrac{3}{2}][N_j+\tfrac{3}{2}](\hbar/M\omega_0)^2\chi_{ij}\equiv(5/4\pi)\nu_i\nu_j\chi_{ij}. \tag{2.4}$$

The operators in Eqs. (2.2) and (2.3) are arranged in a specific order to facilitate the spectral decomposition into the amplitudes discussed in the Introduction.

If we take the matrix elements of (2.2) between states $|IMS(A)\rangle$ of an even nucleus with A particles and states $|J\bar{\mu}\nu(A-1)\rangle$ of an odd nucleus with $(A-1)$ particles and the matrix element of (2.3) between states $|IMS(A-2)\rangle$ of a neighboring even nucleus and $|J\bar{\mu}\nu(A-1)\rangle$, we obtain, respectively,[7]

$$\begin{aligned}&[W_{IS}(A)-W_{J\nu}(A-1)-h\alpha_i-2F_{ai}]\langle J\bar{\mu}\nu(A-1)|a_{\alpha i}|IMS(A)\rangle\\&=-\tfrac{1}{2}G_i s_\alpha\sum_n\langle J\bar{\mu}\nu(A-1)|a_{-\alpha i}{}^\dagger|n(A-2)\rangle\langle n(A-2)|\sum_\beta s_\beta a_{-\beta i}a_{\beta i}|IMS(A)\rangle-X_i\sum_{\beta q}F_i(a,b)s_\beta(j_a j_b m_\alpha\bar{m}_\beta|2q)\\&\qquad\times\sum_n\langle J\bar{\mu}\nu(A-1)|a_{\beta i}|n(A)\rangle\langle n(A)|\Lambda_q{}^i|IMS(A)\rangle,\end{aligned} \tag{2.5}$$

$$\begin{aligned}&[W_{IS}(A-2)-W_{J\nu}(A-1)+h_{\alpha i}-G_i]\langle J\bar{\mu}\nu(A-1)|a_{-\alpha i}{}^\dagger|IMS(A)\rangle\\&=-\tfrac{1}{2}G_i s\alpha\sum_n\langle J\bar{\mu}\nu(A-1)|a_{\alpha i}|n(A)\rangle\langle n(A)|\sum_\beta s_\beta a_{\beta i}{}^\dagger a_{-\beta i}{}^\dagger|IMS(A-2)\rangle+X_i\sum_{\beta q}F_i(a,b)(j_a j_b m_\alpha\bar{m}_\beta|2q)\\&\qquad\times\sum_n\langle J\bar{\mu}\nu(A-1)|a_{-\beta i}{}^\dagger|n(A-2)\rangle\langle n(A-2)|\Lambda_q{}^i|IMS(A-2)\rangle,\end{aligned} \tag{2.6}$$

where $W_N(B)=\langle N(B)|H|N(B)\rangle$. The sum over n should be extended over all contributing intermediate states. However, the number of such states is limited by the fact that the operator $\hat{\Delta}_i=\sum_\alpha s_\alpha a_{-\alpha i}a_{\alpha i}$ carries zero angular momentum and the other operator $\Lambda_q{}^i$ carries angular momentum 2. In terms of the amplitudes defined by Eqs. (1.1) and (1.2), the equations of motion (2.5) and (2.6) can be written in the form

$$\begin{aligned}&[W_{IS}(A)-W_{J\nu}(A-1)-h_{\alpha i}-2F_{ai}]\Psi_{J\mu\nu}{}^i(\alpha,IMS)\\&=-\tfrac{1}{2}G_i s_\alpha\sum_{s'}[\sum_{J'\mu'\nu'\beta}s_\beta\phi_{J'\mu'\nu'}{}^i(\bar{\beta},IMS')\Psi_{J'\mu'\nu'}{}^i(\beta,IMS)]\phi_{J\bar{\mu}\nu}{}^{i*}(\bar{\alpha},IMS')-\sum_{I'M'S'q\beta}[\sum_j X_{ij}\sum_{\gamma\delta}F_j(c,d)s_\delta\\&\qquad\times(j_c j_d m_\gamma\bar{m}_\delta|2q)\sum_{J'\mu'\nu'}\Psi_{J'\mu'\nu'}{}^{j*}(\delta,I'M'S')\Psi_{J'\mu'\nu'}{}^j(\gamma,IMS)]F_i(a,b)s_\beta(j_a j_b m_\alpha\bar{m}_\beta|2q)\Psi_{J\mu\nu}{}^i(\beta,I'M'S'),\end{aligned} \tag{2.7}$$

$$\begin{aligned}&[W_{IS}(A-2)-W_{J\nu}(A-1)+h_{\alpha i}-G_i]\phi_{J\bar{\mu}\nu}{}^{i*}(\bar{\alpha},IMS)\\&=-\tfrac{1}{2}G_i s_\alpha\sum_{S'}[\sum_{J'\mu'\nu'\beta}s_\beta\Psi_{J'\mu'\nu'}{}^{i*}(\beta,IMS')\phi_{J'\bar{\mu}'\nu'}{}^{i*}(\beta,IMS)]\Psi_{J\mu\nu}{}^i(\alpha,IMS')-\sum_{I'M'S'q\beta}[\sum_j X_{ij}\sum_{\delta\gamma}F_j(c,d)s_\delta\\&\qquad\times(j_c j_d m_\gamma\bar{m}_\delta|2q)\sum_{J'\mu'\nu'}\phi_{J'\bar{\mu}'\nu'}{}^{j*}(\gamma,IMS)\phi_{J'\bar{\mu}'\nu'}{}^j(\delta,I'M'S')]F_i(a,b)s_\beta(j_a j_b m_\alpha\bar{m}_\beta|2q)\phi_{J\bar{\mu}\nu}{}^{i*}(\bar{\beta},I'M'S').\end{aligned} \tag{2.8}$$

In addition to the equations of motion (2.7) and (2.8), we have the following sum rules for the amplitudes Ψ and ϕ^*:

$$\begin{aligned}\langle I'M'S'|\{a_{\alpha i}{}^\dagger,a_{\beta i}\}|IMS\rangle&=\sum_{J\mu\nu}[\Psi_{J\mu\nu}{}^{i*}(\alpha,I'M'S')\Psi_{J\mu\nu}{}^i(\beta,IMS)+\phi_{J\mu\nu}{}^i(\beta,I'M'S')\phi_{J\mu\nu}{}^{i*}(\alpha,IMS)]\\&=\delta_{\alpha,\beta}\delta_{II'}\delta_{MM'}\delta_{SS'},\end{aligned} \tag{2.9}$$

$$\langle IMS(A)|\sum_\alpha a_{\alpha i}{}^\dagger a_{\alpha i}|IMS(A)\rangle=\sum_{J\mu\nu}|\Psi_{J\mu\nu}{}^i(\alpha,IMS)|^2=A_i. \tag{2.10}$$

[7] Note that we are using two odd systems. If the even system is specified by the total number of particles A, the neutron number N, and the proton number Z, the two systems are $[(A-1),N,(Z-1)]$, $[(A-1),(N-1),Z]$. The $(A-2)$ system has N, $(Z-2)$ or $(N-2)$, Z.

Furthermore, we have self-consistency conditions for the energies

$$W_{IS}(A)=\langle IMS(A)|H|IMS(A)\rangle,$$
$$W_{IS}(A-2)=\langle IMS(A-2)|H|IMS(A-2)\rangle, \qquad (2.11)$$

which can be expanded in the same manner as the equations of motion.

Equations (2.7) and (2.8) here constitute a set of coupled nonlinear equations for the amplitudes Ψ and ϕ^* and the energies $W_{J\nu}(A-1)$. The conditions (2.9) and (2.10) serve as normalization conditions and consistency checks for the amplitudes.

The only approximation made so far is

$$\langle J\bar{\mu}\nu(A+1)|a_\alpha^\dagger|IMS(A)\rangle \cong \langle J\bar{\mu}\nu(A-1)|a_\alpha^\dagger|IMS(A-2)\rangle,$$

which is used to obtain (2.9). An exact treatment of number conservation should, however, be aspired to in a more complete theory.

Even so, an exact solution of the equations of motion is a rather formidable task and we have to resort to a series of further approximations using available experimental information as a guide.

III. APPROXIMATION SCHEMES

This experimental guidance is supplied, e.g., by a consideration of the quadrupole operator Q_{2q}. Its matrix elements between the states $|IMS(A)\rangle$ can be expressed as

$$\langle IMS(A)|Q_{2q}|I'M'S'(A)\rangle = \sum_{\alpha\beta i}\langle\alpha i|Q_{2q}{}^i|\beta i\rangle\sum_{J\mu\nu}\langle IMS(A)|a_{\alpha i}{}^\dagger|J\bar{\mu}\nu(A-1)\rangle \times\langle J\bar{\mu}\nu(A-1)|a_{\beta i}|I'M'S'(A)\rangle. \qquad (3.1)$$

Here $\langle\alpha i|Q_{2q}{}^i|\beta_i\rangle$ is a shell-model matrix element of either the $E2$ transition operator or the static quadrupole moment operator.

Having specified a set of single-particle states j_a, j_b, j_c, $\cdots$, the question to be considered is which states of the $(A-1)$-nucleon systems contribute to the intermediate sum. For the sake of simplicity we restrict ourselves to the ground state and the first excited 2^+ state of the A-nucleon system. Several situations now obtain.

If each of the amplitudes in Eq. (3.1) is appreciable only for one choice of j_a, we are in the weak-coupling limit. The states of the $(A-1)$-nucleon systems can be classified by the "parent" state of the A-nucleon core and the hole coupled to it.

$$|J\bar{\mu}\nu\rangle\cong|J\bar{\mu}(j_a,IS)\rangle. \qquad (3.2)$$

The dominant amplitudes are then

$$\langle J\bar{\mu}\nu|a_\alpha|IMS\rangle\cong\langle J\bar{\mu}(j_aI_s)|a_\alpha|IMS\rangle. \qquad (3.3)$$

In this limit one finds for the density in Eq. (3.1)

$$\langle IMS|a_\alpha{}^\dagger a_\beta|I'M'S'\rangle \cong\sum_{J=|j_a-I|}^{j_a+I}\sum_\mu\langle IMS|a_\alpha{}^\dagger|J\bar{\mu}(j_aIS)\rangle \times\langle J\bar{\mu}(j_a,IS)|a_\alpha|IMS\rangle\delta_{\alpha\beta}\delta_{II'}\delta_{SS'}\delta_{MM'}. \qquad (3.4)$$

It is borne out by our subsequent calculation that the densities of the ground state and the first excited state are approximately equal in this limit,

$$\langle 2M|a_\alpha{}^\dagger a_\alpha|2M\rangle\cong\langle 00|a_\alpha{}^\dagger a_\alpha|00\rangle, \qquad (3.5)$$

which is the assumption of the BCS theory. Referring to Eqs. (3.1), (3.4), and (3.5), we see that this theory does not allow for either a quadrupole moment of the 2^+ state or an $E2$ transition from the 2^+ to the ground state.

If one goes on to the random phase approximation (RPA) one mixes in the (presumably first-order) off-diagonal amplitudes

$$\langle J\bar{\mu}(j_a\nu_{I'S'})|a_\alpha|IMS\rangle, \quad (I'S'\neq I,S) \qquad (3.6a)$$

besides the diagonal ones (zero order)

$$\langle J\bar{\mu}(j_a\nu_{IS})|a_\alpha|IMS\rangle. \qquad (3.6b)$$

The notation for the states of the odd system indicates that one effectively has a weak mixing of the states found in the previous limit with respect to the core parentage. The subscript stresses the main core parent. This limit allows for an $E2$ transition (of first order) and as noted in the previous paper, a correction to the quadrupole moment of the 2^+ state of second order. It can be characterized as phonon mixing in the weak-coupling limit.

A third possibility arises when there is mixing such that each of the states $|J\mu\nu\rangle$ can be reached easily by coupling *different* holes to the same core state. The dominant amplitudes are now of the form

$$\langle J\bar{\mu}\nu|a_\alpha|IMS\rangle\cong\langle J\bar{\mu}\nu(a,IS)|a_\alpha|IMS\rangle, \qquad (3.7)$$

where the notation of the odd states indicates that there is mixing with respect to the multiple hole parentage. This situation can be obtained in both the intermediate- and strong-coupling limits and can be described as particle mixing. In this case the angular momentum coupling of one hole to the core is closely related to that of the other holes present, and we can thus expect a coherence effect leading to a permanent quadrupole deformation.

In the remainder of this article we will investigate the consequences of the assumption that amplitudes of the type (3.7) are the only dominant ones. The solution of the equations of motion then decomposes into separate problems for each core state. This is clearly not a good approximation to the physical situation, as the value of the $E2$ transition rate for the 2^+ to ground-state transition requires

$$\langle 2^+M|a_\alpha{}^\dagger a_\beta|00\rangle \cong \langle 2^+2|a_\alpha{}^\dagger a_\beta|2^+2\rangle. \quad (3.8)$$

This condition cannot be satisfied with the amplitudes (3.7) alone. In fact

$$\langle 2^+M|a_\alpha{}^\dagger a_\beta|00\rangle \cong 0$$

in this approximation.

The preceding arguments and the results of Paper I indicate that a fully adequate solution of the problem has to include both phonon and particle mixing at the same level. The results of Tamura and Udagawa[2] show that it is necessary to include the effect of "higher-phonon" states. As a typical value of the quadrupole moment of a "vibrational" nucleus like Cd^{114} is approximately 6 single-particle units, we are in an intermediate-coupling situation.

IV. HARTREE-BOGOLIUBOV EQUATIONS FOR THE 2^+ STATE

It was mentioned in the preceding section that under the assumption of only "particle mixing," we obtain separate sets of equations of motion for the different A-nucleon core states. For the ground state we thus retain the usual BCS equations.

For the first excited 2^+ state, we then have only amplitudes of the type

$$\Psi_{J\mu\nu}{}^i(\alpha,2q)=\langle J\bar{\mu}\nu(A-1)|a_{\alpha i}|2q(A)\rangle$$

and (4.1)

$$\phi_{J\bar{\mu}\nu}{}^{i*}(\bar{\alpha},2q)=\langle J\bar{\mu}\nu(A-1)|a_{-\alpha i}{}^\dagger|2q(A-2)\rangle,$$

where the states $|J\bar{\mu}\nu(A-1)\rangle$ are an admixture of states of a one-phonon state coupled with a hole (particle). Therefore, the angular momentum $\mathbf{J}$ satisfies

$$\mathbf{J}=\mathbf{j}_a+\mathbf{2}, \quad (4.2)$$

where $\mathbf{j}_a$ is the angular momentum of the single particle. For convenience, we introduce the following definitions:

$$\begin{aligned} e_{J\nu}&=W_0(A)-W_{J\nu}(A-1),\\ \omega_I(A)&=W_I(A)-W_0(A), \quad (4.3)\\ 2\lambda(A)&=W_0(A)-W_0(A-2),\\ 2\lambda_1{}^i(A)&=2\lambda(A)+G_i,\\ \epsilon_{\alpha i}&=h_{\alpha i}+F_{\alpha i}-\lambda_1{}^i,\\ E_{J\nu i}&=-e_{J\nu}+\lambda_1{}^i. \end{aligned}$$

We also introduce the reduced amplitudes u and v by

$$\Psi_{J\mu\nu}{}^i(\alpha,2q)\equiv s_\alpha(j_aJm_\alpha-\mu|2q)v_i(J\nu,a), \quad (4.4)$$

$$\phi_{J\bar{\mu}\nu}{}^{i*}(\bar{\alpha},2q)\equiv(j_aJm_\alpha-\mu|2q)u_i(J\nu,a). \quad (4.5)$$

Equations (2.9)–(2.12) are then reduced to the simple forms

$$[-E_{J\nu i}-F_{ai}+\omega_2(A)]v_i(J\nu,a)=\epsilon_{ai}v_i(J\nu,a) -\Delta_2{}^iu_i(J\nu,a)+\sum_b \Lambda_{J\nu}{}^i(a,b)v_i(J\nu,b), \quad (4.6)$$

$$[-E_{J\nu i}-F_{ai}+\omega_2(A-2)]u_i(J\nu,a)=-\epsilon_{ai}u_i(J\nu,a) -\Delta_2{}^iv_i(J\nu,a)+\sum_b \Lambda_{J\nu}{}^{i'}(a,b)u_i(J\nu,b), \quad (4.7)$$

$$\sum_\nu\left\{|v_i(J\nu,a)|^2-\sum_{J'}(2J+1)\begin{Bmatrix}2 & j_a & J\\ 2 & j_a & J'\end{Bmatrix} \times|u_i(J'\nu,a)|^2\right\}=\tfrac{1}{5}(2J+1), \quad (4.8)$$

$$\sum_{J\nu a}|v_i(J\nu,a)|^2=A_i, \quad (4.9)$$

where

$$\Delta_2{}^i=\tfrac{1}{2}G_i\sum_{J\nu b}u_i(J\nu,b)v_i(J\nu,b), \quad (4.10)$$

$$\Lambda_{J\nu}{}^i(a,b)=-25\sum_j X_{ij}\left[\sum_{j_cj_dJ'\nu'}(-)^{J'+j_d}\begin{Bmatrix}2 & 2 & 2\\ j_c & j_d & J'\end{Bmatrix} \times F_j(c,d)v_j(J'\nu',j_c)v_j(J'\nu',j_d)\right](-)^{J+j_b} \times\begin{Bmatrix}2 & 2 & 2\\ j_a & j_b & J\end{Bmatrix}F_i(a,b). \quad (4.11)$$

$\Lambda_{J\nu}{}^{i'}(a,b)$ has the same form as $\Lambda_{J\nu}{}^i(a,b)$ except that $v_i(J'\nu',j_c)$, $v_i(J'\nu',j_d)$ are replaced by $u_i(J'\nu',j_c)$, $u_i(J'\nu',j_d)$, respectively.

If we ignore the difference between $\omega_2(A)$ and $\omega_2(A-2)$, Eqs. (4.6) and (4.7) can be solved to determine the eigenvectors

$$\begin{pmatrix}v\\u\end{pmatrix}$$

with the eigenvalues $(-E+\omega_2)$. Equation (4.8) serves as a normalization condition. Equation (4.9) is used as a check on the solution. We shall not in this simplified theory utilize the self-consistency condition (2.11) for the even nuclei energies. With the final solution one can calculate the quadrupole moment of the 2^+ state by the equation

$$Q_2=10(2220|22)\left[\sum_i e_{\text{eff}}{}^i\sum_{J\nu ab}(-)^{J+j_b} \times\begin{Bmatrix}2 & 2 & 2\\ j_a & j_b & J\end{Bmatrix}\nu_iF_i(ab)v_i(J\nu,a)v_i(J\nu,b)\right], \quad (4.12a)$$

or, alternatively (to be used as a check),

$$Q_2=-10(2220|22)\Bigg[\sum_i e_{\rm eff}{}^i \sum_{J\nu ab}(-)^{J+j_b}\times\begin{Bmatrix}2 & 2 & 2\\ j_a & j_b & J\end{Bmatrix}v_iF_i(ab)u_i(J\nu,a)u_i(J\nu,b)\Bigg]. \quad (4.12b)$$

The actual solution of Eqs. (4.6) and (4.7), however, involves a number of subtleties which require further consideration. The general method of solution is an iteration process. We determine a reasonable initial set of values $v^{(0)}$, $u^{(0)}$ to calculate $\Delta_2{}^i$, $\Lambda_{J\nu}{}^i$, and $\Lambda_{J\nu}{}^{i\prime}$ in the zeroth-order iteration. This set is obtained by spreading out the solution of the ground-state calculation [see I, Eqs. (3.8) and (3.9)] for each j_a over all the J states

$$J=j_a+2,\cdots,|j_a-2|. \quad (4.13)$$

The ground-state calculation provides at the same time values for $\lambda_1{}^i$. In principle, a value of $\lambda_1{}^i$ could, as in the ground-state calculation, be determined using the condition (4.9). Because of the approximations involved, this value would generally deviate from the ground-state value.

With the calculation of the Hartree-Fock pairing and quadrupole potentials $\Delta^{(0)}$ and $\Lambda^{(0)}$ ($\Lambda^{(0)\prime}$), we have reduced the problem to a linear one which can be solved with standard methods. With the usual matrix diagonalization process, we obtain a normalization of the form (the eigenstates are labeled by $J\nu$)

$$\sum_a [|v_i{}^{(1)\prime}(J\nu,a)|^2+|u_i{}^{(1)\prime}(J\nu,a)|^2]=1. \quad (4.14)$$

The superscript indicates the first iteration, the prime preliminary normalization.

It is a particularity of the pairing Hamiltonian to give redundant solutions. The selection of the "physical" states was carred out using the following equivalent criteria:

$$(E_{J\nu i}-\omega_2)_{\rm physical}>(E_{J\nu i}-\omega_2)_{\rm unphysical},$$

$$[\sum_a u_i'(J\nu,a)v_i'(J\nu,a)]_{\rm physical} >[\sum_a u_i'(J\nu,a)v_i'(J\nu,a)]_{\rm unphysical} \quad (4.15)$$

at any state of the iteration. These criteria are in analogy to the ones used in the BCS ground-state calculation.

After the selection of the physical states, we have to connect the normalization (4.14) with the normalization (4.8). From Eq. (4.14) we can extract that the preliminary eigenvectors v' and u' can differ from the properly normalized ones only by a factor depending on J and ν. We express this fact by the relations

$$|v_i{}^{(1)}(J\nu,a)|^2=(N_{J\nu i}{}^{(1)})^2\tfrac{1}{5}(2J+1)|v_i{}^{(1)\prime}(J\nu,a)|^2,$$
$$|u_i{}^{(1)}(J\nu,a)|^2=(N_{J\nu i}{}^{(1)2})^2\tfrac{1}{5}(2J+1)|u_i{}^{(1)\prime}(J\nu,a)|^2. \quad (4.16)$$

Substituting (4.16) into (4.8), one obtains systems of linear inhomogeneous equations for $(N_{J\nu i}{}^{(1)})^2$. We have to keep in mind though that the relations (4.8) involve two approximations, the replacement of $u(A)$ by $u(A-2)$ and the truncation of the intermediate sum to a special set of states $|J\bar{\mu}\nu\rangle$. The error involved can be expressed generally by multiplying the right-hand side of each of the Eq. (4.8) by an appropriate factor $n_{ai}<1$. A brief investigation showed that the solution $(N_{J\nu i})^2$ can in some cases depend very sensitively on the values of n_{ai}. For example, a variation of the inhomogeneous terms by maximally 5% gave a variation of some of the $N_{J\nu i}{}^2$ of more than 100% in a model case, adapted to our calculation for Cd^{114}. This point will be taken up again in the presentation of our results.

With the properly normalized solution of the first iteration $v^{(1)}$, $u^{(1)}$ we can repeat the cycle described above, until the nth solution differs only by a prescribed amount from the $(n-1)$th solution.

V. RESULTS AND DISCUSSION

Utilizing the approximations described in the previous sections, we calculated the quadrupole moment of Cd^{114} and Ni^{62}. All single-particle levels are taken from Kisslinger and Sorensen.[5]

For Cd^{114}, the pairing force constants G_i are fixed at the values of Kisslinger and Sorensen, and the quadrupole force constants χ_{ij} are taken to be $\chi_{nn}=\chi_{pp}=\chi_{np}=\chi$. The quadrupole moment of Cd^{114} is calculated for various values of χ by using an effective charge $e_{\rm eff}{}^n=0.8$. The results are shown in Table I. We see

TABLE I. Quadrupole moment of Cd^{114} calculated by means of a self-consistent theory of the 2^+ state. With the exception of line 2,[a] the parameters χ_{ij} are all set equal in this calculation, and X is defined by $X=(5/4\pi)b^4\chi$, where b is the fundamental length of the harmonic-oscillator problem. The effective charge for neutron $e_{\rm eff}{}^{(n)}$ is taken as 0.8.

X (MeV)	Q_2 (10^{-24} cm^2)
0.034[b]	−0.00121
See caption[a]	−0.00126
0.0352[c]	−0.00292
0.037	−1.83
0.038	−1.86
0.042	−1.92
0.051	−1.95

[a] χ_{ij} are the same as those in line 3, Table I, of Paper I. The χ value was fitted to the energy at the 2^+ state using the RPA.
[b] The X value was fitted to the energy at the 2^+ state using the RPA.
[c] This value was chosen to give a 2^+ energy 25% smaller than the experimental value.

TABLE II. Quadrupole moment of Ni^{62} calculated by using the parameters $G_n = 0.3$ and $e_{eff}^{(n)} = 1.0$.

X (MeV)	Q_2 (10^{-24} cm^2)
0.0864	−0.000227
0.0987	−0.000371
0.111	−0.00390
0.123	−0.117
0.136	−0.212

a sharp phase transition at about $X = 0.036$. While the first three lines show almost spherical solutions, the quadrupole moment increases sharply from almost zero to a large value within only a few percent change in X, and then it stays nearly constant for a further increase of this coupling constant. It is interesting to note that the value of X which yields $\omega_2 = 0$ in the RPA is 0.0363. Thus the deformation due to the mechanism considered in this paper occurs in the range of X where the RPA no longer yields physically acceptable results. This is an indication that the particle mixing alone is insufficient to produce the experimentally observed large deformation of the first excited 2^+ state (at least for Cd^{114}). However, we consider the closeness of the value of X needed to produce a large deformation to the value which yields the correct 2^+ state energy to be an encouragement for a more ambitious study.

For Ni^{62}, Thankappan and True[8] have argued from a study of Cu^{63} using a core-particle coupling model that the quadrupole moment of the 2^+ state of Ni^{62} should be about 0.191 b. Although their treatment may be open to some question, it is probable that the first 2^+ state of Ni^{62} has a large quadrupole moment. The suggested value of the quadrupole moment again is about the same magnitude as the quadrupole transition matrix element $\langle 0|Q_2|2\rangle$. A calculation using $X = 0.151$, $G_n = 0.42$, and $e_{eff}^n = 1.0$, which are normally accepted values in the RPA, yields $Q_{2^+} = -0.0424$ b. A series of calculations using $G_n = 0.3$ and variable X yields the results shown in Table II. The small G value is used because of the fast convergence in computer calculation and for the purpose of seeing the variation of Q_{2^+} with X. Again we see a sharp phase transition at around $X = 0.12$. Comparing the values of Q_2 in Table II, we see that the physical values of the force constants quoted above lie in the transition region.

We used the normalization $N_{J\nu i}^2 = 1$ in the calculation of Cd^{114} since the more satisfactory normalization (4.8) gave imaginary roots for $N_{J\nu i}$. A countercheck of the normalization (4.8) showed that it was satisfied to within an average of 15% by the choice of $N_{J\nu i}^2 = 1$. Such difficulty in the normalization should disappear eventually in a more complete treatment in which the particle number conservation and off-diagonal amplitudes are taken into account. However, the tentative normalization employed in this case probably does not affect the quadrupole moment too much. For Ni^{62} where such difficulty did not arise, the difference in the quadrupole moments between the two normalizations was less than 4%.

The results of this calculation and the results reported in I indicate strongly that both phonon mixing (mechanism of Paper I) and particle mixing (mechanism of this paper) whould be included simultaneously to account for the quadrupole deformation of the first excited 2^+ state of so-called spherical nuclei. Such a treatment is possible within the framework of the general formalism given in Sec. II of this paper by retaining off-diagonal amplitudes and higher excited states, possibly the two-phonon states. We shall report our progress in such a direction in future papers.

[8] V. K. Thankappan and W. W. True, Phys. Rev. **137**, B793 (1965).