Collective coordinates, shape transitions, and shape coexistence: A microscopic approach

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We investigate a description of shape mixing and shape transitions using collective coordinates. To that end we apply a theory of adiabatic large-amplitude motion to a simplified nuclear shell model, where the approximate results can be contrasted with exact diagonalizations. We find excellent agreement for different regimes, and contrast the results with those from a more standard calculation using a quadrupole constraint. We show that the method employed in this work selects diabatic (crossing) potential energy curves where these are appropriate, and discuss the implications for a microscopic study of shape coexistence.
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I. INTRODUCTION

In order to describe processes in nuclei involving large excursions from equilibrium, such as shape coexistence or fission, we cannot use the small-amplitude harmonic expansion about a stationary mean-field state provided by the random-phase approximation (RPA). Various methods exist to deal with large-amplitude motion, many of which are reviewed in Ref. [1]. This reference also sets out the basic formalism on which our work is based.

We have recently embarked on a study into the properties of collective motion in systems with pairing. In a first application we have analyzed properties of collective motion in a semimicroscopic model of nucleons interacting through a pairing force, coupled to a single harmonic variable giving a macroscopic description of the remaining degrees of freedom [2]. We have used the local-harmonic approximation, which is equivalent to the generalized valley approximation for a single collective coordinate [1], to analyze the collective motion. To our surprise it has turned out that the system automatically selects either diabatic or adiabatic collective surfaces according to the strength of the pairing interaction. However, since this model is not fully microscopic, we feel that it would be beneficial to study a fully microscopic Hamiltonian. This does not mean that we wish to fully ignore the success of the unified model by Bohr and Mottelson, which indicates that the semimacroscopic approach describes many nuclear phenomena quite well, but rather that we wish to understand such behavior from a microscopic viewpoint. We thus feel that it is desirable to test the methodology for a fully microscopic Hamiltonian which is able to describe nuclear systems from vibrational to deformed.

To this end we investigate the collective motion in a microscopic model which describes a system of nucleons interacting through a simplified version of the pairing-plus-quadruple force [3]. Although the Hamiltonian has a very simple form, we shall see that the model can reproduce the qualitative features of many kinds of interesting situations observed in real nuclei. In this work we shall concentrate on the spherical-to-deformed transition, and nuclei with shape coexistence, where more than one equilibrium shape plays a role.

In the case of a single-j shell the model Hamiltonian is built from the generators of an o(4) algebra, which makes exact diagonalization feasible. The model has been originally developed to describe $K^\pi=0^+$ excitations in deformed nuclei [3], and has also been used as a test-bed for various methods used in the calculation of collective excitations such as the boson expansion method [4], the self-consistent collective coordinate method [5], and a semiclassical method [6]. The model can be generalized to multiple shells, where it has been used to investigate shape-coexistence phenomena [7]. Finally, a similar model has been used to study the collective mass parameter in finite superconducting systems [8].

Although the low-lying spectra in nuclei are mostly dominated by the quadrupole phonon ($J^\pi=2^+$) excitations, the anharmonicity is very important for many nuclei, especially in a shape-transition region, where the nature of the ground-state changes rapidly with particle number. For instance, the even-even Sm isotopes show a typical example of the spherical to deformed shape transition in which the spectrum shows a strong anharmonicity between the spherical ($N \leqslant 84$) and deformed ($N \geqslant 90$) nuclei, especially for ^{148,150}Sm. These phenomena are primarily related to the competition between the monopole and quadrupole interactions among the valence particles outside a closed core. The pairing-plus-quadrupole model, originally proposed by Bohr and Mottelson, was designed to describe this competition and is quite well able to reproduce the most important aspects of the experimental data (see Ref. [9], and references therein). Later the boson expansion method has been applied to the same model (with an additional quadrupole pairing interaction) for the description of the shape transition in the Sm isotopes [10], which shows excellent agreement with the experimental data. Since the $O(4)$ model is very similar to the pairing-plus-quadrupole model, it would be of significant interest to see whether our method of large amplitude collective motion is able to properly describe the shape transition phenomena in this exactly solvable model.

The importance of shape-coexistence in nuclear physics can be seen from the multitude of theoretical approaches and the amount of experimental data as compiled in Ref. [11].

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An important example can be found in even semimagic Sn and Pb isotopes, where the ground states are spherical. However, deformed excited $J^\pi = 0^+$ states have been observed at low-excitation energies in many of these nuclei. These excited states are regarded as states associated with proton two-particle-two-hole ($2p$-$2h$) excitations across the closed shell. Using the Nilsson picture, which shows down-sloping single-particle levels above the proton closed shell, and up-sloping levels below it, it is possible to assign a configuration of two particles lying on down-sloping levels and two holes on up-sloping levels. The configuration-constrained Nilsson-Strutinsky calculations as performed by Bengtsson and Nazarewicz [12] have suggested that the diabatic potential-energy curve obtained by switching off the interaction between the $2p$-$2h$ and the ground-state ($0p$-$0h$) configuration gives more accurate picture than the conventional adiabatic potential energy. This question, whether the nuclear collective potential is adiabatic or diabatic, is quite old, and was originally raised by Hill and Wheeler [13]. We have shown in our previous work [2] that, using a method to self-consistently determine collective coordinates, the system itself selects either an adiabatic or a diabatic collective path according to the properties of the interaction. It is our aim to investigate in the $O(4)$ model whether the method is able to provide us with useful information about shape mixing, and to test whether it makes useful predictions whether the collective potential energy is diabatic or adiabatic.

In Sec. II, the theory of adiabatic large amplitude collective motion is briefly reviewed. A problem peculiar to the model under consideration, related to the special character of the zero modes, is dealt with by a prescription to remove the zero-mode degrees of freedom. In Sec. III, the $O(4)$ model in a single-j shell is described, and we discuss the applications of our methodology to the model. In Sec. IV, a generalization of the $O(4)$ model to multiple shells is introduced. We then investigate the large amplitude collective motion for a set of parameters which describe transitional (from vibrational to deformed) nuclei. In Sec. V, we use a proton-neutron form of the Hamiltonian, which can be used to describe shape coexistence. We show how our method selects a diabatic or adiabatic potential energy curve. Finally, we give some conclusion and present an outlook in Sec. VI.

II. FORMALISM

A. Review of methodology for the local harmonic approximation

We briefly review the local harmonic approximation (LHA), as a method in adiabatic large amplitude collective motion (ALACM). A full discussion of the method can be found in Ref. [1]. We use the convention that the repeated appearance of the same symbol $(\alpha,\beta,\ldots;i,j,\ldots)$ as an upper and lower index denotes a sum over the relevant index over all allowed values. We also use the convention that a comma in a lower index denotes the derivative with respect to a coordinate, thus $F_{,\alpha} = \partial F/\partial \xi^\alpha$.

Our approach to large amplitude collective motion is applicable for classical Hamiltonian systems which have a kinetic energy quadratic in momentum only. Since most systems, especially the mean-field problems of nuclear physics, do not satisfy this requirement, we are forced to truncate the full Hamiltonian $\mathcal{H}(\xi,\pi)$ to second order,

$$\mathcal{H}_{ad}(\xi,\pi) = \frac{1}{2} B^{\alpha\beta}\pi_\alpha\pi_\beta + V(\xi), \quad \alpha,\beta = 1,\ldots,n. \tag{2.1}$$

Here the mass tensor $B^{\alpha\beta}$ depends in general on the coordinates ξ^α and is defined by expansion of the Hamiltonian to second order in momenta

$$B^{\alpha\beta} = \left.\frac{\partial^2 \mathcal{H}}{\partial\pi_\alpha \partial\pi_\beta}\right|_{\pi=0}. \tag{2.2}$$

Thus all terms of more than quadratic order in momenta are neglected. This is only possible when the higher-order terms are small, which is definitely true in the small (zero) velocity limit. It is in this sense that the theory may be regarded as an *adiabatic* theory. The tensor $B_{\alpha\beta}$, which is defined as the inverse of $B^{\alpha\beta}$ ($B^{\alpha\gamma}B_{\gamma\beta} = \delta^\alpha_\beta$), plays the role of metric tensor in the Riemannian formulation of the local harmonic approximation below.

Collective coordinates x^i and intrinsic (noncollective) coordinates x^a which are decoupled from each other, are assumed to be reached by making a point transformation, conserving the quadratic nature of Eq. (2.1),

$$x^i = f^i(\xi) \quad (i = 1,\ldots,K), \tag{2.3}$$

$$x^a = f^a(\xi) \quad (a = K+1,\ldots,n). \tag{2.4}$$

In this section, we use symbols $(\alpha,\beta,\ldots)$ as indices of the original coordinates, $(\mu,\nu,\ldots)$ for the new coordinates after the transformation, $(i,j,\ldots)$ for collective coordinates, and $(a,b,\ldots)$ for intrinsic coordinates. The requirement that the motion is exactly restricted to a collective subspace Σ (defined by $x^a = 0$), yields three conditions

$$\overline{B^{ai}} = 0, \quad \overline{V}_{,a} = 0, \tag{2.5}$$

$$\overline{B^{ij}_{,a}} = 0. \tag{2.6}$$

These three conditions are only satisfied for exactly decoupled collective motion, a rare occurrence indeed. It is therefore practical to combine these three decoupling conditions into two sets of conditions, that are satisfied even when no exact collective subspace exists. The conditions chosen are those that determine the bottom of a valley in the potential landscape, which is, under certain conditions, an approximation to a decoupled subspace. The quality of this decoupling can be measured, see below. In this work we prefer to work with the LHA. In the default case of a single collective coordinate only ($K=1$), the basic equations of this formalism can be written as

$$V_{,\alpha} = \lambda f^1_{,\alpha}, \tag{2.7}$$

$$B^{\beta\gamma}V_{;\alpha\gamma}f^1_{,\beta} = \omega^2 f^1_{,\alpha}. \tag{2.8}$$

The second of these equations is the local harmonic (or local RPA) equation from which the method derives its name. The covariant derivative (denoted by a semicolon) in the left-hand side of Eq. (2.8) is defined by

$$V_{;\alpha\beta}\equiv V_{,\alpha\beta}-\Gamma^{\gamma}_{\alpha\beta}V_{,\gamma}, \tag{2.9}$$

with the affine connection Γ defined in the standard way in terms of the metric tensor $B_{\alpha\beta}$ as

$$\Gamma^{\alpha}_{\beta\gamma}=\frac{1}{2}B^{\alpha\delta}(B_{\delta\beta,\gamma}+B_{\delta\gamma,\beta}-B_{\beta\gamma,\delta}). \tag{2.10}$$

Equations (2.7) and (2.8) must be solved as a self-consistent pair, except at stationary points, where the RPA (2.8) is independent of the force equation (2.7). This allows us to bootstrap our way up from such a stationary point. This procedure constructs a path by finding successive points at which an eigenvector $f^{1}_{,\alpha}$ of the covariant RPA equation (2.8) satisfies the force condition (2.7) at the same time. It is worth noting that since the equations at every point can be solved independently, no computational error is accumulated while calculating the collective path, which is a problem with, e.g., the formalism of Goeke and Reinhard [14].

The quality of decoupling can be measured by comparing two different collective mass parameters that can be calculated in the theory. If we calculate the derivatives $d\xi^{\alpha}/dx^{1}$ in terms of the tangents of the path, we find

$$\check{B}_{11}=\frac{d\xi^{\alpha}}{dx^{1}}B_{\alpha\beta}\frac{d\xi^{\beta}}{dx^{1}}. \tag{2.11}$$

The other mass parameter can be obtained by using the eigenvectors $f^{1}_{,\alpha}$ obtained from the covariant RPA equation

$$\overline{B}^{11}=f^{1}_{,\alpha}B^{\alpha\beta}f^{1}_{,\beta}. \tag{2.12}$$

This is equal to $(\overline{B}_{11})^{-1}$ if the decoupling is exact. Therefore, we define the decoupling measure D as

$$D=(\check{B}_{11})\overline{B}^{11}-1. \tag{2.13}$$

The size of this measure D indicates the quality of decoupling. The smaller its value, the better the decoupling.

B. Removal of spurious modes

In this section we discuss how to treat the spurious modes. A typical example is given by the Nambu-Goldstone (NG) mode associated with the violation of particle-number conservation. We have presented a method adding a constraint to the original LHA formalism, in order to find a collective subspace orthogonal to the NG modes [2]. However, in the model to be discussed here this method does not work because of a divergence problem associated with the fact that the model has an exact zero mass parameter, since $\det(B^{\alpha\beta})=0$. Instead, in this paper, we choose to remove the NG degrees of freedom explicitly.

For the models to be discussed in the following sections, the modes associated with a change in average particle number are given by a linear combination of coordinates:

$$\tilde{f}^{\mathrm{NG}}(\xi)=\sum_{\alpha=1}^{n}c_{\alpha}\xi^{\alpha}, \tag{2.14}$$

where c_{α} is a constant. The problem is that this mode leads to a zero eigenvalue of the mass

$$B^{\alpha\beta}\tilde{f}^{\mathrm{NG}}_{,\beta}=B^{\alpha\beta}c_{\beta}=0. \tag{2.15}$$

This means that we cannot invert the mass matrix. The only sensible way to deal with this is to remove these degrees of freedom from our space, by defining a new set of coordinates, $\tilde{\xi}^{\mu}=\tilde{f}^{\mu}(\xi)$. These are required to satisfy

$$B^{\alpha\beta}\tilde{f}^{\mu}_{,\beta}\neq 0 \quad \text{for} \quad \forall\alpha \ \text{ and } \mu=1,\ldots,n-M, \tag{2.16}$$

$$B^{\alpha\beta}\tilde{f}^{\mu}_{,\beta}=0 \quad \text{for} \quad \forall\alpha \ \text{ and } \mu=n-M+1,\ldots,n, \tag{2.17}$$

where we assume that there are M NG modes ($\mu>n-M$). Then, we may formulate the LHA in the space of $n-M$ dimension, $\{\tilde{\xi}^{\mu}\}_{\mu=1,\ldots,n-M}$, in which $\det(B^{\mu\nu})\neq 0$:

$$\mathcal{M}^{\nu}_{\mu}f^{i}_{,\nu}=(\omega^{i})^{2}f^{i}_{,\mu}, \tag{2.18}$$

$$\mathcal{M}^{\nu}_{\mu}\equiv\tilde{V}^{;\nu}_{;\mu}=\tilde{B}^{\nu\nu'}\tilde{V}_{;\nu'\mu}, \tag{2.19}$$

where indices $\mu,\nu,\ldots,$ are running only from 1 to $n-M$. Our aim is to provide a feasible method to calculate this LHA, namely to calculate the mass parameter $\tilde{B}^{\nu\nu'}$, potential $\tilde{V}(\tilde{\xi})$, and their derivatives.

The second equation (2.17) determines tangent vectors of the NG modes. The rest of coordinates $\tilde{f}^{\mu}$ for $\mu=1,\ldots,n-M$ are arbitrary as long as their derivatives are linearly independent from the others. The full Jacobian matrix $\tilde{f}^{\mu}_{,\alpha}$ allows us to define the derivatives of inverse transformation, $\tilde{g}^{\alpha}_{,\mu}$ as the inverse of $\tilde{f}$,

$$\tilde{f}^{\mu}_{,\beta}\tilde{g}^{\beta}_{,\nu}=\delta^{\mu}_{\nu}, \quad \tilde{f}^{\mu}_{,\beta}\tilde{g}^{\alpha}_{,\mu}=\delta^{\alpha}_{\beta}. \tag{2.20}$$

Since all $\tilde{f}^{\mu}_{,\alpha}$ are constant (independent of coordinates), all $\tilde{g}^{\alpha}_{,\mu}$ are also constant and the derivatives $\tilde{f}^{\mu}_{,\alpha\beta}$ (or $\tilde{g}^{\mu}_{,\alpha\beta}$) all vanish. This implies that within the NG subspace the connection vanishes, $\Gamma=0$, and the geometric character of the transformation of any tensor is fully determined in the subspace that does not contain the NG modes. One can use this to calculate the new mass parameter and its derivatives as

$$\tilde{B}^{\mu\nu}=\tilde{f}^{\mu}_{,\alpha}B^{\alpha\beta}\tilde{f}^{\nu}_{,\beta}, \tag{2.21}$$

$$\tilde{B}^{\mu\nu}_{,\lambda}=\tilde{f}^{\mu}_{,\alpha}B^{\alpha\beta}_{,\gamma}\tilde{f}^{\nu}_{,\beta}\tilde{g}^{\gamma}_{,\lambda} \tag{2.22}$$

and the derivatives of potential as

$$\tilde{V}_{,\mu}=\tilde{g}^{\alpha}_{,\mu}V_{,\alpha}, \tag{2.23}$$

$$\tilde{V}_{,\mu\nu}=\tilde{g}^{\alpha}_{,\mu}\tilde{g}^{\beta}_{,\nu}V_{,\alpha\beta}. \tag{2.24}$$

III. THE $O(4)$ MODEL

We shall first study the properties of the single-shell $O(4)$ model. We define fermionic operators $c^{\dagger}_{jm}$ and c_{jm} that create or annihilate a particle in the $J_z=m$ substate. In terms of these operators we define four pairing (P, $P^{\dagger}$, $\tilde{P}$, and $\tilde{P}^{\dagger}$)

and two multipole operators (N and Q) that close under commutation, and generate the algebra o(4),

$$P^\dagger=\sum_{m>0} c^\dagger_{jm}c^\dagger_{j\bar{m}},\quad \tilde{P}^\dagger=\sum_{m>0}\sigma_{jm}c^\dagger_{jm}c^\dagger_{j\bar{m}}, \tag{3.1}$$

$$N=\sum_m c^\dagger_{jm}c_{jm},\quad Q=\sum_m \sigma_{jm}c^\dagger_{jm}c_{jm}, \tag{3.2}$$

$$\sigma_{jm}=\begin{cases}+1 & \text{for } |m|<\Omega/2,\\ -1 & \text{for } |m|\geqslant\Omega/2.\end{cases} \tag{3.3}$$

Here we need to require that the pair multiplicity $\Omega=j+1/2$ is an *even* integer in order for the algebra to close. The sign of σ_{jm} is chosen so as to mimic the behavior of the matrix elements of the axial quadrupole operator $\langle jm|r^2Y_{20}|jm\rangle$, and we shall call Q the quadrupole operator in the remainder of this work, even though it does not carry the correct multipolarity.

As is well-known, the algebra o(4) is isomorphic to su(2)$\oplus$su(2). This can be made explicit in terms of the quasispin operators

$$A_+=\tfrac{1}{2}(P^\dagger+\tilde{P}^\dagger)=A^\dagger_-,\quad A_0=\tfrac{1}{4}(N+Q-\Omega), \tag{3.4}$$

$$B_+=\tfrac{1}{2}(P^\dagger-\tilde{P}^\dagger)=B^\dagger_-,\quad B_0=\tfrac{1}{4}(N-Q-\Omega), \tag{3.5}$$

which generate two independent su(2) algebras

$$[A_+,A_-]=2A_0,\quad [B_+,B_-]=2B_0, \tag{3.6}$$

$$[A_0,A_\pm]=\pm A_\pm,\quad [B_0,B_\pm]=\pm B_\pm, \tag{3.7}$$

$$[A_\mu,B_{\mu'}]=0. \tag{3.8}$$

The Hamiltonian of the model is chosen as a simple quadratic form in (some of) the generators of o(4),

$$H=-GP^\dagger P-\tfrac{1}{2}\kappa Q^2, \tag{3.9}$$

and mimics the pairing-plus-quadrupole model that has been such a successful phenomenological model in heavy nuclei [9]. Even though the Hamiltonian looks simple, it does not have a closed-form solution [it does not have $O(4)$ dynamical symmetry]. Nevertheless a numerically exact solution for the Hamiltonian (3.9) can be obtained by simple diagonalization. To this end one rewrites the Hamiltonian in terms of the quasispin operators **A** and **B**

$$H=-G(A_++B_+)(A_-+B_-)-2\kappa(A_0-B_0)^2. \tag{3.10}$$

This Hamiltonian commutes with the total particle number $N=2(A_0+B_0)+\Omega$, and there are no further constants of the motion. The pairing force tends to align the two quasispin vectors **A** and **B**, so as to obtain the maximal pairing matrix elements, while the quadrupole force tends to dealign them [to maximize $(A_0-B_0)^2$]. In this picture, the nonintegrability of the model, as well as the physics described, is related to the competition between the pairing and the quadrupole force. This is identical to a competition between alignment and dealignment of the quasispins.

For a fixed number of particles $N=2n_0$, we construct from the vacuum state $|0\rangle$ all states with a constant number of generators A_+ and B_+

$$|n_0,k_a\rangle=\left[\frac{(\Omega/2-k_a)!(\Omega/2-n_0+k_a)!}{\{(\Omega/2)!\}^2k_a!(n_0-k_a)!}\right]^{1/2}A_+^{k_a}B_+^{n_0-k_a}|0\rangle, \tag{3.11}$$

where $0\leqslant k_a\leqslant n_0$. Finding the eigenvectors of the Hamiltonian now involves a trivial matrix diagonalization in this basis of dimension (n_0+1).

A. The coherent-state representation and the TDHFB equations of motion

The mean-field description of the Hamiltonian (3.10) is most easily based on the use of a product of su(2) coherent states, one for the A_μ subalgebra, and another for the B_μ one. Each of these states is characterized by a complex variable, z_a and z_b [15]. The time-dependent mean-field dynamics in this parametrization is the classical Hamiltonian problem we shall apply our methodology to. We can also parametrize the coherent state with four real angles [6,15]

$$|z_a,z_b\rangle=\exp[z_aA_+-z_a^*A_-+z_bB_+-z_b^*B_-]|0\rangle, \tag{3.12}$$

$$=\left(\cos\frac{\theta}{2}\cos\frac{\chi}{2}\right)^{\Omega/2}\exp\left[\tan\frac{\theta}{2}\exp(-i\phi)A_+ +\tan\frac{\chi}{2}\exp(-i\psi)B_+\right]|0\rangle, \tag{3.13}$$

where we have used

$$z_a=\frac{\theta}{2}\exp(-i\phi),\quad z_b=\frac{\chi}{2}\exp(-i\psi). \tag{3.14}$$

The time-dependent Hartree-Fock Bogoliubov (TDHFB) equations are in this case the classical equations of motion obtained from the stationary condition of the coherent-state action $\delta S=0$, where

$$S[z]=\int^t dt\langle z_a,z_b|i\partial_t-H|z_a,z_b\rangle, \tag{3.15}$$

$$=\int^t dt\frac{\Omega}{2}\left(\dot{\phi}\sin^2\frac{\theta}{2}+\dot{\psi}\sin^2\frac{\chi}{2}\right)-\int^t dt\,\mathcal{H}(\theta,\chi;\phi,\psi), \tag{3.16}$$

and

$$\mathcal{H}=\langle z_a,z_b|H|z_a,z_b\rangle. \tag{3.17}$$

In order to facilitate our work we introduce real canonical variables ξ^α and π_α,

$$\xi^1=\frac{\Omega}{2}\sin^2|z_a|=\frac{\Omega}{2}\sin^2\frac{\theta}{2},\quad \xi^2=\frac{\Omega}{2}\sin^2|z_b|=\frac{\Omega}{2}\sin^2\frac{\chi}{2}, \tag{3.18}$$

$$\pi_1=\arg(z_a)=-\phi,\quad \pi_2=\arg(z_b)=-\psi. \tag{3.19}$$

Since these variables are canonical, the equations of motion are of Hamiltonian form

$$\dot{\pi}_\alpha = -\frac{\partial \mathcal{H}}{\partial \xi^\alpha}, \quad \dot{\xi}^\alpha = \frac{\partial \mathcal{H}}{\partial \pi_\alpha}, \tag{3.20}$$

where the classical Hamiltonian (3.17) is the coherent state expectation value of the Hamiltonian rewritten in terms of canonical variables [the explicit form can be found from that of the more general Hamiltonian discussed in the following section, Eqs. (4.9)–(4.14), upon substitution of $q_\alpha = 1$]. The adiabatic Hamiltonian is then found by expanding the full Hamiltonian with respect to π up to second order, and is defined in Eqs. (4.15)–(4.18).

B. Requantization

In this section, we discuss the problem of defining a requantisation procedure and the consequences of the adiabatic truncation with respect to momentum. The classical limit of the single-j Hamiltonian has two constants of motion $\mathcal{H} = E$ and $\langle N \rangle = 2\Sigma_\alpha \xi^\alpha = N_0$. Since the phase space is four dimensional, this implies the complete integrability of the system, and there is a two dimensional torus on which all classical orbits lie. Due to this special feature of this model, one can apply the Einstein-Brillouin-Keller (EBK) quantization condition. This has been done in Ref. [6] and good agreement with the exact results has been obtained for both energy spectra and transition amplitudes. However, it is impossible to extend this quantization method to non-integrable systems like the ones we will discuss in the following sections. We wish to use the same quantization procedure for the simplest form of the model and the more complicated cases discussed later on, and shall turn to our favorite technique first.

After truncation of the Hamiltonian up to second order in momentum, we can define a collective Hamiltonian by evaluating its value for points on the collective space Σ which is parametrized by x^1 and p^1 (strictly this is the cotangent bundle over Σ), since we have chosen $x^a = p^a = 0; a = 1, \ldots, n-1$,

$$\overline{\mathcal{H}}_{\rm col} = \overline{\mathcal{H}}_{\rm ad}|_\Sigma = \frac{1}{2}\overline{B}^{11}(x^1) p_1^2 + \overline{V}(x^1), \tag{3.21}$$

$$\overline{B}^{11}(x^1) = \sum_{\alpha\beta} f^1_{,\alpha} f^1_{,\beta} B^{\alpha\beta}[\xi^\alpha = g^\alpha(x^1, x^a = 0)], \tag{3.22}$$

$$\overline{V}(x^1) = V[\xi^\alpha = g^\alpha(x^1, x^a = 0)]. \tag{3.23}$$

Since the scale of collective coordinate x^1 is arbitrary, we choose to normalize $f^1_{,\alpha}$ so as to make $\overline{B}^{11} = 1$. Subsequently, the Hamiltonian $\overline{\mathcal{H}}_{\rm col}$ is quantized in this flat space as [2]

$$\hat{H}_{\rm col} = -\frac{1}{2}\frac{d^2}{dx^2} + \overline{V}(x), \tag{3.24}$$

where we have replaced (x^1, p_1) by (x, p).

In order to evaluate the matrix elements of a one-body operator F (either diagonal or transition matrix elements), we first obtain the collective classical representation of the operator F, which in keeping with the adiabatic approximation is expanded in powers of momentum,

$$\overline{\mathcal{F}}(x,p) = \mathcal{F}(\xi,\pi)|_\Sigma = \langle z|F|z\rangle|_\Sigma = \sum_{i=0}^{\infty} \mathcal{F}^{(i)}(\xi,\pi)\Big|_\Sigma = \sum_{i=0}^{\infty} \overline{\mathcal{F}}^{(i)}(x,p). \tag{3.25}$$

Here $\mathcal{F}^{(i)}$ is the term of ith order in π. The function $\overline{\mathcal{F}}$ is requantized, by making the replacement $\overline{\mathcal{F}}(x,p) \rightarrow \overline{F}(x, d/dx)$, at which point one will have to confront the problem of operator ordering between x and p. We shall avoid this problem by keeping, invoking once again the assumption of slow collective motion, only the zeroth order term $\overline{\mathcal{F}}^{(0)}$. It is an interesting question what the effect of higher order terms will be. This is clearly outside the scope of the present work, and requires further investigation. Fortunately, in the current model, we have no ambiguity for the quadrupole operator Q because $\mathcal{Q}^{(i)} = 0$ for $i \neq 0$. For convenience we denote the classical limit of the quadrupole operator by q. The transition matrix elements can thus be calculated by the one-dimensional integral

$$\langle n'|F|n\rangle = \int dx\, \Psi^*_{n'}(x) \overline{F}^{(0)}(x) \Psi_n(x), \tag{3.26}$$

where Ψ_n are the eigenfunctions of the collective Hamiltonian (3.24).

From the number of coordinates and momenta found (2 +2) we see that the configuration space of the single-j shell model is two dimensional. Since there is a zero mode [$\det(B^{\alpha\beta}) = 0$] corresponding to the NG mode associated with the particle number violation, one may obtain a one-dimensional path Σ by simply applying the prescription in Sec. II B (without the application of LHA). Rather than plotting this path we have chosen to represent the results of requantization for energies and transition strengths. These results are presented in panel (1) of Fig. 1, and as the dotted lines in Fig. 2. We obtain good agreement with the exact results over a wide range of parameters except very close to a pure quadrupole force. Due to the peculiar nature of the quadrupole operator the mass parameter goes to zero in this limit ($G = 0$), and there is no kinetic term. Thus an eigenstate of Hamiltonian is a coordinate eigenstate $|x\rangle$ at the same time. Then, the periodic nature of the momentum becomes important, which we have ignored in our calculations. Taking account of the periodicity of momentum, one finds that coordinate operator x should have discrete eigenvalues. In order to check that it is possible to deal with this problem, we have expanded the Hamiltonian up to second order with respect to the coordinates rather than momenta, keeping all order in momenta. We have also imposed periodic boundary conditions on the wave function $\Psi(p) = \Psi(p + \pi/2)$. The result of this quantization is shown in panel (2) of Fig. 1, and as the dashed lines in Fig. 2. The agreement is good in the no-pairing limit $G = 0$, while it is not as good as the standard quantization anywhere else. Since we are not really interested in the (integrable) pure quadrupole model, but rather in competition between the pairing and quadrupole forces, we shall ignore the $G = 0$ limit in the rest of this work. We shall

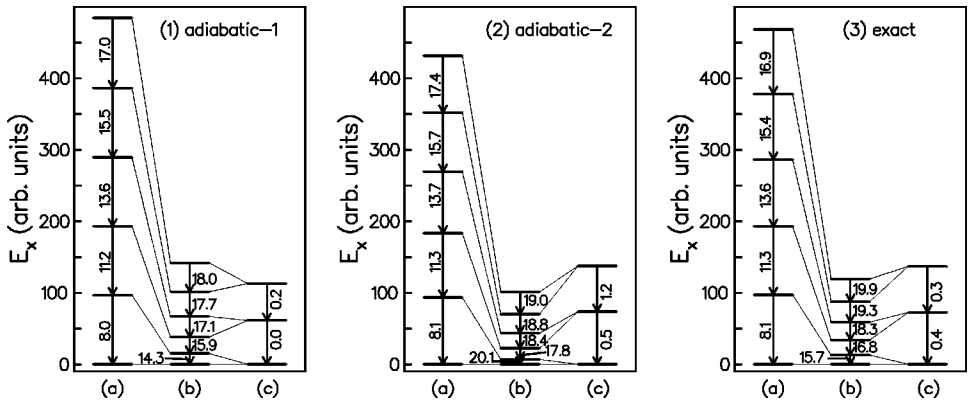

FIG. 1. The excitation energies and transition matrix elements $|\langle n-1|Q|n\rangle|$, all in arbitrary units, in the single-j shell $O(4)$ model as a function of the ratio between the strength of the pairing and that of the quadrupole force. The case (a) is a weak quadrupole force, $2\kappa/G=0.079$, (b) a medium sized one, $2\kappa/G=1.63$, and (c) a very strong one, $2\kappa/G=12.7$. We have constrained $G^2+(2\chi)^2=1$. The three panels give our standard adiabatic quantization (1), the results from the ''adiabatic in coordinates'' method (2), and the exact results (3).

thus follow the conventional adiabatic quantization procedure in coordinate space as described above.

IV. THE MULTI-$O(4)$ MODEL

A. The model and the Hamilton's form of TDHFB equation

It is a greater challenge to our approach to study the multishell case. There exists a straightforward extension of the model, by addition of the individual pairing generators, and summing the quadrupole operators of each shell with a weight factor (we shall thus not have a direct coupling between the different shells). The operators are, for $j=j_1,j_2,\ldots,j_\Lambda$ (for each shell j_i we take the pair degeneracy $\Omega_i=j_i+1/2$ to be even)

$$P^\dagger=\sum_{i,m_i>0} c^\dagger_{j_i m} c^\dagger_{j_i \bar{m}_i}, \quad \tilde{P}^\dagger=\sum_{i,m_i>0} \sigma_{j_i m_i} c^\dagger_{j_i m_i} c^\dagger_{j_i \bar{m}_i}, \tag{4.1}$$

$$N=\sum_{i m_i} c^\dagger_{j_i m_i} c_{j_i m_i}, \quad Q=\sum_{i m_i} q_i \sigma_{j_i m_i} c^\dagger_{j_i m_i} c_{j_i m_i}, \tag{4.2}$$

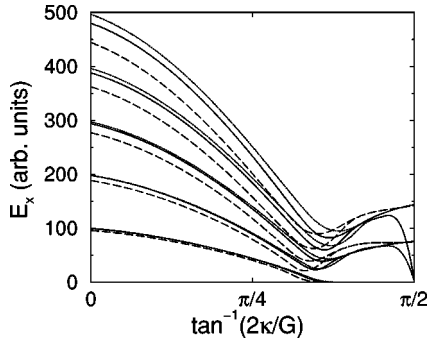

FIG. 2. The excitation energies in the single-j shell $O(4)$ model for 40 particles in a shell with $\Omega=100$ as a function of the parameter essentially the ratio between the strength of the pairing and that of the quadrupole force. The left end corresponds to the case of pure pairing force and the right end to the pure quadrupole force. The solid lines are the exact results, and the dotted lines represent the standard requantization of the adiabatic collective Hamiltonian. The dashed lines represent the expansion in terms of coordinates discussed in the text.

where q_i represents the magnitude of quadrupole moment carried by single-particle states. For each shell we can define quasispin $[\mathrm{su}(2)\oplus\mathrm{su}(2)]$ generators $\mathbf{A}^i$ and $\mathbf{B}^i$ in a manner similar to Eqs. (3.4) and (3.5). We choose a slightly more general Hamiltonian than in the previous chapter by adding a term containing spherical single-particle energies

$$H=\sum_{jm} \epsilon_j c^\dagger_{jm} c_{jm} - G P^\dagger P - \frac{1}{2}\kappa Q^2. \tag{4.3}$$

The exact solution can also be obtained by diagonalization in a basis set

$$\bigotimes_{i=1}^{\Lambda} |k_a^i, k_b^i\rangle = \prod_{i=1}^{\Lambda} (A_+^i)^{k_a^i} (B_+^i)^{k_b^i} |0\rangle, \tag{4.4}$$

where $0\leqslant k_a^i, k_b^i \leqslant \Omega_i/2$ and $\Sigma_i(k_a^i+k_b^i)=n_0=N_0/2$. This is no longer as trivial a calculation as before, since the dimension of the basis increases rapidly with the number of shells Λ, but can still be done, provided that one chooses Λ sufficiently small. On the other hand, since the dimension of TDHFB configuration space increases only linearly with Λ, the amount of effort required for the ALACM calculation is still rather small. The time-dependent mean-field state is obtained through the use of the coherent-state representation as before, and is given by the product of states (3.13)

$$|\mathbf{z}\rangle=\prod_{i}^{\Lambda} |z_i\rangle. \tag{4.5}$$

We choose the canonical variables as

$$\xi^\alpha=\begin{cases} \dfrac{\Omega_i}{2}\sin^2\dfrac{\theta_i}{2} & \text{for } \alpha=i=1,\ldots,\Lambda, \\ \dfrac{\Omega_i}{2}\sin^2\dfrac{\chi_i}{2} & \text{for } \alpha=\Lambda+i=\Lambda+1,\ldots,2\Lambda, \end{cases} \tag{4.6}$$

$$\pi_\alpha=\begin{cases} -\phi_i & \text{for } \alpha=i=1,\ldots,\Lambda, \\ -\psi_i & \text{for } \alpha=\Lambda+i=\Lambda+1,\ldots,2\Lambda. \end{cases} \tag{4.7}$$

It is convenient to allow the indices of e, q, and Ω to range from 1 to 2Λ by copying the original list of parameters, e.g.,

$$e_\alpha=\begin{cases} e_i \ \ (i=\alpha) & \text{for } \alpha=1,\ldots,\Lambda, \\ e_i \ \ (i=\alpha-\Lambda) & \text{for } \alpha=\Lambda+1,\ldots,2\Lambda. \end{cases} \tag{4.8}$$

Using these definitions, the classical Hamiltonian can be given in the compact form

$$\mathcal{H}=h_{\rm sp}+\mathcal{H}_P+\mathcal{H}_Q, \tag{4.9}$$

$$h_{\rm sp}=2\sum_\alpha e_\alpha \xi^\alpha, \tag{4.10}$$

$$\mathcal{H}_P(\xi,\pi)=-\frac{G}{16}\left\{\left|\sum_\alpha e^{i\pi_\alpha}S_\alpha\right|^2+32\sum_\alpha \Omega_\alpha^{-1}(\xi^\alpha)^2\right\}, \tag{4.11}$$

$$\mathcal{H}_Q(\xi)=-2\kappa\left\{\left(\sum_\alpha \sigma_\alpha q_\alpha \xi_\alpha\right)^2+\sum_\alpha \Omega_\alpha^{-1} q_\alpha \xi^\alpha(\Omega_\alpha-\xi^\alpha)\right\}, \tag{4.12}$$

$$S_\alpha=2\sqrt{2\xi^\alpha(\Omega_\alpha-2\xi^\alpha)}, \tag{4.13}$$

$$\sigma_\alpha=\begin{cases} +1 & \text{for } \alpha=1,\ldots,\Lambda, \\ -1 & \text{for } \alpha=\Lambda+1,\ldots,2\Lambda. \end{cases} \tag{4.14}$$

The adiabatic limit of this Hamiltonian is

$$\mathcal{H}_{\rm ad}=\frac{1}{2}\sum_{\alpha\beta} B^{\alpha\beta}\pi_\alpha\pi_\beta+V(\xi), \tag{4.15}$$

$$B^{\alpha\beta}=\frac{G}{8}\left[\delta_{\alpha\beta}\left(S_\alpha\sum_\gamma S_\gamma\right)-S_\alpha S_\beta\right], \tag{4.16}$$

$$V(\xi)=V_P(\xi)+V_Q(\xi), \tag{4.17}$$

$$V_P(\xi)=\mathcal{H}_P(\xi,\pi=0), \ \ V_Q(\xi)=\mathcal{H}_Q(\xi). \tag{4.18}$$

The terms in Eqs. (4.11) and (4.12) proportional to Ω_α^{-1} arise from the exchange contributions, and will be neglected.

B. Results for transitional nuclei

Using the LHA we identify the collective degree of freedom amongst the 2Λ coordinates. As before we first must remove the NG mode corresponding to a change in particle number explicitly, due to the zero mass parameter associated with this mode. The particle number is simply given by the sum of the numbers for the individual shells, $\mathcal{N}=2\Sigma_\alpha\xi^\alpha$. It is easy to show that

$$\sum_\beta B^{\alpha\beta}\mathcal{N}_{,\beta}=2\sum_\beta B^{\alpha\beta}=0. \tag{4.19}$$

Thus we apply the prescription discussed in Sec. II B to this model, and use the LHA to determine the collective path in the remaining $(2\Lambda-1)$-dimensional coordinate space. Since we shall mainly investigate how the LHA can deal with the transition spherical to deformed, it is sufficient to study only two shells. We take the size of these shells to be equal, $\Omega_1=\Omega_2=10$, and put 16 particles in the available space. We split the degeneracy by taking $e_1=0$ and $e_2=1$, and we use a different value of the ''quadrupole moment'' for each shell as well, $q_1=3$ and $q_2=1$. The pairing force is fixed at $G=0.3$, and we only vary the quadrupole force strength κ.

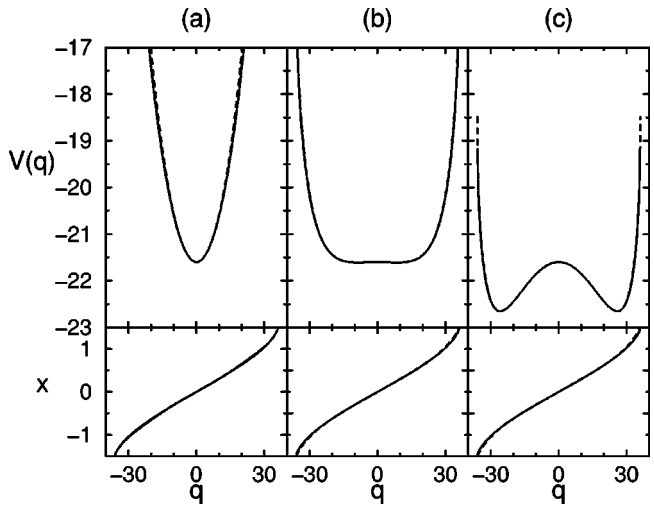

FIG. 3. The collective potential energy $V(q)$ and the collective coordinate x (normalized to unit mass) as a function of the quadrupole moment $q=\langle\hat{Q}\rangle$. We show both the LHA (dashed line) and the CHB (solid line) results in each figure. These results are, for this model, essentially indistinguishable. The case (a) corresponds to a weak quadrupole force ($\kappa=0.01$), (b) to a slightly stronger force ($\kappa=0.03$), and (c) to the strongest, $\kappa=0.035$. The units of all displayed quantities are arbitrary.

We show a representation of the collective potential energy and the collective coordinate in Fig. 3. We represent these quantities as a function of the expectation value of the quadrupole operator. As an alternative to the LHA approach, we have also performed a simple constrained Hartree-Bogoliubov (CHB) calculation, where one imposes a value for the expectation value of the quadrupole operator. We determine the mass for this case by replacing the RPA eigenvector by the coordinate derivative of the quadrupole expectation value. We then renormalize the coordinate to obtain a constant mass.

We have investigated a full shape transition scenario, where we have changed the strength of the quadrupole interaction so that the collective Hamiltonian changes from spherical and harmonic for case (a) to flat for case (b) to deformed for case (c). We see that the difference between the LHA and CHB calculations is relatively small. This is also borne out by the spectra and transition strength in Fig. 4. We can see the similarity between the two approximate calculations. If anything, the LHA gives slightly better results than the CHB based calculations. We seem to be unable to reproduce the large density of states found in the exact calculation for ''deformed'' nuclei, where there are indications from the transition strengths that some of the states in the approximate calculations are split into several of the exact states. Note, however, that at an excitation energy of 6, we are 5 units above the barrier, so this may just be due to our choice of parameters. The shape mixing in the low-lying excited states appears to be described sensibly, however. We would have liked to be able to choose an even large value of κ, but if we do that the system collapses to the largest possible quadrupole moment in the model space, which leads to all kinds of unphysical complications.

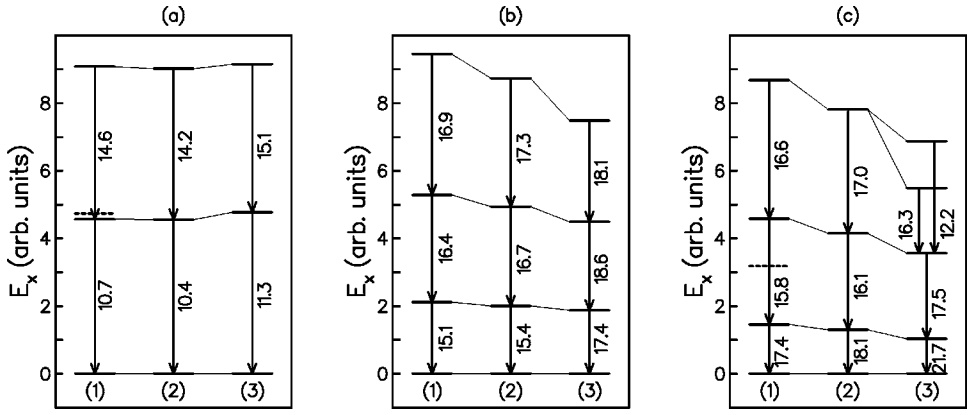

FIG. 4. The excitation energies E_x and transition matrix elements $|\langle n'|Q|n\rangle|$ (numbers next to arrows) in the two-shell case discussed in the text. The three cases (a), (b), and (c) correspond to those discussed in Fig. 3. In each of the three panels the left one (1) is obtained from requantizing the CHB, the middle one (2) is obtained from requantizing the LHA result, and the right one corresponds to exact diagonalization. The dashed line shows the lowest RPA eigenvalue.

V. A MULTISHELL $O(4)$ MODEL WITH NEUTRONS AND PROTONS

In heavy nuclei, the number of neutrons is normally (much) larger than that of protons, which often leads to a radically different shell structure at the Fermi surface for neutrons and protons. In order to perform a model study of such phenomena, where we can still perform an exact calculation, we adapt the multishell $O(4)$ model introduced in the previous section to one describing systems with both neutrons and protons [7]. We shall then use this model to analyze the collective dynamics of shape-coexistence nuclei, as observed for instance in semimagic nuclei. At the same time we shall concentrate on the diabatic/adiabatic dichotomy already mentioned in the Introduction.

The model is a simple extension of the multishell $O(4)$ model in the previous section, with the main difference that we do not have pairing between proton and neutron orbitals

$$H = H_n + H_p + H_{np}, \tag{5.1}$$

$$H_n = \sum_{i \in n, m_i} \epsilon_i c^\dagger_{j_i m_i} c_{j_i m_i} - G_n P_n^\dagger P_n - \tfrac{1}{2}\kappa Q_n^2, \tag{5.2}$$

$$H_p = \sum_{i \in p, m_i} \epsilon_i c^\dagger_{j_i m_i} c_{j_i m_i} - G_p P_p^\dagger P_p - \tfrac{1}{2}\kappa Q_p^2, \tag{5.3}$$

$$H_{np} = -\kappa Q_n Q_p, \tag{5.4}$$

where $P_{n(p)}$ and $Q_{n(p)}$ are the pairing and quadrupole operators for neutrons (protons) (see the definitions in Sec. IV). In this model there are two trivial NG modes associated with the change of neutron and of proton number, which can both be removed explicitly in the manner discussed before.

We study this model for a single-shell for neutrons, with pair degeneracy $\Omega_n = 50$, containing 40 particles (see Fig. 5). We take the single-particle quadrupole matrix element $q_n = 1$, and use a pairing strength $G_n = 0.3$, and assume zero single-particle energy. For protons we take two shells, both with $\Omega_{p1} = \Omega_{p2} = 2$, $q_{p1} = q_{p2} = 2$, having single-particle energies $e_{p1} = -e_{p2} = 5$. We study two different sets of interaction parameters, both with $\kappa = 0.1$. The first is $G_n = G_p = 0.3$, the second has the same neutron pairing strength, but $G_p = 10$.

The collective potential energy for the weaker pairing strength shows a very interesting behavior, with two shoulders appearing in the CHB collective potential energy. This is what is normally called the adiabatic potential energy, and the shoulders arise from an avoided crossing. As in our previous work [2] the adiabatic LHA method chooses a diabatic (crossing) set of potential energy curves. These shape-coexistence minima are related to $2p$-$2h$ excitation in the proton model space, promoting two particles from the lowest Nilsson orbitals to the down-sloping ones. This is of course very similar to the phenomena observed in shape coexistence in semimagic nuclei.

We get another surprise for the strong pairing case. Here the collective potentials look very similar, and rather structureless, but the collective coordinates are different. This can be traced back to the fact that the collective coordinate in the

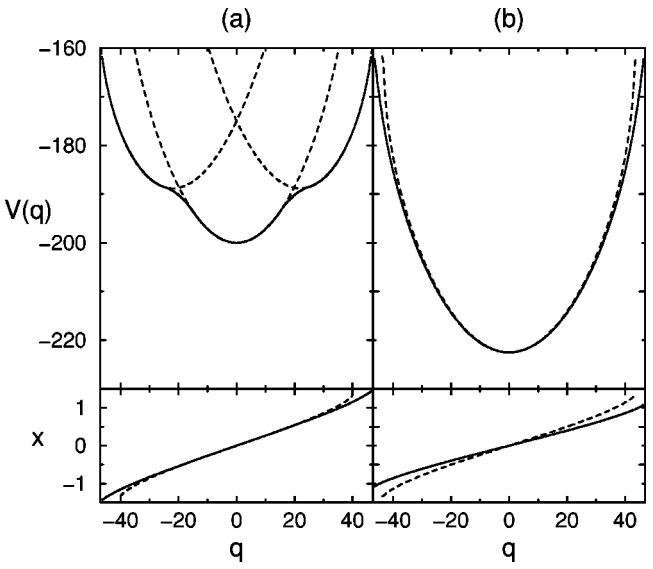

FIG. 5. The collective potential energy $V(q)$ and the collective coordinate x as a function of the quadrupole moment $q = q_p + q_n$. We show both the LHA (dashed lines) and the CHB results (solid line) in each figure. The case (a) corresponds to a weak proton pairing force ($G_p = 0.3$), (b) to a strong pairing force ($G_p = 10$). The rest of the parameters are given in the main text. The units of all quantities displayed are arbitrary.

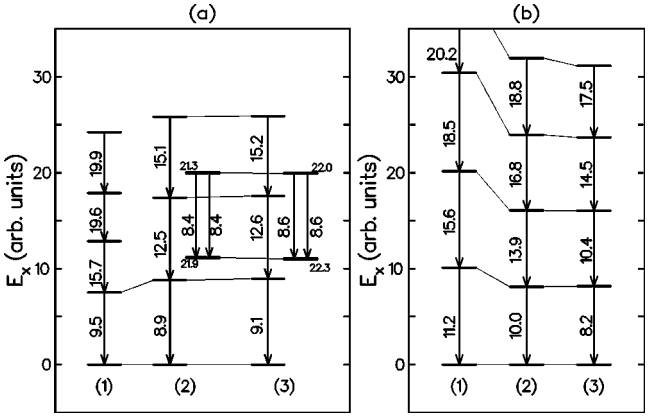

FIG. 6. The excitation energies E_x and transition matrix elements $|\langle n'|Q|n\rangle|$ (numbers next to arrows), in arbitrary units, for the proton-neutron model discussed in the text. The two cases (a) and (b) correspond to those discussed in Fig. 5. In each of the panels the left one (1) is obtained from requantizing the CHB, the middle one (2) is obtained from requantizing the LHA result, and the right one (3) corresponds to the exact diagonalization. Levels denoted by thick lines are doubly degenerate. The numbers next to the arrows denote the size of the transition matrix elements.

LHA is not q_p+q_n, but a different combination. At the minimum, the lowest RPA mode corresponds approximately to $q_n+\frac{1}{10}q_p$. This is similar to the situation analyzed in great detail in Ref. [16], and once again shows the importance of self-consistency in the selection of the collective coordinate. The real collective coordinate is *not* the mass-quadrupole operator.

In Fig. 6 we show the consequences of these results for the requantization. For the weak pairing case the diabatic picture obtained through the LHA gives almost perfect results, whereas the CHB potential energy curve fails to provide the correct answer. In the case of the strong pairing the incorrect choice of the collective coordinate leads to too large a level spacing in the CHB calculations, whereas the LHA and exact calculations agree again.

For the weak pairing case the exact calculation almost exhibits the doublet structure found from the diabatic potential energy curves; the splitting is less than one part in 10^5 in the exact calculation. Nevertheless, the exact calculation consists of symmetric and antisymmetric states, which leads to the transition matrix element 22.3 between these two states. Since in the LHA calculation the states do not mix, we have printed the *diagonal* matrix element instead. For very weak mixing this is the correct comparison, as is borne out by the results.

The decoupling measure D, Eq. (2.13), is small for all these cases. The worst case is the strong pairing case, where it rises from 0 for $q=0$ to 3×10^{-3} for $q=40$. For this reason we also believe that the ''scalar Berry potential'' [2] will be small, and we have not included this, or any other quantum corrections, in our calculations.

VI. CONCLUSION

In the area of shape coexistence, as studied by the model calculations discussed in this paper, it seems that on the whole the LHA is an excellent method to obtain sensible results, with reasonable effort. Even though the size of the space is much smaller than that used in a straightforward diagonalization, the use of the local RPA, which needs to be performed many times at every point along the collective path, may seem prohibitive for realistic calculations. Fortunately, many problems can be studied with simplified separable forces, as in the model discussed here. We are at the moment considering the old pairing-plus-quadrupole model, that has been applied so successfully in the physics of heavy nuclei. Such a model can be dealt with much more straightforwardly than more microscopic Skyrme or Gogny-force based approaches. This will allow us to shed light on a good treatment of shape coexistence, as well as on the interesting question on the choice of the collective (cranking) operator, which was already found to be nontrivial in certain limits of the $O(4)$ model.

One might argue that even that is not enough, and we should really adopt a fully microscopic quantum many-body approach. We believe that we can address this problem, and are actively considering the approaches available to us. As must be obvious from the discussion given above, an efficient calculation hinges on efficient solution of the RPA. We are investigating two approaches to this problem, the use of iterative diagonalization of the RPA using Lanczos procedures, or the approximation of the RPA by using separable forces [17], which can be diagonalized much more efficiently.

In the present work we have not included any quantum corrections, nor the ''scalar Berry potential'' arising from choosing a slow degree of freedom. In our previous work [2] we have shown that these corrections tend to improve the spectrum, so that the results presented can even be improved slightly. We are strongly encouraged by the ability of our method to choose the right coordinate and the correct potential energy curves for problems that involve pairing and ''quadrupole'' degrees of freedom, and we expect results for realistic nuclear models in the near future.

ACKNOWLEDGMENTS

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