Diabatic Approach to Shape Coexistence Phenomena in Semi-Magic Nuclei. I

Illustration of Basic Ideas

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A new microscopic method based on the diabatic picture is proposed to describe the low-lying deformed excited 0+ states in semi-magic nuclei. In this method, the couplings between anharmonic shape vibrations associated with different Hartree-Fock-Bogoliubov minima are diagonalized after constructing the diabatic basis. Basic ideas are illustrated for three kinds of exactly solvable models. Several examples are given which exhibit well localized deformed wave functions around the second minimum of the collective potential. It is possible that such deformed excited states well retain their identities against the mixing with the spherical configurations, even when their existence can hardly be expected from the properties of the adiabatic potential-energy functions.

§ 1. Introduction

In recent years, deformed excited states with $I^*=0^+$ have been systematically observed in semi-magic Sn isotopes$^{11-15}$ and Pb isotopes$^{6-10}$ whose ground states are spherical. They appear very low in excitation energy and retain their identities suggesting that mixings with the spherical ground states are small. These experimental data may therefore be regarded as typical examples of shape coexistence phenomena. The deformed excited 0+ states are associated with proton two-particle-two-hole (2p-2h) excitations across the closed shells ($Z=50$ or 82)$^{11-15}$ Their excitation energies are drastically lowered mainly by the pairing correlations among the protons and by the quadrupole correlations between the protons and the neutrons$^{11-15}$. In the Nilsson picture, we have down-sloping and up-sloping single-particle levels as functions of quadrupole deformation. It is then easily confirmed that the 2p-2h excited configurations, where two particles lie in the down-sloping levels and two holes in the up-sloping levels, have finite equilibrium deformations. In the adiabatic potential energy surface plotted as a function of quadrupole deformation, we expect to have second minimum corresponding to the 2p-2h excited configurations. The excitation energy of deformed excited state may be roughly estimated from the energy difference between the first and the second minima.

Quite recently, Bengtsson and Nazarewicz$^{16}$ have shown that the diabatic potential-energy functions defined by switching off the interaction between the 2p-2h configuration and the ground-state configuration give more accurate estimate for the excitation energies of the deformed excited 0+ states in Pb isotopes than the conventional adiabatic potential-energy functions. This suggests that the couplings between the deformed and the spherical states in semi-magic nuclei of interest will not be correctly described in terms of the conventional adiabatic theory of collective motions.
In this paper, we propose a new microscopic approach for treating the shape coexistence phenomena. This approach is based on the diabatic picture. Namely, we first define two diabatic configurations which correspond to the deformed and the spherical states, neglecting the couplings between them. The coupling between two kinds of states is then diagonalized in the second step. We use the \((\eta^*, \eta)\) expansion method based on the selfconsistent-collective-coordinate (SCC) method\(^{17}\) in order to describe collective motions associated with individual diabatic configurations. The couplings between the two kinds of collective motion are then treated in a manner similar to the well-known coupled channel method. Our method may thus be regarded as a coupled channel version of the SCC method. For convenience, in this paper we call our method “coupled-configuration SCC method”. The formulation is given in \(\S\ 2\). We shall illustrate usefulness of our approach by applying our method to three kinds of exactly solvable models; i.e., the particle-plus-harmonic-core model (\(\S\ 3\)), the particle-plus-anharmonic-core model (\(\S\ 4\)) and the multi-O(4) model (\(\S\ 5\)). These models may be useful to study various problems of collective dynamics accompanying level crossings in the single-particle spectrum. We shall present in \(\S\S\ 3\sim 5\) typical examples that exhibit deformed excited states with localized wave functions. It is worth emphasizing that such localized wave functions exist even when their existence can hardly be expected from the properties of the adiabatic potential-energy functions. Conclusions are given in \(\S\ 6\).

\(\S\ 2\). Outline of the method

We assume that the system under consideration has two local minima in the collective potential energy function. We proceed in two steps. In the first step, we construct classical collective Hamiltonians describing diabatic collective vibrations about the individual local minima. For this purpose, we use the \((\eta^*, \eta)\) expansion method\(^{17}\) about the individual Hartree-Bogoliubov (HB) stationary states corresponding to the local minima. In the second step, we construct the total Hamiltonian taking into account the coupling between the two diabatic collective vibrations and quantize it.

2.1. Diabatic collective Hamiltonian for each configuration

Let us express the individual HB vacua by \(|\phi_i(0)\rangle\) with \(i=1\) and \(2\). The time-dependent (TD) HB state vectors evolving from these static HB vacua can be written in the following form:

\[
|\psi(\eta^*_i, \eta_i, \phi_i, N_i)\rangle = e^{-i\phi_i N_i} e^{i\tilde{G}_i(\eta^*_i, \eta_i, N_i)} |\phi_i(0)\rangle , \quad i=1, 2 ,
\]  
(2.1)

where \(\eta^*_i\) and \(\eta_i\) are time-dependent collective variables describing the collective vibrations around the \(i\)-th local minima. The operator \(e^{-i\phi_i N_i}\), \(N_i\) being the number operator, is introduced in order to eliminate the spurious number-fluctuations associated with the use of the TDHB approximation.\(^{18}\) Here \(\phi_i\) are the angle variables conjugate to the nucleon number \(N_i\). They are treated as classical dynamical variables. The operator \(i\tilde{G}_i\) can be written in terms of the quasiparticle creation and
Diabatic Approach to Shape Coexistence Phenomena in Semi-Magic Nuclei. I

annihilation operators \((a_{\nu}^\dagger, a_{\nu})\), defined with respect to the individual static HB solutions \(|\phi_i(0)\rangle\) and satisfying \(a_{\nu}|\phi_i(0)\rangle = 0\), as follows:

\[
i \tilde{G}(\eta_i^*, \eta_i, N_i) = \sum_{\mu, \nu} \{ G_{\mu\nu}(\eta_i^*, \eta_i, N_i) a_{\nu}^\dagger a_{\nu} - G_{\mu\nu}^*(\eta_i^*, \eta_i, N_i) a_{\nu} a_{\nu}^\dagger \}.
\]

Note that the TDHB state vectors are normalized to unity and their time developments are here treated as a unitary transformation parametrized by the time-dependent collective variables \((\eta_i^*, \eta_i, \phi_i)\). The basic equations of the SCC method that determine the unknown functions \(G_{\mu\nu}(\eta_i^*, \eta_i, N_i)\) are

1) Equations of collective submanifold

\[
\delta \langle \phi_i(0) | e^{-i\tilde{G}((H - i\tilde{\eta}_i \frac{\partial}{\partial \eta_i} - i\tilde{\eta}_i^* \frac{\partial}{\partial \eta_i^*} - i\tilde{N})} e^{i\tilde{G}} | \phi_i(0) \rangle = 0,
\]

where \(\tilde{\eta}_i = d\eta_i/dt = -i \partial \mathcal{H}_i/\partial \eta_i, \tilde{\eta}_i^* = d\eta_i^*/dt = i \partial \mathcal{H}_i/\partial \eta_i^*\) and \(\tilde{N} = d\phi_i/dt = \partial \mathcal{H}_i/\partial N_i\).

2) Canonical variables conditions

\[
\begin{align*}
\langle \phi_i(0) | e^{-i\tilde{G}} \frac{\partial}{\partial \eta_i} e^{i\tilde{G}} | \phi_i(0) \rangle & = \frac{1}{2} \eta_i^* , \\
\langle \phi_i(0) | e^{-i\tilde{G}} \frac{\partial}{\partial \eta_i^*} e^{i\tilde{G}} | \phi_i(0) \rangle & = -\frac{1}{2} \eta_i, \\
\langle \phi_i(0) | e^{-i\tilde{N}} e^{i\tilde{G}} | \phi_i(0) \rangle & = N_i, \\
\langle \phi_i(0) | e^{-i\tilde{N}} \frac{\partial}{\partial N_i} e^{i\tilde{G}} | \phi_i(0) \rangle & = 0,
\end{align*}
\]

where \(H\) is the microscopic Hamiltonian for the system under consideration. The collective Hamiltonian describing the vibrations about the individual HB local minima are defined as

\[
\mathcal{H}_i(\eta_i^*, \eta_i, N_i) = \langle \phi_i(0) | e^{-i\tilde{G}} H e^{i\tilde{G}} | \phi_i(0) \rangle.
\]

The above basic equations are solved by expanding the unknown functions \(G_{\mu\nu}(\eta_i^*, \eta_i, N_i)\) in power series of the collective variables \(\eta_i^*, \eta_i\) and \((N_i - N_0)\) as

\[
G_{\mu\nu}(\eta_i^*, \eta_i, N_i) = \sum_{r,s} g_{\mu\nu}^{(r,s)}(\eta_i^*)^r(\eta_i)^s(N_i - N_0)^t,
\]

where \(N_0 = \langle \phi_i(0) | \hat{N} | \phi_i(0) \rangle\). Correspondingly, the collective Hamiltonian \(\mathcal{H}_i(\eta_i^*, \eta_i, N_i)\) are also expanded as

\[
\mathcal{H}_i(\eta_i^*, \eta_i, N_i) = \sum_{r,s} h_{\mu\nu}^{(r,s)}(\eta_i^*)^r(\eta_i)^s(N_i - N_0)^t.
\]

The unknown coefficients \(g_{\mu\nu}^{(r,s)}\) and \(h_{\mu\nu}^{(r,s)}\) are determined such that the basic equations, (2.3) and (2.4), are satisfied in each order of the expansion. In fact, we can put \(N_i - N_0 = 0\) so that the \(t \neq 0\) terms in the above expansions are unnecessary below. The lowest-order terms of the expansion can be determined by the RPA type boundary condition. In this paper, we consider up to the third order \((r + s \leq 3)\) for \(G_{\mu\nu}\) and to the fourth order \((r + s \leq 4)\) for \(\mathcal{H}_i\). We shall see in §§ 3~5 that \(\mathcal{H}_i\) thus constructed indeed describe diabatic collective vibrations about the individual HB
2.2. Coupled-configuration collective Schrödinger equation

Let us next consider the coupling between the collective vibrations \(\{|\varphi_i(\eta^*, \eta_i, \phi_i, N_i)\rangle; i=1,2\rangle\) associated with the different diabatic configurations (coexisting HB minima). Now we suppose that the two collective variables, \((\eta^*, \eta_i)\) and \((\eta^*_i, \eta)\), describe essentially the same collective degrees of freedom which are connected with the quadrupole shape. The collective variables \((\phi_i, N_i)\) representing the pairing rotations should also be the same irrespective of the configuration \(i\). On the basis of this idea, we introduce the collective coordinates \((\eta^*, \eta, \phi, N)\) which are globally defined over all the diabatic vibrations. The global collective coordinates \((\eta^*, \eta, \phi, N)\) must be connected with the diabatic collective coordinates \((\eta^*_i, \eta_i, \phi_i, N_i)\) by canonical transformations. Taking into account up to the linear order of the transformation, we assume the following relations:

\[
\begin{align*}
(\eta_i, \eta^*_i) &= (x_i, y_i) \begin{pmatrix} \eta - \eta^*_i \\ \eta^* - \eta^*_i \end{pmatrix}, \\
(\phi_i, N_i) &= (\phi, N), \\
(x_i, y_i) &= \frac{z_i \pm z_i^{-1}}{2}.
\end{align*}
\tag{2.8}
\]

\[
(\eta^* = \eta^*_i, \eta = \eta_i, \phi = \phi_i, N = N_i) = (\eta^*_i, \eta_i, \phi_i, N_i). \tag{2.9}
\]

Here the variables \((\eta^*, \eta)\) represent the collective degrees of freedom related with the quadrupole shape motion of the nucleus, and \((\phi, N)\) represent the gauge angle and the nucleon number. The constants \(\eta^*_i\) represent the equilibrium quadrupole deformations of the \(i\)-th HB states \(|\varphi_i(0)\rangle\), and are real because the HB states are static and time-even. The parameters \(z_i(>0)\) are introduced so that scales of the collective coordinates \((\eta^*_i, \eta_i)\) can be adjusted.

The constants \(\eta^*_i\) and \(z_i\) can be determined in the following way. Expectation value \(\langle\varphi_i(\eta^*_i, \eta_i, \phi_i, N_i)|\hat{Q}|\varphi_i(\eta^*_i, \eta_i, \phi_i, N_i)\rangle\) of the quadrupole moment \(\hat{Q}\), which represents the shape of the nucleus, can be calculated for each diabatic configuration by means of the \((\eta^*_i, \eta_i)\) expansion. It is then expressed in terms of the global collective coordinates \((\eta^*, \eta, \phi, N)\) by using Eq. (2.8) and can be Taylor-expanded:

\[
\begin{align*}
Q_i(\eta^*, \eta) &= \langle\varphi_i(\eta^*, \eta_i, \phi_i, N_i)|\hat{Q}|\varphi_i(\eta^*, \eta_i, \phi_i, N_i)\rangle \\
&= Q \big|_{\eta^* = \eta = 0} + \frac{\partial Q}{\partial \eta} \bigg|_{\eta^* = \eta = 0} (\eta^* + \eta) + \cdots, \tag{2.10}
\end{align*}
\]

where \(\eta_i(\eta^*, \eta)\) represents the right-hand side of Eq. (2.8) and we put \(N = N_0\). The quadrupole moment should be zero at \(\eta^* = \eta = 0\) (spherical limit), and it should have the same dependence on the collective coordinates irrespective of the configurations.
Diabatic Approach to Shape Coexistence Phenomena in Semi-Magic Nuclei. I

because it corresponds to the collective degree of freedom which is common to the diabatic configurations. Imposing these requirements on Eq. (2·10) up to the linear order, we get

\[ Q_{ij}\eta^*\eta=0 , \]
\[ \left. \frac{\partial Q_{ij}}{\partial \eta} \right|_{\eta^*=0} = \left. \frac{\partial Q_{ij}}{\partial \eta} \right|_{\eta^*=0} (i \neq j) \]  

(2·11)

These equations are enough to determine \( \eta^i \) and \( z_i \), provided that the scale of the global collective coordinates \( (\eta^*, \eta) \) is fixed. In the case when we have an \( (\eta^*, \eta_i) \) expansion expression for the quadrupole moment,

\[ \langle \phi_i(\eta^*, \eta_i, \phi_i, N_i) | \bar{Q} | \phi_i(\eta^*, \eta_i, \phi_i, N_i) \rangle |_{N_i=N_0} = q_i^{(0)} + q_i^{(1)}(\eta_i + \eta) + \cdots \]  

(2·12)

Eq. (2·11) reads

\[ q_i^{(0)} - 2q_i^{(0)}z_i = 0 , \]
\[ q_i^{(1)}z_i = q_j^{(1)}z_j . \quad (i \neq j) \]  

(2·13)

Thus \( \eta^i \) and \( z_i \) are determined.

We can then express the diabatic wave packets associated with the \( i \)-th HB states in terms of the newly defined collective coordinates \( (\eta^*, \eta, \phi, N) \):

\[ | \tilde{\phi}_i(\eta^*, \eta, \phi, N) \rangle = e^{i\Gamma_i(\eta^*, \eta, \phi, N)} | \phi_i(\eta^*, \eta_i, \phi_i, N_i) \rangle |_{\eta^*=\eta^*, \eta=\eta^*+\eta} \]  

(2·14)

Here we introduced a phase factor \( \Gamma_i(\eta^*, \eta, N) \) which is real and accounts for the relative phase of the diabatic wave packets (2·14) between different configurations. The canonical variable condition is known to restrict the phase of the wave packet, while Eq. (2·4) requires this condition to be fulfilled independently for each diabatic collective variables \( (\eta^*, \eta_i) \). We demand here that the diabatic wave packet \( | \tilde{\phi}_i(\eta^*, \eta, \phi, N) \rangle \) expressed in terms of the global collective coordinates \( (\eta^*, \eta, \phi, N) \) should satisfy the same canonical variable condition for all the diabatic configurations.

\[ \langle \tilde{\phi}_i(\eta^*, \eta, \phi, N) | \frac{\partial}{\partial \eta} \rangle | \tilde{\phi}_i(\eta^*, \eta, \phi, N) \rangle = \frac{1}{2} \eta^* , \]
\[ \langle \tilde{\phi}_i(\eta^*, \eta, \phi, N) | \frac{\partial}{\partial \eta^*} \rangle | \tilde{\phi}_i(\eta^*, \eta, \phi, N) \rangle = -\frac{1}{2} \eta , \]
\[ \langle \tilde{\phi}_i(\eta^*, \eta, \phi, N) | \frac{\partial}{\partial N} \rangle | \tilde{\phi}_i(\eta^*, \eta, \phi, N) \rangle = N , \]
\[ \langle \tilde{\phi}_i(\eta^*, \eta, \phi, N) | \frac{\partial}{\partial N} \rangle | \tilde{\phi}_i(\eta^*, \eta, \phi, N) \rangle = 0 . \]  

(2·15)

These canonical variable conditions reduce to the equations for the phase factor \( \Gamma_i(\eta^*, \eta, N) \):

\[ \frac{\partial}{\partial \eta} \Gamma_i = \frac{1}{2i} \eta^i , \]
\[
\frac{\partial}{\partial \eta^*} \Gamma_i = -\frac{1}{2i} \eta_i ,
\]
\[
\frac{\partial}{\partial N} \Gamma_i = 0 ,
\]
(2.16)

where Eqs. (2.14), (2.8) and (2.4) are substituted in Eq. (2.15). Thus we get the phase factor
\[
\Gamma_i(\eta^*, \eta, N) = \frac{1}{2i} \eta_i(\eta - \eta^*) .
\]
(2.17)

In Eq. (2.17) we neglected an arbitrary constant because the constant phase has no relevant effect.

Next, let us consider the interaction energy between the diabatic wave packets \(|\Psi_i(\eta^*, \eta, \phi, N)\rangle\). It is expressed by
\[
\mathcal{R}_i(\eta^*, \eta) = \langle \Psi_i(\eta^*, \eta, \phi, N) | H | \Psi_j(\eta^*, \eta, \phi, N) \rangle |_{N=N_0}
\]
\[= e^{-i\tau r + i\tau} \langle \Psi_i(\eta^*, \eta), \eta_1(\eta^*, \eta), \phi, N_0 | H | \Psi_j(\eta^*, \eta), \eta_1(\eta^*, \eta), \phi, N_0 \rangle .
\]
(2.18)

On the other hand, the energy expectation value of the \(i\)-th diabatic wave packet is given by
\[
\mathcal{R}_i(\eta^*, \eta) = \langle \Psi_i(\eta^*, \eta, \phi, N) | H | \Psi_i(\eta^*, \eta, \phi, N) \rangle |_{N=N_0}
\]
\[= \mathcal{R}_i(\eta^*, \eta), \eta_1(\eta^*, \eta), N_0 .
\]
(2.19)

With use of these quantities, we introduce a quantized Schrödinger equation for eigenstates of the collective excitation incorporating the couplings between the diabatic configurations:
\[
\begin{pmatrix}
H_1(b^*, b) & H_{12}(b^*, b) \\
H_{21}(b^*, b) & H_2(b^*, b)
\end{pmatrix}
\begin{pmatrix}
|\phi_1\rangle_b \\
|\phi_2\rangle_b
\end{pmatrix}
= E
\begin{pmatrix}
|\phi_1\rangle_b \\
|\phi_2\rangle_b
\end{pmatrix},
\]
(2.20)

where \(H_1(b^*, b)\) and \(H_2(b^*, b)\) are defined by replacing the collective variables \((\eta^*, \eta)\) in \(\mathcal{R}_i(\eta^*, \eta)\) and \(\mathcal{R}_i(\eta^*, \eta)\) with the boson operators \((b^*, b)\) and taking the normal ordering. That is,
\[
H_1(b^*, b) = : \mathcal{R}_i(\eta^*, \eta) \mid_{\eta=b^*} : ,
\]
\[
H_2(b^*, b) = : \mathcal{R}_i(\eta^*, \eta) \mid_{\eta=b^*} : .
\]
(2.21)

The coupled configuration collective Schrödinger equation (2.20) may be justified, provided that the orthogonality between the different diabatic configurations holds well. We are in fact interested in such cases where the orthogonality condition is fulfilled exactly or almost exactly. On the other hand, if the overlap between the two wave packets is not negligible, it might be necessary to generalize the above equations. In this connection, it would be interesting to investigate the relation of this
approach to the time-dependent resonating Hartree-Bogoliubov theory recently proposed by Fukutome and Nishiyama.\textsuperscript{24,25}

The coupled-configuration collective Schrödinger equation can be solved by expanding the boson basis states:

$$|\psi_i\rangle_b = \sum_{n=0}^{N_{b,i}} C_n |n, i\rangle_b.$$  \hspace{1cm} (2·22)

In defining the boson basis states

$$|n, i\rangle_b = \frac{1}{\sqrt{n!}} (b_i^\dagger)^n |0, i\rangle_b, \quad b_i |0, i\rangle_b = 0,$$  \hspace{1cm} (2·23)

we use boson operators ($b_i$, $b_i^\dagger$) which are the quantum counterpart of the collective variables ($\eta_i^*, \eta_i$) associated with the $i$-th HB state ($|\psi_i\rangle_b, i=1, 2$). Namely,

$$\begin{pmatrix} b_i \\ b_i^\dagger \end{pmatrix} = \begin{pmatrix} x_i & y_i \\ y_i & x_i \end{pmatrix} \begin{pmatrix} b - \eta_i^* \\ b^\dagger - \eta_i^* \end{pmatrix},$$  \hspace{1cm} (2·24)

which should be compared with Eq. (2·8). The maximum numbers $N_{b,i}$ of the boson basis in Eq. (2·22) represent the cutoff of the boson space (physical boson space) which may arise from the same origin as in the boson expansion theory.

For any one-body operator $F$ which acts on many-fermion state space we can introduce a corresponding operator $F_{cc}$ which acts on the coupled-configuration collective boson space ($|\psi_i\rangle_b, i=1, 2$). It can be defined by

$$F_{cc} = \begin{pmatrix} F_{11}(b^\dagger, b) & F_{12}(b^\dagger, b) \\ F_{21}(b^\dagger, b) & F_{22}(b^\dagger, b) \end{pmatrix},$$

$$F_{i\delta}(b^\dagger, b) = \mathcal{F}_{i\delta} (\eta^*, \eta)|_{\eta=b^\dagger},$$

$$\mathcal{F}_{i\delta} (\eta^*, \eta) = \langle \bar{\phi}_i(\eta^*, \eta, \phi, N) | \bar{F} | \bar{\phi}_i(\eta^*, \eta, \phi, N) \rangle |_{N=N_0}.$$  \hspace{1cm} (2·25)

The matrix element of $F_{cc}$ between the collective excited states can be calculated in terms of the collective boson state vectors.

§ 3. Particle-plus-harmonic-core model

Let us consider a simple model system consisting of two valence particles and a deformable core. We explicitly consider two valence levels which cross with each other as the deformation of the core increases. The two valence particles can jump between the two levels by the monopole pairing force. In this section, we assume that the vibration of the core is harmonic. The case of anharmonic vibration will be treated in the next section.

The model Hamiltonian consists of four parts,

$$H = H_{\text{core}} + H_{\text{sp}} + H_{\text{coup}} + H_{\text{int}},$$  \hspace{1cm} (3·1)

where
\[ H_{\text{core}} = \frac{1}{2}(P^2 + Q^2), \quad H_{\text{sp}} = \varepsilon_e \sum_{k=1,2} \sigma_k \tilde{N}_k, \]
\[ H_{\text{coup}} = -\chi Q \sum_{k=1,2} \sigma_k \tilde{N}_k, \quad H_{\text{int}} = -G A^\dagger A, \]

with
\[ A^\dagger = \sum_{k=1,2} A_k^\dagger, \quad A_k^\dagger = \sum_{m>0} c_{km} c_m^\dagger, \quad \tilde{N}_k = \sum_m c_{km} c_{km}. \]

Here \( P = -i(\partial / \partial Q) \) is the momentum conjugate to the deformation coordinate \( Q \) of the core. In the above Hamiltonian, \( H_{\text{core}} \) describes the harmonic vibration of the core, \( H_{\text{sp}} \) the shell-model single-particle energies for the valence nucleons, \( H_{\text{coup}} \) the coupling between the valence nucleons and the core deformation \( Q \), and \( H_{\text{int}} \) the monopole pairing interaction between the valence nucleons. The particle-core coupling strength and the pairing-force strength are denoted by \( \chi \) and \( G \), respectively. The suffix \( k \) labels different valence levels. We consider only two levels, and set \( \sigma_k = -1 \) and +1 for \( k=1 \) and 2, respectively. In the monopole-pair creation operator \( A_k^\dagger \) and the nucleon-number operator \( \tilde{N}_k \) for level \( k \), the suffix \( m \) labels degenerate single-particle states and \( k m \) denotes the time reversed state of \( k \bar{m} \). We assume, for simplicity, that the degeneracy is two-fold, i.e., \( m = -1/2 \) and 1/2. The single-particle energies \( \varepsilon_k(Q) \) including the particle-core coupling are defined by
\[ H_{\text{sp}}(Q) = H_{\text{sp}}^* + H_{\text{coup}}(Q) = \sum_k \varepsilon_k(Q) \tilde{N}_k \]
as functions of the deformation of the core. Due to the particle-core coupling, the first level \( \varepsilon_1(Q) = -\varepsilon_e + \chi Q \) is up-sloping while the second level \( \varepsilon_2(Q) = \varepsilon_e - \chi Q \) is down-sloping as a function of \( Q \). They cross at \( Q = \varepsilon_e / \chi \). The two diabatic configurations are simply given by \( A_1^\dagger |0\rangle \otimes |\psi_{\text{core}}\rangle \) and \( A_2^\dagger |0\rangle \otimes |\psi_{\text{core}}\rangle \), where \( |0\rangle \) represents the vacuum for valence nucleons and \( |\psi_{\text{core}}\rangle \) the time dependent wave packets describing the collective vibration of the core. They are apparently orthogonal to each other, and are mixed by the pairing interaction \( H_{\text{int}} \).

It is known that the equation of the collective manifold in the SCC method reduces to the ordinary time-dependent variational principle when we consider simple models involving only single boson-degree of freedom. For the present model with harmonic-vibrational core, the solutions of the time-dependent variational principle are obviously given by the time-dependent coherent states
\[ |\phi_{i,\text{core}}(\eta_i, \eta_i)\rangle = e^{\eta_i b_i^\dagger - \eta_i^* b_i} |\phi_{i,\text{core}}(0)\rangle, \]
where time-dependence of the vibrational amplitudes \( \eta_i(t) \) are given by \( \eta_i(t) = \eta_i(0) e^{-i\omega t} \), and where
\[ |\phi_{i,\text{core}}(0)\rangle = e^{\eta_i (b_i^\dagger - b_i)} |0\rangle \]
with \( b = (Q + iP) / \sqrt{2} \), represent the equilibrium states of the core whose deformations are given by \( \eta_i = -\chi \) and \( \chi \) for \( i=1 \) and 2, respectively. They are the vacua for the shifted boson operators \( b_i = b - \eta_i \) appearing in Eq. (3.6) and satisfying \( b_i |\phi_{i,\text{core}}(0)\rangle = 0 \).
The relation (2.8) between the local collective variables \((\eta^*, \eta)\) and the global ones \((\eta^*, \eta)\) becomes very simple in this model, and is given by \(\eta_i = \eta - \eta_i\). With respect to the diabatic configurations \(A_1|0\> \otimes |\phi, \text{core}\>\), the diagonal and off-diagonal matrix elements of the Hamiltonian are easily calculated to be \(\hat{\mathcal{H}} = (\eta^* \eta + 1/2) + 2\varepsilon \sigma \chi \sigma (\eta^* \eta) - G\) and \(\langle \phi_1(\eta^*, \eta, \phi, \phi_0)|H|\phi_2(\eta^*, \eta, \phi, \phi_0)\rangle = -Ge^{-(\eta^* - \eta)}\). Taking into account the phase factor defined by (2.14) and given by (2.17), we finally obtain the coupling matrix elements defined by (2.18) as \(\hat{\mathcal{R}}_{12} = \hat{\mathcal{R}}_{21} = -G\).

Replacing the \((\eta^*, \eta)\) with the boson operators \((b^*, b)\), we obtain the quantized Hamiltonian

\[
H = \begin{pmatrix} b^* b + \frac{1}{2} - 2\varepsilon e^{-b^* b} - G & -G \\ -G & b^* b + \frac{1}{2} + 2\varepsilon e^{-b^* b} - G \end{pmatrix}
\]

\[
= \frac{1}{2}(P^2 + Q^2) \mathbf{I} + \varepsilon \sum \sigma_i N_i + \chi Q \sum \sigma_i N_i + H_{\text{int}},
\]

where \(\mathbf{I}\) is the 2x2 unit matrix,

\[
N_i = \begin{pmatrix} \langle 0|A_1 \tilde{N}_i A_1^\dagger |0\rangle & \langle 0|A_2 \tilde{N}_i A_2^\dagger |0\rangle \\ \langle 0|A_2 \tilde{N}_i A_1^\dagger |0\rangle & \langle 0|A_2 \tilde{N}_i A_2^\dagger |0\rangle \end{pmatrix} = 2 \begin{pmatrix} \delta_{k1} & 0 \\ 0 & \delta_{k2} \end{pmatrix},
\]

\[
H_{\text{int}} = \begin{pmatrix} \langle 0|A_1 \tilde{H}_{\text{int}} A_1^\dagger |0\rangle & \langle 0|A_2 \tilde{H}_{\text{int}} A_1^\dagger |0\rangle \\ \langle 0|A_2 \tilde{H}_{\text{int}} A_1^\dagger |0\rangle & \langle 0|A_2 \tilde{H}_{\text{int}} A_2^\dagger |0\rangle \end{pmatrix} = -G \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix},
\]

which exactly coincides with the original Hamiltonian (3.1). Thus, we have

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Examples of the potential-energy functions and exact energy levels for the particle-plus-harmonic-core model. Thick and thin lines represent the adiabatic and the diabatic potentials, respectively. Energy levels are drawn with respect to the adiabatic potential in cases (a) and (b), and with respect to the adiabatic ones in case (c). The numbers on individual levels indicate the percentages of the main diabatic configurations in the wave functions obtained by diagonalizing the total Hamiltonian. The parameters used are \(G=0.2, \chi=1.0\) for case (a), \(G=0.2, \chi=0.5\) for case (b), \(G=2.0, \chi=1.0\) for case (c), and \(\varepsilon=0.375\) for all cases.}
\end{figure}
confirmed that our theoretical scheme outlined in § 2 gives exact solutions for the case of simple model under consideration. It should be noted here that the matrix elements of the coupling Hamiltonian $H_{\text{int}}$ become $-G$, in agreement with the exact solutions, owing to the phase factors $e^{i\pi}$ defined by (2.14) and given by Eq. (2.17).

We can simulate various situations concerning shape coexistence phenomena by varying three parameters $\epsilon_0$, $G$ and $\chi$ of this model. In Fig. 1 we present typical examples of the collective potential-energy functions and the quantum levels obtained by exact diagonalizations. Cases (a) and (b) represent the situation with relatively weak pairing-force strength $G$, while case (c) that with very strong pairing force. Except for case (c), we can very clearly distinguish two kinds of vibrational states associated with the first and the second minima of the collective potential. They retain their identities even after the mixings due to the pairing force. It is striking that this characteristic holds for levels whose excitation energies lie much higher than the barrier of the adiabatic potential between the two local minima. Such phenomena, i.e., the existence of well localized wave functions around the local minima can hardly be expected from the properties of the adiabatic potential.

In Fig. 2 we compare the spectra obtained by means of the adiabatic approximation (Born-Oppenheimer approximation) with the exact solutions. They are obtained as follows. First we calculate the adiabatic potential by diagonalizing $H$ for a given value of $Q$ neglecting the collective kinetic energy of $H_{\text{core}}$. It is given by

$$V_{\text{ad}}(Q) = \frac{1}{2} Q^2 + V_{\text{particle}}(Q)$$

with

$$V_{\text{particle}}(Q) = -G - \sqrt{4(\epsilon_0 - \chi Q)^2 + G^2},$$

\[ (3.11) \]

\[ (3.12) \]

Fig. 2. Examples of excitation spectra and transition matrix elements $|\langle m | Q | n \rangle|$ for the particle-plus-harmonic-core model. Parameters used are the same as in Fig. 1, for cases (a), (b) and (c), respectively. “Exa.” represents the spectra obtained by exact diagonalization of the Hamiltonian, and “Adi.” those obtained by the adiabatic approximation. Numbers in parenthesis on each level indicate the expectation value of $Q_\sigma = \sum_\sigma n_\sigma$. Note that we get $\langle Q_\sigma \rangle = \pm 2.0$ when there is no mixing between the lower and the upper configurations. Thus, these numbers indicate the diabaticity of the levels.
where the local minima occurs at $Q=\pm \chi$, when $G=0$. Secondly, we diagonalize $H_{ad}=(1/2)P^2+V_{ad}(Q)$ and obtain adiabatic spectra and wave functions. We see in Fig. 2 that the transition matrix elements are rather poorly reproduced by the adiabatic approximation in cases (a) and (b), while they are well reproduced in case (c) when we have very strong pairing force mixing the two diabatic configurations. The adiabatic approximation is thus found to overestimate the mixing between the two kinds of vibrations around the local minima in situations like cases (a) and (b) where the pairing-force strength $G$ is relatively weak.

The following considerations may be helpful to understand the above result. The Landau-Zener transition probability $P_{LZ}$ at the level crossing point between the down-sloping and up-sloping single-particle levels is given by

$$P_{LZ}=e^{-2\gamma} \quad (3.13)$$

with

$$\gamma=\frac{\pi |V_{int}|}{\dot{Q} \frac{\partial}{\partial Q}(\epsilon_2-\epsilon_1)} \quad (3.14)$$

In the model under consideration, the interaction $V_{int}$ between the two diabatic configurations is given by the pairing-force strength $G$. The single-particle-energy difference $\epsilon_2-\epsilon_1$ is given by $2(\epsilon_2-\chi Q)$. The time-dependence of the core deformation $Q$ is given by $Q=Q_0 e^{i\omega t}$ so that $|Q|=\omega Q_0$, where we can set $Q_0=\omega=1$ for the ground state of $H_{core}=(P^2+Q^2)/2$. For the parameters adopted in Fig. 1, we obtain $\gamma=0.17$, $0.34$ and $1.7$ for cases (a), (b) and (c), respectively. Thus, the condition for the validity of the adiabatic approximation, $\gamma>1$, is violated except for case (c). Namely, the Landau-Zener transition probability is rather large and the particles do not always follow the adiabatic level.

It should be mentioned here that we would also obtain $\gamma<1$ for the level crossings associated with the shape coexistence in Sn and Pb isotopes by making an analysis similar to above.

**§ 4. Particle-plus-anharmonic-core model**

Instead of postulating the collective variables $(Q, P)$ for the core as in the previous section, we now derive them by means of the SCC method for a single-$j$ model Hamiltonian with $O(4)$ symmetry. Namely, we consider the core whose Hamiltonian is given by

$$H_{core}=-G_e A_c^+ A_c-\frac{1}{2} \chi Q_0^* Q_c, \quad (4.1)$$

$$A_c^+ = \sum_{n>0} c_{cm}^+ c_{cm}^-, \quad Q_c = \sum_{m} \sigma_{cm} c_{cm}^+ c_{cm}, \quad (4.2)$$

where $\sigma_{cm}=+1$ for $|m|<Q/2$ and $\sigma_{cm}=-1$ for $|m|>Q/2$ with $Q=j+(1/2)$. The $c_{cm}$ and $c_{cm}^+$ are creation and annihilation operators of nucleons in the core. This model Hamiltonian may be regarded as a simplified version of the familiar pairing-plus-
quadrupole \((P+QQ)\)-force model for the single \(j\)-shell. The operators \(A_j^\sharp\), \(A_c\), \(Q_c\) and their commutators form a Lie algebra of \(O(4)\) symmetry. This model Hamiltonian has been used for schematic analysis of anharmonic quadrupole vibrations in transitional nuclei.\(^{18,20,21}\) It was shown in Ref. 18) that the fourth-order approximation of the \((\eta^*, \eta)\) expansion well reproduces the low-lying collective states for the Hamiltonian (4·1). In accordance with the above \(H_{\text{core}}\), we consider the single-particle Hamiltonian

\[
H_{sp} = H_{sp}^c + H_{\text{coup}} = (\epsilon_i - \chi \vec{Q}_c) \sum_{i} \sigma_i \vec{N}_i ,
\]

where \(H_{sp}^c\) is given by (3·2). Note that \(Q\) in the previous subsection is here replaced with the simplified "quadrupole" operator \(\vec{Q}_c\) for the core. The total Hamiltonian of this model is defined by \(H = H_{\text{core}} + H_{sp} + H_{\text{int}}\), where the interaction \(H_{\text{int}}\) between the valence particles is the same as in (3·3).

We apply our theoretical scheme outlined in § 2 to the model system consisting of two particles plus core with the \(O(4)\) symmetry defined above. It is easily seen that there exists two HB minima corresponding to two valence configurations. The two diabatic configurations may be explicitly constructed as

\[
|\phi_i(\eta^*, \eta_i, \phi_i, N_i)\rangle = A_i^\dagger |0\rangle \otimes |\phi_{\text{core}}(\eta^*, \eta_i, \phi_i, N_i)\rangle , \quad (i=1, 2) \quad (4·4)
\]

\[
|\phi_{\text{core}}(\eta^*, \eta_i, \phi_i, N_i)\rangle = e^{-i\phi_i \hat{N}_i} e^{G(\eta^*, \eta_i, N_i)B_{ii} - G^*(\eta^*, \eta_i, N_i)B_{ii}} |\phi_i(0)\rangle , \quad (4·5)
\]

\[
B_i^\dagger = \sum_{m>0} \sigma_{im} a_{im}^\dagger a_{im}^\dagger , \quad B_i = \sum_{m>0} \sigma_{im} a_{im} a_{im}^\dagger \quad (4·6)
\]

where \(|\phi_i(0)\rangle\) are the HB vacua and \(a_{im}\) are the quasiparticles defined with respect to them:

\[
a_{im}^\dagger = u_{im} c_{im}^\dagger - v_{im} c_{im}^\dagger , \quad a_{im} |\phi_i(0)\rangle = 0 . \quad (4·7)
\]

The diabatic configurations (4·4) are obviously orthogonal to each other.

The unknown function \(G_i(\eta^*, \eta, N_i)\) in Eq. (4·5) is determined by the \((\eta^*, \eta)\) expansion method based on the SCC method. Assuming the existence of global collective variables \((\eta^*, \eta)\) related with the collective variable \((\eta^*, \eta_i)\) by Eq. (2·8), we then derive the coupled-configuration Schrödinger equation for the model under consideration following the procedure described in § 2. We adopt the fourth-order approximation in the \((\eta^*, \eta)\) expansion when evaluating the diabatic collective Hamiltonians \(\mathcal{H}(\eta^*, \eta)\), while the \((\eta^*, \eta)\) dependence of the coupling matrix elements \(\mathcal{R}^\dagger(\eta^*, \eta)\) is taken into account up to the first order in \((\eta^*, \eta)\).

We show in Fig. 3 typical examples of the calculated potential-energy functions. In this figure, thin lines show the diabatic potentials while thick lines the adiabatic potentials. The horizontal lines indicate the zero-point vibrational amplitudes evaluated by means of the RPA based on the local HB minima. The adiabatic potentials are calculated in terms of the conventional Born-Oppenheimer approximation scheme. On the other hand, the diabatic potentials are calculated in the following way. First, we rewrite the collective Hamiltonian \(\mathcal{H}(\eta^*, \eta_i)\) defined by (2·5) in terms of the collective coordinates \(q_i = (\eta_i^* + \eta_i)/\sqrt{2}\) and the momenta \(p_i = i(\eta_i^* - \eta_i)/\sqrt{2}\),
Diabatic Approach to Shape Coexistence Phenomena in Semi-Magic Nuclei. I

Fig. 3. Examples of the potential-energy functions for the particle-plus-anharmonic-core model. Thick lines represent the adiabatic potentials, while thin lines the diabatic potentials obtained by means of the SCC method. Parameters used are $e_c=0.375$, $G_c=0.06$, $\Omega=40$, $N_c=30$, and $G=0.1$, $\chi=0.03$ for case (a), $G=0.1$, $\chi=0.025$ for case (b), $G=1.0$, $\chi=0.03$ for case (c). The calculated pairing gap $\Delta$ of the core is 1.16 at the spherical point.

Fig. 4. Examples of excitation spectra and transition matrix elements $|\langle m|\hat{Q}_c|n\rangle|$ for the particle-plus-anharmonic-core model. The spectra denoted as “SCC” are obtained by means of the coupled-configuration SCC method, “Exa.” by exact diagonalization, and those denoted as “Adi.” are obtained by means of adiabatic approximation. Parameters used are the same as in Fig. 3, for cases (a), (b) and (c), respectively.

and define the momentum-independent part of it as the collective potential $V_i(q_i)$ associated with the $i$-th diabatic configuration. Secondly, we evaluate the expectation value $Q_c$ of the “quadrupole operator” $\hat{Q}_c$ with respect to the core wave function (4.5), and expand it in terms of the collective coordinate up to the third order in $q_i$. Using the relation between $q_i$ and $Q_c$, we rewrite the $V_i(q_i)$ as a function of $Q_c$.

Cases (a), (b) and (c) in Fig. 3 correspond to those in Fig. 1. Namely, Figs. 3(a) and (b) represent the case of relatively weak pairing-force strength $G$, while Fig. 3(c) that of very strong $G$. We see that the fourth-order ($\eta^4$, $\eta^3$) expansion successfully yields the diabatic potential-energy functions incorporating the anharmonic effects of the core vibrations. It should be noted here that zero-point amplitude washes out the
second minimum that exists in case (a) in the adiabatic potential-energy function.

In Fig. 4 are compared the excitation spectra and transition moments obtained by the coupled-configuration SCC method with those of the exact solutions. Expectation values of the "quadrupole" operator \( Q_c \) and the percentages of the first diabatic configurations in the final wave functions obtained after taking the couplings into account are listed in Table I. Cases (a), (b) and (c) in Fig. 4 and Table I correspond to cases (a), (b) and (c) of Fig. 3, respectively. In Table I, \( Q_c \) represent the expectation values of the operator \( Q_c \) for the core, while \( Q_p \) those for the valence operator \( Q_p \) defined by \( \hat{Q}_p = \sum_{k=1,2} \hat{Q}_k \) with \( \hat{Q}_k = \sum_m \sigma_{km} C_{km}^* C_{km} \). Note that \( Q_p = -2\ ) and \(+2\ ) for the first and the second diabatic configurations, respectively. They can therefore be used

<table>
<thead>
<tr>
<th>Case</th>
<th>Exact</th>
<th>SCC</th>
<th>Adiabatic</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>%</td>
<td>( Q_c )</td>
<td>( Q_p )</td>
</tr>
<tr>
<td>(a)</td>
<td>1</td>
<td>100</td>
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<tr>
<td></td>
<td>2</td>
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<td>-7.9</td>
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<td>14.6</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>98</td>
<td>-2.9</td>
</tr>
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<td></td>
<td>5</td>
<td>1</td>
<td>8.2</td>
</tr>
</tbody>
</table>

| (b)  |      |     |       |     |     |       |     |     |       |
|      | %     | \( Q_c \) | \( Q_p \) | % | \( Q_c \) | \( Q_p \) | % | \( Q_c \) | \( Q_p \) |
|      | 1     | 100 | -6.8  | -2.0 | 100 | -7.2  | -2.0 | -6.1  | -1.9 |
|      | 2     | 97  | -5.4  | -1.9 | 97  | -6.5  | -1.9 | -3.5  | -1.6 |
|      | 3     | 3   | 6.5   | 1.9  | 3   | 6.8   | 1.9  | 0.2   | 0.7 |
|      | 4     | 97  | -4.0  | -1.9 | 98  | -6.1  | -1.9 | -     | -     |
|      | 5     | 3   | 5.5   | 1.9  | 3   | 6.5   | 1.9  | -     | -     |

| (c)  |      |     |       |     |     |       |     |     |       |
|      | %     | \( Q_c \) | \( Q_p \) | % | \( Q_c \) | \( Q_p \) | % | \( Q_c \) | \( Q_p \) |
|      | 1     | 90  | -12.8 | -1.6 | 92  | -15.0 | -1.6 | -10.1 | -1.5 |
|      | 2     | 70  | -1.1  | -0.8 | 72  | -5.0  | -0.9 | 0.5   | -0.7 |
|      | 3     | 58  | 2.3   | -0.3 | 53  | 2.4   | -0.1 | 1.7   | -0.5 |
|      | 4     | 63  | 1.2   | -0.5 | 62  | 0.4   | -0.5 | -0.6  | -0.5 |
as a measure of the mixings of the two configurations in the total wave functions.

In Fig. 4, we also show the result calculated in terms of the adiabatic (Born-Oppenheimer) approximation. This calculation was done in the following way. We first apply the conventional constrained Hartree-Bogoliubov (CHB) method to the model under consideration by choosing the expectation value \( Q_c \) of the core "quadrupole" operator \( \hat{Q}_c \) as a constraint. For a given value of \( Q_c \), we diagonalize the pairing interaction \( H_{\text{int}} \) which mixes different eigenstates of the single-particle Hamiltonian \( H_{sp} = (\epsilon_k - \chi Q_c) \sum_{k=1,2} \sigma_k \tilde{N}_k \), and select the lowest energy configuration. The collective potential energy is then obtained as a sum of the core and the valence-particle contributions as follows:

\[
V_{\text{ad}}(Q_c) = V_{\text{core}}(Q_c) + V_{\text{particle}}(Q_c),
\]

where

\[
V_{\text{core}}(Q_c) = -\frac{G}{8} \left\{ N_c (2\Omega - N_c) - Q_c^2 + \sqrt{(N_c^2 - Q_c^2)(2\Omega - N_c)^2 - Q_c^2} \right\} - \frac{1}{2} \chi Q_c^2 \tag{4.9}
\]

with \( N_c \) being the number of particles in the core, and \( V_{\text{particle}}(Q_c) \) is the same as in Eq. (3.12). Next, we evaluate the collective mass parameter as a function of \( Q_c \) by means of the conventional cranking procedure. Diagonalizing the Schrödinger equation obtained after quantization, we get the collective spectra in the adiabatic approximation.

It is clearly seen in Fig. 4 and Table I that the coupled-configuration SCC method successfully reproduces the main features of the exact spectra. In Figs. 4(a) and (b), the 1st, 2nd and 4th eigenstates are associated with the first (lower) diabatic configurations, while 3rd and 5th eigenstates correspond to the second (higher) configurations. It is striking that the diabatic collective vibrations well retain their identities in the 3rd and 5th eigenstates in spite of the fact that the second HB minima are completely washed out by the zero-point vibrational amplitudes (see Figs. 3(a) and (b)). As shown in Table I, the mixing probabilities of the first diabatic configurations are only a few percent in the 3rd and 5th eigenstates. This result is totally unexpected from the properties of the adiabatic potential energy functions. Indeed, the adiabatic (Born-Oppenheimer) approximation completely fails in reproducing the main characteristics of the 3rd and 5th eigenstates which are seen in the exact spectra and in the coupled-configuration SCC method. On the other hand, the adiabatic approximation works fairly well when the coupling matrix elements between the two diabatic configurations become stronger. This is shown in Fig. 4(c) and Table I(c) which exhibit the result for the case with very strong pairing force. In contrast to the adiabatic (Born-Oppenheimer) approximation, the coupled-configuration SCC method nicely reproduces the transition moments as well as the excitation spectra over the whole range of the pairing-force strength \( G \).

§ 5. Multi-\( O(4) \) model

The \( O(4) \) model Hamiltonian for nucleons in a single j-shell, discussed in § 4 in
relation to the particle-plus-anharmonic-core model, may be easily generalized to the case of many j-shells as

$$ H = \sum_k \epsilon_k \hat{N}_k - GA^\dagger A - \frac{1}{2} \chi \hat{Q}^\dagger \hat{Q}, $$

$$ A^\dagger = \sum_k A^\dagger_k, \quad \hat{Q} = \sum_k \hat{q}_k \hat{Q}_k, \quad \hat{N} = \sum_k \hat{N}_k, $$

$$ A^\dagger_k = \sum_{m>0} c^\dagger_{km} c_{km}^k, \quad \hat{Q}_k = \sum_m \sigma_{km} c_{km}^k c_{km}, \quad \hat{N}_k = \sum_m c_{km}^k c_{km}, $$

where the suffix k distinguishes different j-shells, and \( \sigma_{km} = \pm 1 \) according to \(|m| \geq \Omega/2\). The coefficients \( q_k \) in \( \hat{Q} \) simulate the magnitude of the reduced quadrupole moments of the j-shell. This model Hamiltonian may be regarded as a simplified version of the conventional \( P+QQ \) force model in the sense that only the \( K=0 \) component of the quadrupole deformation is considered. In the special case that single-particle levels \( \epsilon_m \) are equidistant, all \( q_k \) are equal, and all \( \Omega_k = j_k + (1/2) = 2 \), this model reduces to the one used by Arve and Bertsch in order to study collective mass parameters in finite superconducting systems. The single-particle energies \( \epsilon_{km}(Q) \) corresponding to the Nilsson diagram may be defined by

$$ H_{sp} = \sum_{km} \epsilon_{km}(Q)c_{km}^\dagger c_{km}, $$

$$ \epsilon_{km}(Q) = \epsilon_k^\star - \chi Q \sigma_{km}, $$

where \( Q \) represents the expectation value of \( \hat{Q} \) with respect to the HB state vector. The levels with positive (negative) \( \sigma_{km} \) are down-sloping (up-sloping) as functions of \( Q \). Corresponding to this classification of single-particle levels, let us define the following operators:

$$ K_{k+} = \frac{1}{2} (A_k^\dagger + B_k^\dagger), \quad L_{k+} = \frac{1}{2} (A_k^\dagger - B_k^\dagger), $$

$$ K_{k-} = \frac{1}{2} (A_k + B_k), \quad L_{k-} = \frac{1}{2} (A_k - B_k), $$

$$ K_{k0} = \frac{1}{4} (\hat{N}_k + \hat{Q}_k - \Omega_k), \quad L_{k0} = \frac{1}{4} (\hat{N}_k - \hat{Q}_k - \Omega_k), $$

where \( B_k^\dagger = \sum_{km>0} \sigma_{km} c_{km}^\dagger c_{km}^k \). The sets \( (K_{k+}, K_{k-}, K_{k0}) \) and \( (L_{k+}, L_{k-}, L_{k0}) \) form \( SU(2) \) algebras, and they commute with each other. The former represents the nucleon pairs in the down-sloping levels, while the latter those in the up-sloping levels. Thus, the multi-\( O(4) \) model is equivalent to the multi-\( SU(2) \times SU(2) \) model. The \( O(4) \) representation corresponds to the seniority-coupling scheme, while the \( SU(2) \times SU(2) \) representation to the Nilsson-plus-BCS picture. By choosing different values for the parameters \( \epsilon_k, q_k, \Omega_k, G \) and \( \chi \), the model may be used to simulate a variety of situations where the pairing and quadrupole correlations compete with each other.

In the following, we consider a special case of the multi-\( O(4) \) model to simulate the shape coexistence phenomena in semi-magic nuclei. For this purpose, we distinguish protons and neutrons, and consider two levels for protons and one level for neutrons.
Diabatic Approach to Shape Coexistence Phenomena in Semi-Magic Nuclei. I

Fig. 5. Schematic illustration of the single-particle energies adopted in the multi-$O(4)$ model. The arrow shows the 2p-2h excitation of the protons.

The lower proton level is assumed to be fully occupied by protons and the neutron level is assumed to have large $j$ and partially filled with neutrons (see Fig. 5). The model Hamiltonian is given by

$$H = H_p + H_n + H_{np},$$

$$H_p = -G_p A_p^+ A_p - \frac{1}{2} \chi \hat{Q}_p^+ \hat{Q}_p,$$

$$H_n = \sum_{k=1,2} e_k^* \hat{N}_{pk} - G_p A_p A_p - \frac{1}{2} \chi \hat{Q}_p^+ \hat{Q}_p,$$

where the suffixes $p$ and $n$ in the operators $A^+$, $\hat{Q}^+$ and $\hat{N}$ denote the levels for protons and neutrons, respectively. Here the proton 2p-2h excitations across the closed shell in Sn and Pb isotopes are simulated as excitations of two protons from the level $k=1$ to $k=2$. In accordance with this physical picture, we shall treat protons as being in normal phase while neutrons are treated as being in superconducting phase. It should be emphasized that the “protons” and “neutrons” in this model do not necessarily correspond to the actual ones. Rather, the “neutron” Hamiltonian $H_n$ in (5·7) may be regarded as simulating not only neutron excitations but also proton excitations in the single-particle levels except for those explicitly treated by $H_p$. From this point of view, we can regard $H_p$, $H_n$ and $H_{pn}$ of (5·7) as corresponding to $H_{sp} + H_{int}$, $H_{core}$ and $H_{coup}$ of the particle-plus-anharmonic-core model Hamiltonian (3·1). It should be emphasized, however, that we are now going to derive collective variables for the total model Hamiltonian (5·7) in contrast to the treatment in previous sections where the collective variables are assumed to describe the collective vibrations of the core. The model Hamiltonian (5·7) is similar to the one used in Ref. 14) in order to study the deformed excited states in Pb isotopes by means of the extended TDHF theory of Yamamura and Kuriyama. A major difference between their approach and ours is that they neglect the mixings between the deformed and spherical configurations while we are interested in the problem how to correctly treat them.

Typical excitation spectra obtained by exact diagonalization of the model Hamiltonian (5·7) are displayed in Fig. 6. Here the parameters $N_p = N_{p1} + N_{p2} = 4$, $\Omega_{p1} = \Omega_{p2} = 2$ and $\Omega_n = 40$ are adopted. We see that model produces the excited deformed configurations associated with the proton 2p-2h excitations, and that their excitation energies decrease with increasing neutron number $N_n$. This is because the model system under consideration becomes softer against deformation as $N_n$ approaches mid-shell, which occurs at $N_n = 40$ for $\Omega_n = j_n + (1/2) = 40$. In this figure, we also see that the excited deformed configuration appears in doublets. This is because of symmetry properties of the multi-$O(4)$ model; namely, the system is invariant under the transformation $\hat{Q}_k \rightarrow -\hat{Q}_k$. This is analogous to the prolate-oblote degeneracy. The small splittings of the doublets may be interpreted as due to the tunnelings.
between the “prolate” and the “oblate” configurations.

To this model we apply the coupled-configuration SCC method. We note here that the “prolate-oblate” symmetry of this model brings about three Hartree-Bogoliubov states $|\phi_i(0)\rangle$, which are spherical, “prolate” and “oblate”. As the exact spectra indicates, however, the doublet states due to the “prolate-oblate” symmetry are almost degenerate. Thus, in applying the coupled-configuration SCC method, we neglect the couplings with the “oblate” configuration for simplicity, and take into account only the couplings between the spherical and the “prolate” configurations. The diabatic configuration $|\psi_i(\eta^*, \eta_i, \phi_i, N_i)\rangle$ associated with the spherical ($i=1$) and the “prolate” ($i=2$) HB states are constructed by the fourth-order $|\eta^*, \eta, \phi, N\rangle$ expansion. They are orthogonal to each other. We use the “quadrupole” operator $\vec{Q} = \vec{Q}_n + \vec{Q}_p$ when making the canonical transformation (2.8) between the diabatic collective coordinate $(r;1; r;i, \phi_i, N_i)$ and the global collective coordinates $(\eta^*, \eta, \phi, N)$. Along the line discussed in § 2, we calculate the coupling Hamiltonian $\mathcal{H}_{ij}(\eta^*, \eta)$ as well as $\mathcal{H}_i(\eta^*, \eta)$. The $(\eta^*, \eta)$ dependence of the coupling matrix elements $\mathcal{H}_{ij}(\eta^*, \eta)$ is taken into account up to the first-order in $(\eta^*, \eta)$, since the $(\eta^*, \eta)$ dependence of them is found to be very weak.

In Fig. 7 we show the calculated potential energy functions. Thin lines represent the diabatic potentials while thick lines the adiabatic potentials calculated by means of the Born-Oppenheimer approximation. The diabatic potentials are evaluated in the same way as in Fig. 3 except that the core “quadrupole” moment $Q_c$ is replaced with the total “quadrupole” moment $Q = \langle \vec{Q}_p + \vec{Q}_n \rangle$ here. It is apparently seen that the multi-$O(4)$ model under consideration produces the excited HB minimum. In this figure, the horizontal lines indicate the zero-point vibrational amplitudes of the RPA modes associated with individual diabatic configurations. It should be noted that the second HB minimum is not deep enough to accommodate the zero-point vibration within the second well. In Figs. 8(a) and (b), excitation spectra and transition matrix elements calculated by means of the coupled-configuration SCC method are denoted as SCC (A) and compared with the exact solutions. Here, the third eigenstates correspond to the deformed excited states associated with the second minima of the collective potential shown in Fig. 7. They involve the proton 2p-2h excitations and correspond to the doublets in the exact spectra. In Tables II(a) and (b), percentages of the first (spherical) diabatic configuration in the total wave functions are listed together with the expectation values of the $\hat{Q}$ operators. It is seen that the mixing
Fig. 7. Examples of the potential-energy functions for the multi-\(O(4)\) model. Thick lines represent the adiabatic potentials, while thin lines the diabatic potentials obtained by means of the SCC method. The neutron numbers are \(N_n=30\) for case (a), and \(N_n=28\) for case (b). Parameters used are the same as in Fig. 6.

Fig. 8. Excitation spectra and transition matrix elements for the multi-\(O(4)\) model calculated by various methods. The spectra denoted as “SCC(A)” and “SCC(B)” are obtained by means of the diabatic approaches described in the text. The deformed excited states are connected by thin lines. The spectra denoted as “Adi.” show the results obtained by means of the adiabatic approximation. The RPA excitation energies are also shown by dashed lines. The numbers on the transition arrows indicate the transition matrix elements of the operator \(\bar{Q}=\bar{Q}_a+\bar{Q}_b\). Parameters used are the same as in Fig. 7 for cases (a) and (b), respectively.
Table II. Properties of the excited states in the multi-$O(4)$ model obtained
by exact diagonalization (Exa.), the coupled-configuration SCC method
(SCC(A)), an alternative application of the SCC method (SCC(B)) and
the adiabatic approximation (Adiabatic). Notations are essentially
the same as in Table I. Parameters used are the same as in Fig. 7 for
cases (a) and (b), respectively. Note that the third eigenstates in the
columns “Exa.”, SCC(A) and SCC(B) correspond to the deformed
excited states, except for the column SCC(B) in case (b) where the
fourth eigenstate corresponds to them. Note also that two numbers
are written for the third eigenstates in the exact spectra, since they are
in fact doublets.

(a)

<table>
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<th>SCC(B)</th>
<th>Adiabatic</th>
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<td></td>
<td>%</td>
<td>%</td>
<td>Q</td>
<td>Qp</td>
</tr>
<tr>
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<td>97</td>
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<td>32.6</td>
<td>7.7</td>
</tr>
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(b)

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between the first and the second (deformed diabatic configurations are small for the
pairing-force strength $G$ adopted, and thus the excited deformed configurations retain
their identities very well in the third eigenstates. Thus, the expectation values of the
$\tilde{Q}$ operator, $Q$, are large only for the third eigenstates demonstrating their characters
as deformed excited states.

For the matrix elements of the $\tilde{Q}$ operators between the eigenstates of the multi-
$O(4)$ model under consideration, the following remarks should be added. Because of
the symmetry property with respect to the transformation $\tilde{Q}_k \rightarrow -\tilde{Q}_k$, the deformed
excited states discussed above are in fact symmetric or antisymmetric superpositions
of the “prolate” and “oblate” configurations. Thus, the expectation values of the $\tilde{Q}$
operator in the exact solution always become zero even if they have large value of $Q$
when the tunnelings are neglected. To indicate the deformed character of the
calculated eigenstates, however, we have written in Tables II(a) and (b) the $Q$ values
that are obtained in the coupled-configuration SCC method by neglecting the tunneling
effects. On the other hand, it is necessary to take into account the above symmetry
property when we discuss the transition matrix elements between the “spherical” and
"deformed" configurations. One can easily confirm that the transition matrix elements of this kind get a factor $\sqrt{2}$ when we replace the "prolate" configuration with the linear combination of the "prolate" and "oblate" configurations satisfying the symmetry property of the Hamiltonian (5.7). This replacement has been done in Figs. 8(a) and (b). Needless to say, other transition matrix elements are unaffected by this replacement.

It is seen in Figs. 8(a) and (b), that the transition matrix elements between the deformed and the spherical configurations are of the same order of magnitude in spite of the small mixings. The reason is that the diagonal matrix elements of $Q$ are much larger than the off-diagonal matrix elements contributing to the transitions between different states in the same diabatic configurations. Thus, even small mixings are sufficient to bring about strong transitions between the deformed and the spherical configurations.

For reference sake, we present in Figs. 8(a), (b), Tables II(a), (b) also the results of an alternative calculation denoted as SCC(B), which is done in the following way. First the SCC method is applied to the neutron Hamiltonian $H_n$, Eq. (5.8), and the fourth-order approximation of the $(\eta^*, \eta)$ expansion on the spherical basis is adopted. The collective representation $\mathcal{H}_n(\eta^*, \eta)$ of $H_n$ is then regarded as a collective Hamiltonian. Second the collective representation $Q_n(\eta^*, \eta)$ of the operator $Q_n$ in $H_{pn}$, Eq. (5.10), is obtained. Third, the total Hamiltonian $\mathcal{H} = \mathcal{H}_n(\eta^*, \eta) + H_p - \chi_{Q_p}Q_n(\eta^*, \eta)$, which corresponds to (5.7), is diagonalized replacing the collective variables $(\eta^*, \eta)$ with the boson operators and treating the proton operators $H_p$ and $Q_p$ exactly. In this approach, the proton and the neutron parts of the model Hamiltonian (5.7) are treated as the valence particles and the core, respectively. In the sense that the particle-core couplings are diagonalized in the spherical basis, this approximation procedure is analogous to the intermediate-coupling scheme. Although this procedure is not selfconsistent since the collective variables are determined by neglecting the valence particles and the particle-core couplings, it may be useful for situations where the division of the many $j$-shell into the valence and the core parts can be done without ambiguities in such a way that the collectivities are essentially attributed to the core part. In addition, it is applicable also to such cases where there are no well-defined second HB minima. It is seen in Figs. 8(a), (b) and Tables II(a) and (b) that this alternative procedure also successfully reproduces the major characteristics of the exact spectra.

In Figs. 8(a), (b), Tables II(a), (b), we also present the results obtained by means of the conventional adiabatic (Born-Oppenheimer) approximation. They are calculated in the following way. First, we adopt the constrained HB method by choosing the expectation value $Q$ of the total "quadrupole" operator $\hat{Q} = \hat{Q}_n + \hat{Q}_p$ as a constraint to obtain the collective potential-energy functions displayed by the thick lines in Fig. 7. Second, we apply the conventional cranking procedure to evaluate the collective mass parameter as a function of $Q$. Finally, we solve the collective Schrödinger equation obtained after quantization. The resulting eigensolutions are denoted as "Adi." in these figures and tables. It is obvious that the adiabatic approximation completely fails in reproducing the deformed excited states that appear as the third eigenstates in the coupled-configuration SCC method.
§ 6. Concluding remarks

We have proposed a new microscopic method on the basis of the diabatic picture in order to study the shape coexistence phenomena in semi-magic nuclei. This method may be regarded as an extension of the SCC method to treating the couplings between diabatic vibrational modes associated with different HB minima. We have applied this method to three kinds of schematic models whose exact solutions exhibit two kinds of vibrational states coexisting in the same energy region. It is shown that our method well reproduces the main characteristics of the exact spectra of the systems, which is beyond the limit of applicability of the conventional adiabatic treatment. A particularly interesting suggestion for future study of the shape coexistence phenomena is that the two kinds of diabatic vibrational states associated with the first and the second minima of the collective potential-energy function may retain their identities even if their excitation energies are much higher than the barrier between the two local minima. A crucial quantity which determines whether such situations are realized or not is the matrix element of the pairing force between the two diabatic configurations. We shall apply the coupled-configuration SCC method proposed in this paper to the deformed excited $0^+$ states in Sn and Pb isotopes in a succeeding paper; with particular attention to the strength of the interaction matrix elements between the spherical and the deformed configurations.

Acknowledgements

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References