Theory of large-amplitude collective motion applied to the structure of ^{28}Si

Niels R. Walet,[1] G. Do Dang,[2] and Abraham Klein[1]
[1] *Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19104*
[2] *Laboratoire de Physique Théorique et Hautes Energies, Université de Paris-Sud, 91405 Orsay, France*
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In recent years we have developed a mathematical treatment of large amplitude collective motion in the adiabatic limit and formulated a set of methods, collectively known as the generalized valley approximation, that were applied to the approximate solution of a series of simplified models. In this paper we report the application of one of our algorithms to the study of the nucleus ^{28}Si, our first successful application to a realistic nuclear physics problem. We determine self-consistently a one-dimensional manifold of triaxial Slater determinants that connects the energy minimum of oblate deformation to the prolate minimum. Upon requantization of the implied collective Hamiltonian in the intrinsic frame, reasonable agreement with a shell-model calculation of the low-lying levels is achieved. Application of a theoretical criterion for assessing the quality of decoupling shows that a one-dimensional path is not sufficiently well decoupled in the model studied, thus suggesting one direction for future improvement. We compare our research with the only comparable previous work, that of Pelet and Letourneux.

I. INTRODUCTION

In this paper we study the possibility of obtaining an approximate solution to the nuclear many-body problem by reducing the number of degrees of freedom to a limited set of collective coordinates ("deformation parameters"). What immediately comes to mind is Bohr's macroscopic approach[1] to nuclear structure through parametrization of the nuclear surface. The idea is to relate this approach to the microscopic description of a many particle system in terms of a mean-field approximation, either Hartree-Fock or, when pairing correlations are important, Hartree-Fock-Bogoliubov. One method to bridge this gap, the theory of large amplitude collective motion, utilizes the time-dependent versions of these theories to derive a classical collective Hamiltonian, involving only a few degrees of freedom, that is subsequently requantized. The procedure consists of moving from one point of the collective surface to the next by solving a set of constrained (or cranked) mean-field equations. In almost all existing literature, where the final goal is a calculation of some properties of realistic nuclei, the choice of the collective coordinates, or what is the same thing, the choice of constraining operators, was based on physical intuition only, with a strong tendency towards choosing the expectation value of simple multipole operators, especially the components of the mass-quadrupole operator $q_m = \langle r^2 Y_m^{(2)} \rangle$. In the well-known work of Kumar and Baranger,[2] where a schematic nuclear Hamiltonian involving the quadrupole-quadrupole interaction was used, the mass quadrupole was the obvious choice of collective coordinate. This choice is not self-evident for more realistic Hamiltonians. In the more fundamental approaches developed during the past two decades, the optimal choice of constraining operators or collective coordinates must be determined by the nuclear Hamiltonian itself, and is not subject to the whims (intuition) of the individual.

Stimulated by the realization that there was an open problem, a large number of different approaches to a self-consistent determination of the collective operators has been developed (see Ref. 3 for a complete set of references). Although none can claim total success, some interesting methods have been proposed. One of the most viable of these[4] has been used for heavy-ion reactions, but suffers from the limitation that no more than one collective coordinate can be treated. We have proposed our own approach to the problem, which has proven to be successful when applied to toy models,[3,5] but the need to test the method for a (semi)realistic nuclear physics problem remained. For this reason we decided to apply our method, the generalized valley approximation (GVA), to the deformed nucleus ^{28}Si. In doing so we encountered some difficulties, which may be due to the fact that a description of collective motion requires a larger model space than just the *sd* shell, but with some slight changes to our approach, as previously applied, these have been overcome. The formulation we are currently using has, compared to all previous work in the literature, the largest overlap with that of Rowe,[6] though the latter has not applied his work to any realistic nuclear physics problems.

It has been known for a long time that the time-dependent mean field theories are equivalent to Hamilton's classical equations of motion. We have emphasized, in particular, the utility of basing an analysis on this framework. We have discussed at length in our previous work our approach to decoupling a few degrees of freedom in a Hamiltonian system and described several versions of our generalized valley approximation (GVA). The ver-

sion that is most useful for nuclear physics problems can be implemented as a combination of a constrained (or cranked) Hartree-Fock equation, that determines a local single-particle coordinate system at each point of the collective manifold, and an RPA-like equation that gives the matrix elements in this basis of the self-consistent cranking operator(s). It is this latter element that was absent from earlier microscopic approaches. From the solution to this set of equations for a single collective coordinate we obtain a collective potential energy, a collective mass, as well as the moments of inertia. [Because of the appearance of an RPA-like equation, which can be obtained through a quadratic expansion of the Hamiltonian, previous versions of this method are usually referred to as the local harmonic approximation.]

In this paper we contrast our theory with one of the few other successful and general methods to calculate nuclear structure from the theory of large amplitude collective motion, the Holzwarth-Yukawa (HY) method.[7] This method seemingly takes a totally different approach: One writes the wave function as a generator coordinate superposition

$$|\phi\rangle = \int_P d\alpha\, f(\alpha)|\alpha\rangle, \tag{1}$$

where α labels a member of the set of Slater determinants. The expectation value of the Hamiltonian is now optimized both with respect to the path P and with respect to the coefficients $f(\alpha)$. The calculation of the path is found to be independent of the function $f(\alpha)$, so that we can first determine the path and then solve the Hill-Wheeler equation for fixed P. A major difference between our theory and that of HY now appears, since Holzwarth and Yukawa only consider real generator coordinates, and thus time-even Slater determinants. It is well-known that such an approach is inadequate to describe mass parameters, since it fails to reproduce the correct classical limits. To generate a spectrum in the HY method one calculates the eigenstates within this approximation by deriving an angular-momentum projected Hill-Wheeler equation for the functions $f_J(\alpha)$ that appear in (1) when we project the generating functions, i.e.,

$$|JM\rangle = \int_P f_J(\alpha) P_{JM}|\alpha\rangle \tag{2}$$

is assumed to be an approximate solution of the Schrödinger equation.

Later on we shall show that our theory leads to a local RPA equation, whereas the HY formalism, in its present formulation, leads to a local set of TDA equations. It should be possible to include complex generator coordinates in the HY method, especially if we take the complex parts to be infinitesimal, corresponding to the adiabatic limit. We expect to find an equivalent derivation of our results in that case, but we shall not pursue such an approach here. The interested reader may benefit from the discussion by Reinhard and Goeke,[8] where the inclusion of small complex pieces is discussed in some detail. The HY theory has only been applied to ^{28}Si,[9] and this is one of the reasons that we have chosen this nucleus for detailed study.

In Sec. II, we give a brief account of the theoretical background needed for this paper. Sec. II A contains a review of the those parts of the theory developed previously that are utilized in the current work, in particular, the local harmonic approximation. In Sec. II B we discuss the symmetries we impose on the Slater determinant. These lead to a reduction in the number of degrees of freedom and thus make the system easier to treat. Finally we discuss the calculation of the moments of inertia in Sec. II C. We then turn to the actual algorithm used in our calculations in Sec. III. We also discuss the calculation of some other quantities of interest. The results are given in Sec. IV, and finally we give some conclusions and an outlook in Sec. V.

II. FORMALISM

A. Recapitulation of old results

Since we have taken considerable pains to describe our ideas fully in a forthcoming paper on decoupling in classical mechanics,[10] and in our previous papers on applications to nuclear physics,[3,5] it would be inappropriate to include here more than the barest details necessary to introduce the appropriate ideas and equations. The reader should note, however, that the formalism is slightly different from that presented in Refs. 3 and 5.

It has been amply documented that the TDHF equations,

$$\begin{aligned} \dot{\rho}_{ph} &= \delta W[\rho]/\delta\rho_{ph}, \\ W[\rho] &= \rho_{ab}\epsilon_{ba} + \tfrac{1}{2}V_{abcd}\rho_{ca}\rho_{db}, \end{aligned} \tag{3}$$

are a disguised form of Hamilton's equations of motion. Here we work in a "local basis," i.e., at each point on the manifold of Slater determinants we introduce a set of single particle labels, h for the orbits occupied in that specific Slater determinant, and p for the unoccupied orbits. The number of degrees of freedom of the classical dynamical system is equal to the number of independent p-h pairs used to label the local coordinates. This is especially clear if we introduce canonical coordinates ξ and momenta π through the "classical Holstein-Primakoff mapping", i.e., when we define

$$\beta_{ph} = \frac{1}{\sqrt{2}}(\xi_{ph} + i\pi_{ph}), \quad \beta^\dagger_{hp} = \frac{1}{\sqrt{2}}(\xi_{ph} - i\pi_{ph}), \tag{4}$$

and

$$\begin{aligned} \rho_{ph} &= (\beta(1-\beta^\dagger\beta)^{1/2})_{ph}, \\ \rho_{hp} &= ((1-\beta^\dagger\beta)^{1/2}\beta^\dagger)_{hp}, \\ \rho_{hh'} &= \delta_{hh'} - (\beta^\dagger\beta)_{hh'}, \\ \rho_{pp'} &= (\beta\beta^\dagger)_{pp'}. \end{aligned} \tag{5}$$

According to (3), the Hartree-Fock energy functional W plays the role of a Hamiltonian. In general this is not a quadratic form in the momenta and this leads to some ambiguity if we wish to truncate up to quadratic order. The problem arises because, as we have emphasized before, the only way to guarantee that the truncation to quadratic order is independent of the choice of canonical coordinates is to include the leading order momentum-dependent corrections in the adiabatic limit of the canonical transformations. This shows that it is not strictly correct to restrict attention to point canonical transformations, even though this approach is taken in almost all the papers on the adiabatic limit. In a previous paper[5] we have shown that for a specific model of a monopole excitation this has important consequences. However, the physics of that model, where the energy of a giant resonance is pushed up from its single-particle value, is not strictly in accord with the definition of adiabaticity. It may well be that for the cases where the appropriate criteria are satisfied, as in the application to the low-lying spectra of deformed nuclei, it will suffice to consider only point transformations. In any event that is the choice made in this paper. Our justification is as follows: In the paper on the monopole, we found that the effects of curvature of the manifold in coordinate space, which can be included within the framework of point transformations, were of the same size as the effects of the leading momentum dependent terms that are omitted in the present paper. Since the curvature terms in the present calculation will be shown to have a small effect on the results, we feel that the same is probably true for the momentum-dependent effects. However, a test of this assertion will have to await future generalizations of the algorithm developed in this paper.

The algorithm described in the previous application[5] hinged on the fact that we could specify a decoupled path by expanding the self-consistent cranking operator in a limited number of basis operators. This may be a good approach to nuclear collective motion described in large model spaces, since it extends the usual cranking approach, but we found from a detailed investigation that it fails for the case of ^{28}Si treated in the very limited *sd* model space. For that reason we decided to return to the fundamental equations of our theory and try to derive a sensible approximation from them, without using a basis of operators. In such an approach it is more difficult to deal with the ambiguity in the definition of the kinetic energy, and it is at least temporarily fortunate that we have good reason to believe such corrections to be small for the current system.

The starting point is the adiabatic Hamiltonian

$$H = \tfrac{1}{2}\pi_{ph} B^{php'h'} \pi_{p'h'} + V(\xi), \tag{6}$$

where

$$B^{php'h'} = \frac{\partial^2 W}{\partial \pi_{ph} \pi_{p'h'}}, \tag{7}$$

and the potential energy V is the value of W for a time-even density matrix, i.e., for zero momentum.

As discussed at length in our previous work we now look for a point transformation[11] to new coordinates q and momenta p,

$$q^\mu = f^\mu(\xi), \quad p_\mu = g^\alpha_{,\mu} \pi_\alpha, \tag{8}$$

such that our new coordinates show decoupling. The coordinates are specified by two sets of functions, f^μ that describe the new coordinates with respect to the old, and g^α that give the inverse transformations, so that we have the chain-rule relations

$$f^\mu_{,\alpha} g^\alpha_{,\nu} = \delta^\mu_\nu, \quad f^\mu_{,\alpha} g^\beta_{,\mu} = \delta^\beta_\alpha. \tag{9}$$

Here we use a comma to indicate a derivative, and the indices $\alpha, \ldots$ are reserved for the old coordinates, whereas we use μ, etc., for the new ones. We also use the summation convention. In a nuclear physics context we shall always replace α by the pair of indices ph, since, as can be see from Eq. (3), these are the natural labels of the dynamical degrees of freedom.

After the transformations discribed above we end up with the collective Hamiltonian

$$\bar{H} = \tfrac{1}{2} p_\mu \bar{B}^{\mu\nu} p_\nu + \bar{V}(q), \tag{10}$$

where the collective potential is obtained by substituting $\xi^\alpha = g^\alpha(q)$ in V, and the collective mass is calculated from the equation

$$\bar{B}^{\mu\nu} = f^\mu_{,\alpha} B^{\alpha\beta} f^\nu_{,\beta}. \tag{11}$$

The local harmonic form of the generalized valley theory consists of two equations. The first expresses the requirement that the force should lie along the collective path. For the case of a single collective coordinate we find the following condition, using the chain-rule relation for the gradient of the potential energy,

$$V_{,\alpha} = (d\bar{V}/dq)(dq/d\xi^\alpha). \tag{12}$$

If we replace the derivative of the collective potential energy by λ and use the fact that $dq/d\xi^\alpha = f^1_{,ph}$ as well as the fact that the derivative of W is just the Hartree-Fock matrix, we find that this equation turns into the familiar, constrained Hartree-Fock or cranking equation

$$\mathcal{H}_{ph} = \lambda f_{ph}. \tag{13}$$

[Note the difference between f_{ph} and $f_{,ph}$. In the first case we mean the matrix element of an effective single-particle operator, in the other case the derivative of the collective coordinate with respect to ξ_{ph}. If the derivative of q with respect to π is zero, the difference between the two is a factor $\sqrt{2}$,

$$f_{ph} = \frac{\delta q}{\delta \rho_{ph}} = (\partial q/\partial \xi_{ph})/\sqrt{2} = f_{,ph}/\sqrt{2}.] \tag{14}$$

The second equation of the method expresses the requirement that geometrical forces should also be along the path for decoupling to occur. This turns out to be

equivalent to the requirement that the cranking matrix elements be the solution of an RPA-like equation

$$M^{p'h'}_{ph} f^{\mu}_{,p'h'} = \Omega^2_{\mu} f^{\mu}_{,ph}, \tag{15}$$

with

$$M^{p'h'}_{ph} = V_{;php''h''} B^{p''h''p'h'} \tag{16}$$

and

$$V_{;php''h''} = V_{php''h''} - V_{,p'h'} \Gamma^{p'h'}_{php''h''}. \tag{17}$$

The affine connection is totally determined by the mass B, which for this system is the Riemannian metric,

$$\begin{aligned}\Gamma^{\gamma}_{\alpha\beta} &= \tfrac{1}{2} B^{\gamma\delta} (B_{\delta\alpha,\beta} + B_{\delta\beta,\alpha} - B_{\alpha\beta,\delta}) \\ &= \tfrac{1}{2} \left(-B^{\gamma\delta}_{,\beta} B_{\delta\alpha} - B^{\gamma\delta}_{,\alpha} B_{\delta\beta} \right. \\ &\quad \left. + B^{\alpha'\beta'}_{,\gamma'} B_{\alpha\alpha'} B_{\beta\beta'} B^{\gamma\gamma'} \right),\end{aligned} \tag{18}$$

and we have used the relation

$$B^{\alpha\beta}_{,\gamma} B_{\beta\delta} = -B^{\alpha\beta} B_{\beta\delta,\gamma}$$

to obtain the second line. The calculation of the covariant derivative requires the inverse of the mass, which may be a very expensive computation in a large model space. In the present case such a computation is almost trivial.

The cranking and local-harmonic equations have to be solved self-consistently: The cranking equation (13) determines, for given f, a set of single-particle wave functions p for empty orbits and h for filled orbits. The local harmonic equation determines f, but depends on the indices p and h. If we neglect the affine connection we obtain a set of equations that is very close to the set derived in the Holzwarth-Yukawa formalism by Pelet and Letourneux,[9] the only difference being that we use RPA where they use TDA. This is due to the use of real generator coordinates in the calculation of Pelet, whereas our parametrization is based on the dynamics, and thus is very similar to, and may be totally equivalent to, using complex generator coordinates. For static properties, such as the calculated collective path, the difference should not be very important. It has a dramatic impact on the dynamical quantities such as the Hamiltonian along the path. Inclusion of the curvature through use of covariant derivatives also has effects on the calculation, as we shall show.

The RPA equation (15) is a linear eigenvalue problem and thus does not fix the scale of the eigenvectors. We propose to make the very convenient choice of normalization

$$f^{\mu}_{,\alpha} B^{\alpha\beta} f^{\nu}_{,\beta} = \delta^{\mu\nu}. \tag{19}$$

For this special choice the inverse $B_{\alpha\beta}$ also takes a very simple form,

$$B_{\alpha\beta} = f^{\mu}_{,\alpha} \delta_{\mu\nu} f^{\nu}_{,\beta}. \tag{20}$$

Since the quantity f_{ph} is symmetric, $f_{ph} = f_{hp}$, and is equal to the derivative $\delta q / \delta \rho_{ph}$, we find that

$$q = \int f_{,ph} d\xi_{ph} = 2 \int f_{ph} \delta\rho_{ph} = \int \mathrm{Tr}(f \delta\rho) \tag{21}$$

for real $\delta\rho$. One may verify the correctness of this equation for a density-independent one-body operator f, where we obtain the familiar relation

$$\begin{aligned} q - q_0 &= \int_{\rho_0}^{\rho} \mathrm{Tr}\,(f \delta\rho) = \mathrm{Tr}(f \int_{\rho_0}^{\rho} \delta\rho) \\ &= \mathrm{Tr}(f\rho) - \mathrm{Tr}(f\rho_0). \end{aligned} \tag{22}$$

The relation (21) will allow us to evaluate the collective coordinate along the path, and thus plays a very important role in the following discussion.

Finally, we would like to be able to measure the quality of decoupling along the path. This can be obtained by comparing two different forms of the collective mass that can be calculated in the theory; one is the definition the reciprocal collective mass as a contravariant tensor in Eq. (11),

$$\bar{B}^{ij} = f^{i}_{,\alpha} B^{\alpha\beta} f^{j}_{,\beta}, \tag{23}$$

and the other can be calculated from a formula for the collective mass itself in terms of the tangents to the path,

$$\breve{B}_{ij} = \frac{\partial \xi^{\alpha}}{\partial q^i} B_{\alpha\beta} \frac{\partial \xi^{\beta}}{\partial q^j}. \tag{24}$$

If we have exact decoupling the second matrix will be the inverse of the first. We use the deviation from this relation as a measure for the quality of decoupling (K is the number of collective coordinates):

$$D = \sum_{ij} \bar{B}^{ij} \breve{B}_{ji} / K - 1. \tag{25}$$

B. Symmetries

In this section we shall discuss two symmetries we impose on the Slater determinants, as well as their consequences.

Taking advantage of the fact that isospin is a good symmetry for light nuclei, we require that proton and neutron orbits be occupied with equal probability. This corresponds to considering only the manifold of $T = 0$ states, which constitute the low-energy part of the spectrum of ^{28}Si. This symmetry reduces the number of active particles we have to consider by a factor of two, so that the effective number of single-particle degrees of freedom is reduced from 12 to 6. As discussed in Appendix A one can easily write a new energy functional in terms of a density matrix with trace equal to six.

Furthermore, following Pelet[9] we impose "ellipsoidal" symmetry, i.e., we require the intrinsic nuclear shape to be invariant under a rotation of 180° about any of the three symmetry axes. It is well known (see, e.g., Ref. 12) that such a symmetry requires that K, the projection of the angular momentum on the intrinsic z axis is even and also relates wave function components with positive K to those with negative K. In the latter regard, it du-

plicates the function of time reversal invariance, which for static solutions of the Hartree-Fock problem for even nuclei already implies that any pair of time-reversed orbits is either occupied or unoccupied. The requirement of ellipsoidal symmetry is indeed a strong limitation in the implementation of our algorithm, since any reasonable interaction (Kuo, Wildenthal, etc.) gives that for ^{28}Si the lowest-energy RPA mode at the Hartree-Fock minimum is a $\Delta K = 3$ state. We thus reject this solution as a possible choice of cranking operator, and choose the lowest even-ΔK solution for this purpose.

The reduction to ellipsoidally symmetric Slater determinants leads to an extra reduction by a factor of two in the number of single-particle degrees of freedom, so that we finally end up with three active "particles." Taking into account a suitably averaged potential $\bar{V}$, we can rewrite W in terms of a density matrix within the restricted space only (so that $\mathrm{Tr}\rho = 3$). The Hartree-Fock Hamiltonian becomes

$$\mathcal{H}_{\alpha\beta} = 4\delta_{\alpha\beta}\epsilon_a + \sum_{\gamma\delta} \bar{V}_{\beta\delta\alpha\gamma}\rho_{\gamma\delta}. \tag{26}$$

We can evaluate the mass and the second derivative of the potential using methods given in Ref. 3, and find (the roman letters p,h are used to denote all the quantum numbers of the particle-hole orbits except the isospin projection)

$$B^{php'h'} = \mathcal{H}_{pp'}\delta_{hh'} - \mathcal{H}_{hh'}\delta_{pp'} + \bar{V}_{hp'ph'} - \bar{V}_{pp'hh'}, \tag{27}$$

$$V_{,php'h'} = \mathcal{H}_{pp'}\delta_{hh'} - \mathcal{H}_{hh'}\delta_{pp'} + \bar{V}_{hp'ph'} + \bar{V}_{pp'hh'}. \tag{28}$$

The derivative of B needed for the calculation of the RPA matrix is evaluated in Appendix B. At the Hartree-Fock minimum the resulting local harmonic equation is indeed the standard RPA equation, e.g., Eq. (8.83) in Ref. 13, as can be seen from Eq. (8.71) in the same reference.

Instead of rewriting the energy density in terms of the reduced density matrix that takes into account all symmetries, let us also consider the general RPA (taking into account the proton-neutron symmetry, though) at a point of ellipsoidal symmetry. Consider, for example, the kinetic energy matrix B, that can be obtained as the second derivative of the energy functional. We separate the basis into two disjoint sets that are mutually conjugate under time reversal, and restrict the indices p and h to label only states in one of these sets, so that the time reversed states $\bar{p}$ and $\bar{h}$ are members of the other set. (In case of a summation we shall later write $\sum'$ to indicate this limitation.) We now can order the states in such a way that B takes the form

$$B^{\alpha\beta} = \begin{pmatrix} B^{php'h'} & B^{ph\bar{p}'\bar{h}'} & B^{ph\bar{p}'h'} & B^{php'\bar{h}'} \\ B^{\bar{p}\bar{h}p'h'} & B^{\bar{p}\bar{h}\bar{p}'\bar{h}'} & B^{\bar{p}\bar{h}\bar{p}'h'} & B^{\bar{p}\bar{h}p'\bar{h}'} \\ B^{\bar{p}hp'h'} & B^{\bar{p}h\bar{p}'\bar{h}'} & B^{\bar{p}h\bar{p}'h'} & B^{\bar{p}hp'\bar{h}'} \\ B^{p\bar{h}p'h'} & B^{p\bar{h}\bar{p}'\bar{h}'} & B^{p\bar{h}\bar{p}'h'} & B^{p\bar{h}p'\bar{h}'} \end{pmatrix}. \tag{29}$$

From the explicit expression for B, Eq. (28), we can easily derive that all the entries in this matrix with an odd number of barred indices are zero, as a consequence of time reversal invariance of the underlying shell-model Hamiltonian. A further consequence of this symmetry is that all entries of B are invariant under the interchange of unbarred with barred indices. If we now introduce the orthogonal transformation

$$O = \frac{1}{\sqrt{2}} \begin{pmatrix} I & -I & 0 & 0 \\ I & I & 0 & 0 \\ 0 & 0 & I & -I \\ 0 & 0 & I & I \end{pmatrix}, \tag{30}$$

we obtain the following block-diagonal form for the transform of B

$$O^T B O = \begin{pmatrix} B^{php'h'} + B^{\bar{p}\bar{h}p'h'} & 0 & 0 & 0 \\ 0 & B^{php'h'} - B^{\bar{p}\bar{h}p'h'} & 0 & 0 \\ 0 & 0 & B^{\bar{p}h\bar{p}'h'} + B^{\bar{p}hp'\bar{h}'} & 0 \\ 0 & 0 & 0 & B^{\bar{p}h\bar{p}'h'} - B^{\bar{p}hp'\bar{h}'} \end{pmatrix}. \tag{31}$$

The second derivative of the potential energy takes the same form. We thus have split the total RPA problem into four disjoint subproblems. From the structure of the matrix O we can infer that the basis vectors that span the upper left block have equal ph and $\bar{p}\bar{h}$ matrix elements (and zero matrix elements between a state and a time reversed one). The eigenvectors of this part of the RPA matrix can serve as cranking operators, since they conserve the ellipsoidal symmetry. The next block to the lower right still has entries in the same space, but the ph entries are minus the $\bar{p}\bar{h}$ entries. The basis vectors for the next two blocks only have entries $\bar{p}h$ and $p\bar{h}$, the first with equal sign, and the last (on the lower right) with opposite sign. As will be discussed in the next subsection the lower three blocks will be very important when calculating the moments of inertia.

C. The inertia tensor

If we study a real nucleus, we know that there exist two (for an axially deformed nucleus) or three (the general triaxial case) cyclic coordinates, which can be identified as the angles conjugate to the angular momenta. On the classical level the momenta are

$$J_i = \mathrm{Tr}(\rho^{\tau_z}\hat{J}_i^{\tau_z}) = 2\mathrm{Tr}(\rho\hat{J}_i). \tag{32}$$

Here we have taken the proton-neutron degeneracy into

account in the last term. We shall not yet use ellipsoidal symmetry. At an axial minimum we can easily find these momenta, since they correspond to zero eigenvalues of the RPA matrix. In the covariant RPA they no longer correspond to zero modes at all points on the collective path, but we shall still assume it is correct to expand the energy to second order in the components of the angular momenta to obtain the inertia tensor. First let us analyze what form the momenta take in the local (ph) basis. From the matrix elements (C^i_α gives the decomposition of the state i in shell model states α)

$$\begin{aligned}\langle p|\hat{J}_m|h\rangle &= C^p_\alpha C^h_\beta \langle (nljm)_a|\hat{J}_m|(nljm)_b\rangle \\ &= \delta_{j_a j_b}\sqrt{j_a(j_a+1)}C^{\ j_a\ 1\ j_b}_{m_a\ m\ m_b} C^p_\alpha C^h_\beta \end{aligned} \tag{33}$$

and the symmetry properties of the Clebsch-Gordan coefficients we find

$$\langle p|\hat{J}_m|h\rangle = \langle h|\hat{J}_{-m}|p\rangle(-1)^m. \tag{34}$$

If we now use

$$\begin{aligned}\hat{J}_x &= (\hat{J}_{-1} - \hat{J}_{+1})/\sqrt{2}, \\ \hat{J}_y &= i(\hat{J}_{+1} + \hat{J}_{-1})/\sqrt{2},\end{aligned} \tag{35}$$

we find $\langle p|\hat{J}_x|h\rangle = \langle h|\hat{J}_x|p\rangle$ is real and $\langle p|\hat{J}_y|h\rangle = -\langle h|\hat{J}_y|p\rangle$ is purely imaginary. To first order in the coordinates and momenta we now have

$$\begin{aligned}J_x &= 2\sqrt{2}\sum_{ph}\xi_{ph}\langle p|\hat{J}_x|h\rangle, \\ J_y &= -2\sqrt{2}\sum_{ph}\pi_{ph} i\langle p|\hat{J}_y|h\rangle, \\ J_z &= 2\sqrt{2}\sum_{ph}\xi_{ph}\langle p|\hat{J}_z|h\rangle.\end{aligned} \tag{36}$$

It is not very hard to show that J_z has zero matrix elements between a state and a time reversed one, whereas $\langle p|\hat{J}_z|h\rangle = -\langle\bar{p}|\hat{J}_z|\bar{h}\rangle$. Similarly J_x and J_y correspond to the last two symmetry classes discussed in the previous subsection.

To calculate the inverse moments of inertia, which corresponds to the calculation of the inverse mass for the kinetic energy, we now have to evaluate $\partial^2 W/\partial J_i \partial J_j$. This quantity can be reexpressed by the chain rule in terms of $B^{php'h'}$ and $V_{,php'h'}$, e.g.,

$$\mathcal{I}_y^{-1} = \frac{\partial\pi_\alpha}{\partial J_y} B^{\alpha\beta}\frac{\partial\pi_\beta}{\partial J_y}. \tag{37}$$

Using the canonicity conditions[11] for J_i and the conjugate angles θ_i, we find that the quantities $\partial\pi_\beta/\partial J_y$ and $\partial\xi_\beta/\partial J_i$, $i = x, z$, can be replaced by $\partial\theta_y/\partial\xi^\alpha$ and $-\partial\theta_i/\partial\pi_\alpha$, respectively. Since we do not have explicit expressions for the matrix elements of the angles, it does not appear feasible to use the resulting expressions, but there exists an alternative. Consider the moments of inertia themselves, instead of their inverses. In analogy with Eq. (24) we can calculate, for $\mathcal{I}_y$,

$$\mathcal{I}_y = \frac{\partial J_y}{\partial\pi_{ph}} B_{php'h'}\frac{\partial J_y}{\partial\pi_{p'h'}}, \tag{38}$$

where we have once more used the canonicity conditions to equate

$$\frac{\partial\xi^\alpha}{\partial\theta_y} = \frac{\partial J_y}{\partial\pi_\alpha}. \tag{39}$$

This term can be obtained through expansion of the energy in terms of $\dot{\theta}_y$. If we apply a similar analysis to the other two moments of inertia we find that they can be evaluated by a similar expression involving the second derivative of the potential energy with respect to coordinates,

$$\mathcal{I}_j = \frac{\partial J_j}{\partial\xi^{ph}} V^{,php'h'}\frac{\partial J_j}{\partial\xi^{p'h'}}. \tag{40}$$

Even though these equations may look unfamiliar, at the Hartree-Fock minimum they correspond to the usual RPA equations for the moments of inertia, see, e.g., Eq. (8.113) in Ref. 13.

It may not appear obvious to the reader that the inertia tensor is diagonal. As noted before, however, each of the vectors of particle-hole matrix elements of the components of J belongs to a different symmetry class discussed in Sec. II B. Since both the mass and potential energy matrix are block-diagonal, we thus can not have off-diagonal matrix elements in the inertia tensor. This is a consequence of ellipsoidal symmetry, and will no longer hold if we would allow, say, octupole components in the cranking operator.

Note that we have not used the covariant derivative of V in (40) for the sake of a consistent treatment of the different moments of inertia. In the general nonadiabatic theory we would expect complete symmetry between the two expressions, which can only be reached for the present case by disregarding the covariant derivative.

Using the explicit expressions for the derivatives of the different J's as can be obtained from Eq. (36) we find that, using the symmetries to restrict the summations over half the single particle states (as indicated by a prime),

$$\begin{aligned}\mathcal{I}_z &= {\sum_{php'h'}}' (2\sqrt{2}\langle p|\hat{J}_z|h\rangle)\sqrt{2}\,(V_{,php'h'} - V_{,\bar{p}\bar{h}p'h'}) \\ &\quad \times\sqrt{2}(\langle p'|\hat{J}_z|h'\rangle 2\sqrt{2}) \\ &= {\sum_{php'h'}}' 16\langle p|\hat{J}_z|h\rangle (V_{,php'h'} - V_{,\bar{p}\bar{h}p'h'})\langle p'|\hat{J}_z|h'\rangle,\end{aligned} \tag{41}$$

$$\mathcal{I}_y = {\sum_{php'h'}}' 16\langle p|i\hat{J}_y|\bar{h}\rangle (B^{p\bar{h}p'\bar{h}'} - B^{\bar{p}hp'\bar{h}'})\langle p'|i\hat{J}_y|\bar{h}'\rangle, \tag{42}$$

$$\mathcal{I}_x = {\sum_{php'h'}}' 16\langle p|\hat{J}_x|\bar{h}\rangle\left(V_{,p\bar{h}p'\bar{h}'} + V_{,\bar{p}hp'\bar{h}'}\right)\langle p'|\hat{J}_x|\bar{h}'\rangle. \tag{43}$$

III. ALGORITHM

The algorithmic solution of Eqs. (13) and (15) are obtained as follows: First we solve the Hartree equation at the HF minimum, where λ is zero. We then solve the RPA equation to obtain f_{ph}. We use this f to solve the cranking equation at a nearby point, which gives a slightly different ph basis, so that we have to solve the RPA again, etc., until convergence. We can then move on the next point.

When we take a step from one point to another, we would like to know how the collective coordinate changes. Using Eq. (21) we find that for small real $\Delta\rho_{ph}$ the change in the collective coordinate is given by (we have not taken into account the proton-neutron degeneracy or the ellipsoidal symmetry in this expression)

$$\begin{aligned}\Delta Q &= 2\int_{\rho_0}^{\rho_1} \mathrm{Tr}(f\delta\rho)\\ &\approx \sum_{ph} f_{ph}(\rho_0)\Delta\rho^0_{ph} + \sum_{ph} f_{ph}(\rho_1)\Delta\rho^1_{ph},\end{aligned} \tag{44}$$

where we have $\Delta\rho = \rho^1 - \rho^0$, and the superscript 0 or 1 on $\Delta\rho$ indicates that we use the particle-hole basis corresponding to the density matrix ρ^0 or ρ^1, respectively. Note that any higher order approximation to ΔQ also involves higher derivatives of the cranking operator. There may be ways to calculate this quantity approximately, but we are not going to do so here. As explained in our previous work we now sum all the small values ΔQ along the collective path to obtain the collective operator.

For the solution of the cranking problem it is useful to recognize that (13) is the expression of a constrained minimization problem. In fact it is equivalent to the variational condition

$$\frac{\delta}{\delta\rho_{ph}}(W - \lambda(Q - q_0)) = 0. \tag{45}$$

We use this, together with (44), to solve the cranking problem. As a first step we take $\rho \to \rho + \Delta\rho$ and take $\Delta\rho_{ph} = \epsilon f_{ph}$, where ϵ is a suitably chosen small number. If we assume that f_{ph} does not change from this point to the next we find that $Q \to Q + 2\epsilon\sum_{ph} f^2_{ph}$, so that we have to change q_0 to $q_0 + 2\epsilon\sum_{ph} f^2_{ph}$ to satisfy the constraint. This new value of ρ does not usually provide a minimum of the constrained energy, so that we now must search further for its lowest value with this new constraint, i.e., without further changes to Q. As usual, the energy changes most strongly if we take a step in the direction of steepest descent, but such a step also changes Q. In order to remain on the constraint surface, we have to introduce a projected steepest descent method,[13] i.e., we need to project out the part of $\Delta\rho$ that changes Q,

$$\Delta\rho_{ph} \propto \mathcal{H}_{ph} - f_{ph}\sum_{p'h'}(H_{p'h'}f_{p'h'})/\sum_{p'h'}(f_{p'h'}f_{p'h'}), \tag{46}$$

so that $\Delta Q \approx \sum_{ph}\Delta\rho_{ph}f_{ph} = 0$. At a constrained minimum the projected gradient is zero,

$$\mathcal{H}_{ph} = f_{ph}\sum_{p'h'}(H_{p'h'}f_{p'h'})/\sum_{p'h'}(f_{p'h'}f_{p'h'}), \tag{47}$$

If we compare this equation with the cranking equation (13) we can immediately identify the Lagrange multiplier,

$$\lambda = \sum_{ph}(H_{ph}f_{ph})/\sum_{ph}(f_{ph}f_{ph}). \tag{48}$$

The algorithm can now be stated in more detail:

(1) Find an extremal point of the Hartree-Fock equations, where $\lambda = 0$.

(2) Solve the RPA at this point and calculate f_{ph}. There is no self-consistency requirement for $\lambda = 0$.

(3) Move to the next point, using the constraint minimization procedure described above. Use the value of f_{ph} calculated in the previous step.

(4) Solve the RPA and find f_{ph}. If this is very close to the previous value of f_{ph}, go to step 3, else continue.

(5) Solve the constraint problem again, now without changing the constraint. Use the new ph basis as input to step 4.

It is furthermore important to calculate the decoupling measure D. Due to the choice of normalization we find that $\bar{B}^{11} = 1$. So we only need to calculate

$$\breve{B}_{11} = \frac{d\xi^\alpha}{dq}B_{\alpha\beta}\frac{d\xi^\beta}{dq}. \tag{49}$$

From our normalization conditions it follows that

$$B_{\alpha\beta} = \sum_\mu f^\mu_{,\alpha}f^\mu_{,\beta}. \tag{50}$$

If we furthermore approximate the derivatives in (49) by finite differences,

$$\frac{d\xi^\alpha}{dq} \approx \sqrt{2}\frac{\Delta\rho^\alpha}{\Delta Q}, \tag{51}$$

we find

$$\begin{aligned}D &= \breve{B}_{11} - 1\\ &= \sum_\mu(\Delta q^\mu/\Delta Q)^2 - 1.\end{aligned} \tag{52}$$

Here we have defined [note that we can also, with slightly more accuracy, generalize Eq. (44)]

$$\Delta q^\mu = \sqrt{2}\sum_{ph}\Delta\rho_{ph}f^\mu_{,ph}. \tag{53}$$

Thus if $\Delta q^1 \equiv \Delta Q$ is the only nonzero number in the sequence $D = 0$. If any of the other coordinates is comparable to Δq^1 we do not have good decoupling.

IV. RESULTS

We have applied the algorithm discussed in the previous section to a description of ^{28}Si in the *sd* shell, using Kuo's interaction,[14] with single-particle energies as given in Table I. This interaction is not the best shell-model interaction available (it is known that Wildenthal's W interaction[15,16] gives a much better description of the *sd*-shell nuclei), but this interaction is as close as possible to the unpublished interaction used by Pelet and Letourneux. Note that we use ellipsoidal symmetry, which is a limitation for the present case, where the lowest RPA mode at the HF minimum is a $|\Delta K| = 3$ mode, so that it may not be totally correct to consider only even multipoles.

The model exhibits a deep deformed minimum on the oblate side built from a Slater determinant in which orbits with $m = \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, -\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}$ are occupied. There is no stable prolate solution with the same orbits occupied. Further study reveals, however, that there is another minimum with positive quadrupole moment when the orbits $m = \frac{3}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{3}{2}, -\frac{1}{2}, -\frac{1}{2}$ are occupied. Since all axially deformed states within this manifold are orthogonal to all states considered previously, we find that there is no path through the subspace of axially deformed Slater determinants from one state to the other. The lowest mode of the RPA is not an axial ($K = 0$) mode, however, but a $K = 2$ mode. It therefore seems plausible that there exist a path going through triaxial shapes from one to the other. Actually this point has already been studied by Pelet and Letourneux, and such a path has been found.

We have applied our algorithm to the same calculation and found the corresponding path. Since each point of the collective path corresponds to a Slater determinant, or equivalently a set of occupied orbits, it is hard to visualize this path. We need projections of the manifold of Slater determinants on some two-dimensional surface in order to represent the path graphically. Guided by Pelet and Letourneux we give the values of the hexadecapole moment $\langle\sqrt{4\pi/9}\, r^4 Y_0^4\rangle$ as a function of the quadrupole moment $\langle\sqrt{4\pi/5}\, r^2 Y_0^2\rangle$ along the path in Fig. 1. The prolate minimum does not have positive quadrupole moment since the symmetry axis of the prolate solution is the x and not the z axis. The oblate minimum is located at the upper left corner and the prolate one at the lower right. The solid line has been calculated using the covariant derivatives, the dashed line using ordinary derivatives, and the dotted line corresponds to a calculation using TDA (the HY method). Clearly there is a smooth and continuous change of the two parameters along the path. The lower right of this plot, however, is not as smooth as it seems. For that reason we give an enlargement in the inset. The region of this large curvature will be shown below to correspond to a region of bad decoupling, a behavior that has also been noted for simple models.

TABLE I. The single particle energies used in the calculation.

Shell	Single particle energies (MeV)
$1d\frac{5}{2}$	−3.9478
$2s\frac{1}{2}$	−3.1635
$1d\frac{3}{2}$	1.6466

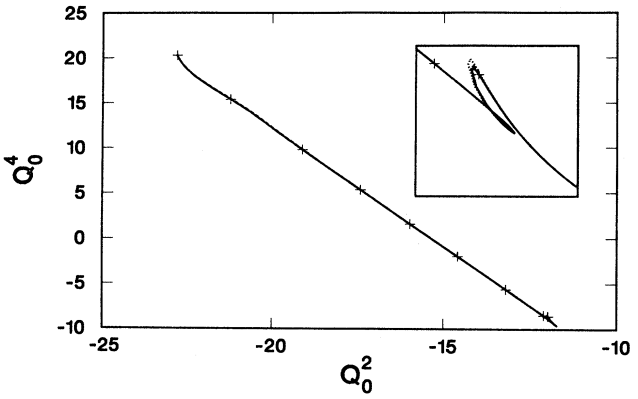

FIG. 1. The value of the hexadecapole moment $\langle r^4 Y_0^4\rangle$ as a function of the quadrupole moment $\langle r^2 Y_0^2\rangle$. The oblate minimum is located at the upper left corner and the prolate one at the lower right. The solid curve is obtained using covariant derivatives, whereas the dashed curve indicates the path obtained in the case of no curvature corrections. The markers are drawn at $Q_i = i/4$, starting from the prolate minimum.

In Fig. 2 we have drawn a different representation of the path, where we plot the quadrupole β and γ parameters along the path, defined as

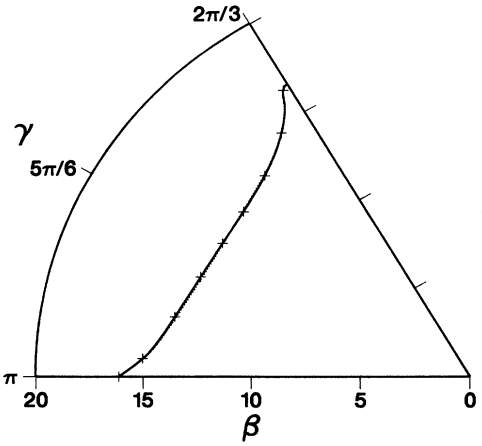

FIG. 2. The value of the (mass) quadrupole deformation parameters β and γ along the collective path. The solid curve is obtained using covariant derivatives, whereas the dashed curve indicates the path obtained in the case of no curvature corrections. The markers are drawn at $Q_i = i/4$, starting from the prolate minimum at $\gamma = \pi/3$.

$$\langle\sqrt{4\pi/5}\, r^2 Y_0^2\rangle = \beta\cos\gamma,$$
$$\langle\sqrt{4\pi/5}\, r^2 Y_2^2\rangle = \beta/\sqrt{2}\sin\gamma. \tag{54}$$

The meaning of the three lines is again the same. The behavior near the prolate minimum is again not as smooth as at all other points. As can be seen from Figs. 1 and 2 the difference between the covariant and noncovariant approaches is surprisingly small. This is even more surprising if one notes that the affine connection does not have small matrix elements. Furthermore, as we have argued before, the difference between TDA and RPA is small as well.

Using the calculated value of the collective coordinate, we can give the collective potential $\bar{V}$ (Fig. 3) and the cranking parameter λ (Fig. 4) (which should be, and is, equal to the derivative of $\bar{V}$) as a function of the collective coordinate Q. In these two figures the curves obtained using the covariant and the noncovariant approach coincide.

Having obtained the path we can now calculate the decoupling measure D. Using Eq. (52) we find in Fig. 5 that the quantity D is not small everywhere along the path. The largest value of D is found near the prolate minimum, but D also exhibits another "bump" not too far from the oblate minimum. This explains the rapid change in properties of the path in Figs. 1 and 2, since the region of rapid change (large curvature) occurs exactly where decoupling is bad. These features seem to indicate that we need to include more than one collective coordinate. To see whether an approach with two coordinates may be able to solve this problem we have separated the contributions $(\Delta q^\mu/\Delta Q)^2$ for the lowest four values of μ. We clearly see in Fig. 6 that the second coordinate (the solid line) gives the most important contribution to this quantity almost everywhere. This seems to hold promise for the calculation of a two-dimensional potential energy surface.

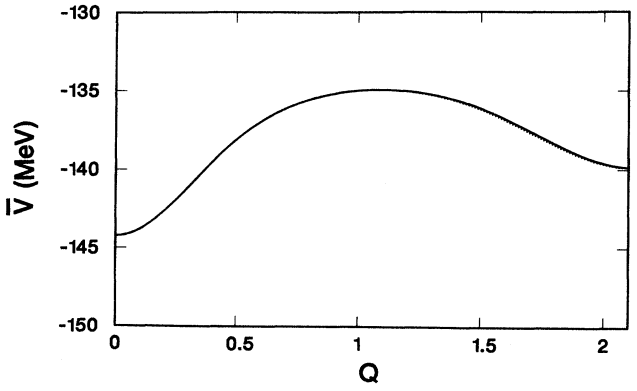

FIG. 3. The potential energy $\bar{V}$ as a function of the collective coordinate Q. The curves with and without use of the covariant derivatives coincide.

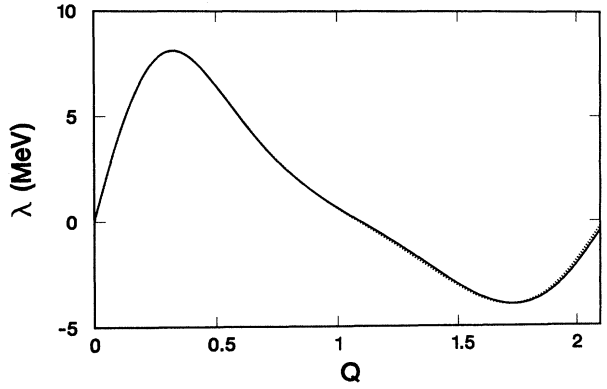

FIG. 4. The quantity λ as a function of the collective coordinate Q. The curves with and without use of the covariant derivatives coincide. λ is numerically very close to $d\bar{V}/dQ$.

To complete the discussion of parameters of the Hamiltonian we have also calculated the moments of inertia, using the approach in Sec. II C. These are displayed in Fig. 7. The moments of inertia behave relatively smoothly (although they do not follow the irrotational pattern). Where D has it largest value the moments of inertia seem to change less smoothly.

Though we have found that decoupling is not good everywhere, we shall nevertheless use the Hamiltonian we have constructed,

$$\mathcal{H} = \tfrac{1}{2}\sum_i \frac{J_i^2}{\mathcal{I}_i} + \tfrac{1}{2}P^2 + \bar{V}(Q), \tag{55}$$

to generate spectra and compare to the full shell-model calculation in the *sd* model space. To that end we need to requantize the Hamiltonian (55). Since we are working in the intrinsic system we have to be very careful. The necessary symmetry properties were, in effect, set out a

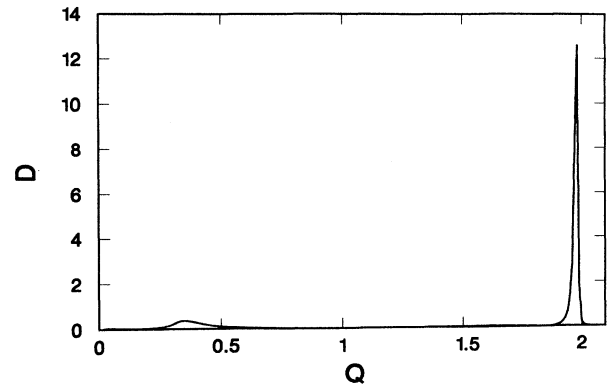

FIG. 5. The decoupling measure D as a function of the collective variable. In this case the path is the one obtained without curvature corrections. As can be seen, decoupling is reasonable, except for the region near $Q = 2$.

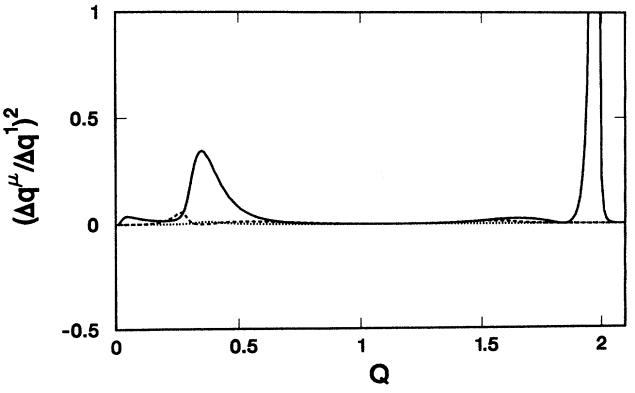

FIG. 6. The quantities $(\Delta q^\mu/\Delta q^1)^2$ for the few lowest eigenvalues of the local RPA. The solid line gives the value for $\mu = 2$, the dashed line for $\mu = 3$ and the dotted line for $\mu = 4$. As can be seen through comparison with the value of D in Fig. 5, the regions of bad decoupling correspond to large Δq^2.

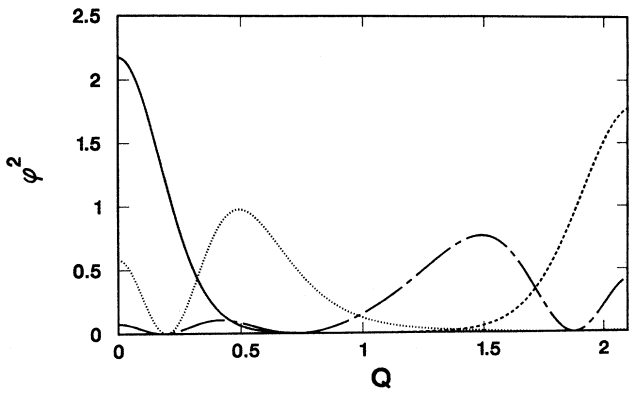

FIG. 8. The square of the four lowest 0^+ eigenfunctions of the collective Hamiltonian. The ground state is the solid line, the dashed line is the first excited state, the dotted line the second excited state, and the short-long dashed line is the third excited state.

long time ago by Bohr,[1] and are discussed in Appendix C. The only thing that needs to concern us here is that we decompose the eigenfunctions as

$$\phi(Q\Omega)_{IMa} = \sum_K \phi_{IKa}(Q)\langle\Omega|IMK\rangle, \tag{56}$$

where $\langle\Omega|IMK\rangle$ are appropriately symmetrized angular functions, and the K summation only runs over positive and even values, and $K = 0$ is excluded for odd I. Using these ideas it is not very hard to write down a finite difference representation for the Hamiltonian matrix (see Appendix C), which in turn can be diagonalized in order to obtain eigenvalues and eigenfunctions. In Fig. 8 we give the eigenfunctions for the states with zero angular momentum. The ground state cannot be very sensitive to the badness of decoupling, since it is very small for $Q > 1$, but the first and other excited states have sizable values in the region of bad decoupling. This means that we do not believe that the corresponding eigenvalues are very good approximations to the shell model values. If we look at the spectrum as given in Fig. 9, we indeed see that the ground state rotational band is reproduced quite well. The band built on the oblate minimum (the second 0^+ state) comes at much too low an excitation energy. Again the moment of inertia of that band is more or less correct. The other 0^+ states also come at a lower energy than their shell-model counterparts. Further note the 3^+ state that is found to lie at too high an excitation

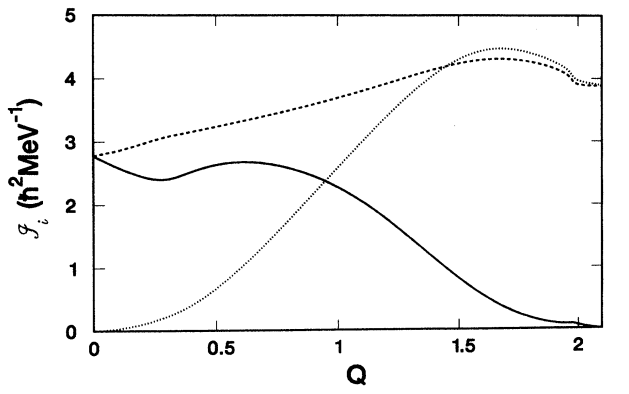

FIG. 7. The moments of inertia, $\mathcal{I}_i$, as a function of Q. The solid line represents $\mathcal{I}_x$, the dashed line represents $\mathcal{I}_y$, and the dotted line represents $\mathcal{I}_z$.

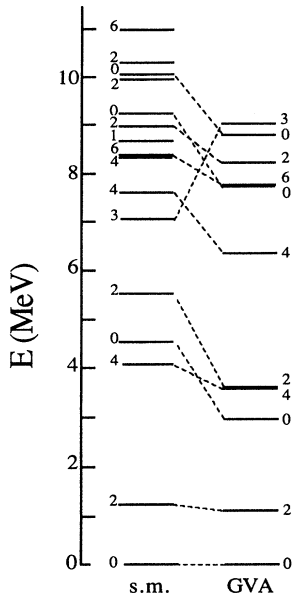

FIG. 9. The spectrum of the shell model calculation (s.m.) compared to that of the generalized valley approximation (GVA).

energy. This is probably partially due to the neglect of odd multipoles in our calculation, which certainly would lower the energy of such a state, but this question requires further study.

V. CONCLUSIONS AND OUTLOOK

We have shown that we can construct a one-dimensional path that, at least for Kuo's interaction, gives a reasonable (but not good) description of the lowest states in ^{28}Si. The major problems are caused by the fact that the path does not really decouple from other degrees of freedom. This has an important impact on the spectrum of 0^+ states, especially in the separation between the ground state and first excited state. We have seen that the second RPA mode is responsible for this lack of decoupling, which leads us to the conclusion that it will be worthwhile to consider the case of two collective coordinates. Formally this problem is very similar to the one we have solved in this paper, so that the only difficulties appear on the numerical side. We are currently studying the feasibility of such a program.

One should notice, however, that the Kuo's interaction that leads to a spectrum with two clearly identifiable rotational bands, does not reproduce the experimental situation, which shows a much less regular and therefore also much more complicated spectrum. For that reason our future calculations should be done both with Kuo's interaction as well with Wildenthal's interaction (the last one gives a much improved description of the spectrum of ^{28}Si). We feel that if we are ever going to see shape mixing, i.e., wave functions that have support in regions of very different nuclear shapes, we will find it for the case of Wildenthal's interaction.

One further problem we would like to mention here is the inclusion of $1/N$ corrections. To understand this it may help to look at the fact that the mean-field approximation becomes exact only in the limit of large particle number. For finite particle number there are corrections, however. One of the easiest ones to evaluate is the rotational zero-point energy. This means that in a general Slater determinant the expectation value of J_i^2 is not zero, so that we have to subtract a term of the form

$$E_{\rm rot} = \tfrac{1}{2}\sum_i \langle J_i^2\rangle/\mathcal{I}_i \tag{57}$$

from the potential energy in order to correct for the finite angular momentum carried by the Hartree-Fock wave function. A further correction would be that due to fluctuations in the noncollective coordinates. In some of our previous papers we have taken that to be $\frac{1}{2}\hbar\omega_a$, the zero-point energy of each of the noncollective modes, which number has to be added to the potential energy. The use of Hartree-Fock, however, masks the fact that there are quantum corrections of the same order of magnitude but opposite sign. We expect to be able to generalize Eq. (8.111) in Ring and Schuck,[13] which would show that the potential energy will be lowered by the zero-point fluctuations. These concepts will be addressed in our next paper.

We started out mentioning the HY approach, which in the case of ^{28}Si has been studied by Pelet and Letourneux.[9] As can been seen from our spectra we have so far not gained too much over that description if we consider only numerical results. It is appropriate to remind the reader once more, however, of the conceptual advantages of our method. We work fully on a classical level, which allows for a clear separation of the decoupling problem from the structure of the nuclear physics. Furthermore, we can calculate and interpret a collective coordinate, and last but not least we know how to gauge the quality (or absence) of decoupling.

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APPENDIX A: FORMALISM

In this appendix we use greek letters to denote all quantum numbers of a single particle orbit except the isospin projection,

$$\alpha = (n_a, l_a, j_a, m_a). \tag{A1}$$

Let us use an isospin-saturated density operator,

$$\rho_{\alpha\tau_a\beta\tau_b} = \delta_{\tau_a\tau_b}\rho^{\tau}_{\alpha\beta} = \delta_{\tau_a\tau_b}\tilde{\rho}_{\alpha\beta}. \tag{A2}$$

It is easy to show that $\mathrm{Tr}\tilde{\rho} = n/2$. As usual we now drop the tilde on ρ. The HF energy functional becomes

$$\begin{aligned} W[\rho] &= \sum_a \epsilon_a \sum_{m_a,\tau_a} \rho^{\tau_a}_{\alpha\alpha} + \tfrac{1}{2}\sum_{\alpha\tau_a\beta\tau_b\gamma\tau_c\delta\tau_d} V_{\alpha\tau_a\beta\tau_b\gamma\tau_c\delta\tau_d}\,\rho^{\tau_d\tau_b}_{\delta\beta}\rho^{\tau_c\tau_a}_{\gamma\alpha} \\ &= 2\sum_a \epsilon_a \sum_{m_a}\rho_{\alpha\alpha} + \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}\left(\sum_{\tau_a=\tau_c,\tau_b\tau_d} V_{\alpha\tau_a\beta\tau_b\gamma\tau_c\delta\tau_d}\right)\rho_{\delta\beta}\rho_{\gamma\alpha} \\ &= 2\sum_a \epsilon_a \sum_{m_a}\rho_{\alpha\alpha} + \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}\bar{V}_{\alpha\beta\gamma\delta}\,\rho_{\delta\beta}\rho_{\gamma\alpha}. \end{aligned} \tag{A3}$$

Here we have introduced $\bar{V}$ by

$$\bar{V}_{\alpha\beta\gamma\delta} = \sum_{\tau_a=\tau_c,\tau_b=\tau_d} V_{\alpha\tau_a\beta\tau_b\gamma\tau_c\delta\tau_d}$$
$$= \sum_{JTM}\left(\sum_{\tau_a=\tau_c,\tau_b=\tau_d,T_z}\begin{pmatrix} C & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ & \tau_a & \tau_b & T_z \end{pmatrix}^2\right) V^{JT}_{abcd}\, C\begin{matrix} j_a & j_b & J \\ m_a & m_b & M \end{matrix} C\begin{matrix} j_c & j_d & J \\ m_c & m_d & M \end{matrix}$$
$$= \sum_{JTM}(2T+1)V^{JT}_{abcd} C\begin{matrix} j_a & j_b & J \\ m_a & m_b & M \end{matrix} C\begin{matrix} j_c & j_d & J \\ m_c & m_d & M \end{matrix}, \tag{A4}$$

and used the common definition of an unnormalized matrix element V^{JT}:

$$V^{JT}_{abcd} = \langle [j_a j_b]^{JT}_{MT_z} | V | [j_c j_d]^{JT}_{MT_z} \rangle. \tag{A5}$$

These equations can be simplified further when we require that for each occupied state the time-reversed state is also occupied. Denoting time reversal by a bar we have, under a choice of phases compatible with ellipsoidal symmetry

$$\rho_{\alpha\beta} = \rho_{\bar{\alpha}\bar{\beta}} = \rho_{\alpha\bar{\beta}} = \rho_{\bar{\alpha}\beta}. \tag{A6}$$

Thus we can limit all summations to half the space, using time reversal to do the other half, and find

$$W[\rho] = 4\sum_a \epsilon_a \sum_{m_a} \rho_{\alpha\alpha} + \tfrac{1}{2}\sum_{\alpha\beta\gamma\delta} \bar{\bar{V}}_{\alpha\beta\gamma\delta}\, \rho_{\delta\beta}\rho_{\gamma\alpha}, \tag{A7}$$

where

$$\bar{\bar{V}}_{\alpha\beta\gamma\delta} = \bar{V}_{\alpha\beta\gamma\delta} + \bar{V}_{\bar{\alpha}\bar{\beta}\gamma\delta} + \bar{V}_{\bar{\alpha}\beta\bar{\gamma}\delta} + \bar{V}_{\bar{\alpha}\beta\gamma\bar{\delta}} + \bar{V}_{\alpha\bar{\beta}\bar{\gamma}\delta} + \bar{V}_{\alpha\bar{\beta}\gamma\bar{\delta}} + \bar{V}_{\alpha\beta\bar{\gamma}\bar{\delta}} + \bar{V}_{\bar{\alpha}\bar{\beta}\bar{\gamma}\bar{\delta}}. \tag{A8}$$

APPENDIX B: DERIVATIVES

In the case of Hartree-Fock the energy functional is

$$W[\rho] = \mathrm{Tr}(\epsilon\rho) + \tfrac{1}{2}\mathrm{Tr}_2(\rho V \rho), \tag{B1}$$

from which we can find the Hartree-Fock Hamiltonian by differentiation,

$$\mathcal{H} = \delta W/\delta\rho. \tag{B2}$$

The two matrices entering in the RPA approximation are

$$V_{,php'h'} = [\delta_{hh'}(\mathcal{H}_{pp'} + \mathcal{H}_{p'p}) - \delta_{pp'}(\mathcal{H}_{hh'} + \mathcal{H}_{h'h})]/2 + (V_{ph'hp'} + V_{hp'ph'} + V_{pp'hh'} + V_{hh'pp'})/2, \tag{B3}$$

and

$$B^{php'h'} = [\delta_{hh'}(\mathcal{H}_{pp'} + \mathcal{H}_{p'p}) - \delta_{pp'}(\mathcal{H}_{hh'} + \mathcal{H}_{h'h})]/2 + (V_{ph'hp'} + V_{hp'ph'} - V_{pp'hh'} - V_{hh'pp'})/2. \tag{B4}$$

Their derivatives — needed in the derivative of the RPA equation — can also be given explicitly. The rules set out in our previous paper,[3] do not apply to third derivatives of expressions like $\mathrm{Tr}H\rho$ (though they do apply to the part that has one derivative due to the explicit density dependence of H). We can easily show that

$$\rho_{ph} = \beta_{ph} - \tfrac{1}{2}\beta_{ph'}\beta^\dagger_{h'p'}\beta_{p'h} + \mathcal{O}(\beta^5),$$
$$\rho_{hp} = \beta^\dagger_{hp} - \tfrac{1}{2}\beta^\dagger_{hp'}\beta_{p'h'}\beta^\dagger_{h'p} + \mathcal{O}(\beta^5), \tag{B5}$$

and the pp' and hh' matrix element of ρ only contain terms up to order β^2. Together with

$$\beta_{ph} = (\beta^\dagger_{hp})^* = (\xi_{ph} + i\pi_{ph})/\sqrt{2} \tag{B6}$$

we find that

$$\frac{\partial^3\mathrm{Tr}(\epsilon\rho)}{\partial\xi^{p_1h_1}\partial\xi^{p_2h_2}\partial\xi^{p_3h_3}} = -\frac{1}{4\sqrt{2}}\{[(\epsilon_{p_1h_2}+\epsilon_{h_2p_1})\delta_{p_2p_3}\delta_{h_1h_3} + (\epsilon_{p_2h_1}+\epsilon_{h_1p_2})\delta_{p_1p_3}\delta_{h_2h_3}] + [(\epsilon_{p_1h_3}+\epsilon_{h_3p_1})\delta_{p_2p_3}\delta_{h_1h_2} + (\epsilon_{p_3h_1}+\epsilon_{h_1p_3})\delta_{p_1p_2}\delta_{h_2h_3}] + [(\epsilon_{p_2h_3}+\epsilon_{h_3p_2})\delta_{p_1p_3}\delta_{h_1h_2} + (\epsilon_{p_3h_2}+\epsilon_{h_2p_3})\delta_{p_1p_2}\delta_{h_1h_3}]\}, \tag{B7}$$

$$\frac{\partial^3\mathrm{Tr}(\epsilon\rho)}{\partial\pi_{p_1h_1}\partial\pi_{p_2h_2}\partial\xi^{p_3h_3}} = -\frac{1}{4\sqrt{2}}\{-[(\epsilon_{p_1h_2}+\epsilon_{h_2p_1})\delta_{p_2p_3}\delta_{h_1h_3} + (\epsilon_{p_2h_1}+\epsilon_{h_1p_2})\delta_{p_1p_3}\delta_{h_2h_3}] + [(\epsilon_{p_1h_3}+\epsilon_{h_3p_1})\delta_{p_2p_3}\delta_{h_1h_2} + (\epsilon_{p_3h_1}+\epsilon_{h_1p_3})\delta_{p_1p_2}\delta_{h_2h_3}] + [(\epsilon_{p_2h_3}+\epsilon_{h_3p_2})\delta_{p_1p_3}\delta_{h_1h_2} + (\epsilon_{p_3h_2}+\epsilon_{h_2p_3})\delta_{p_1p_2}\delta_{h_1h_3}]\}. \tag{B8}$$

We now find

$$V_{php'h',p''h''} = Z^{p''h''}_{php'h'} + Z^{ph}_{p'h'p''h''} + Z^{p'h'}_{p''h''ph} + X^{p''h''}_{php'h'} + X^{ph}_{p'h'p''h''} + X^{p'h'}_{p''h''ph}, \tag{B9}$$

$$(B^{php'h'})_{,p''h''} = -Z^{p''h''}_{php'h'} + Z^{ph}_{p'h'p''h''} + Z^{p'h'}_{p''h''ph} + X^{p''h''}_{php'h'} + Y^{ph}_{p'h'p''h''} + Y^{p'h'}_{p''h''ph}. \tag{B10}$$

Here we have introduced a shorthand for a combination of matrix elements of V and Kronecker-δ's that occurs several times,

$$X^{p''h''}_{php'h'} = [\delta_{hh'}(V_{ph''p'p''} + V_{pp''p'h''}) - \delta_{pp'}(V_{hh''h'p''} + V_{h'h''hp''})]/\sqrt{2}, \tag{B11}$$

$$Y^{p'h'}_{p''h''ph} = -[\delta_{hh''}(-V_{ph'p''p'} + V_{pp'p''h'}) + \delta_{pp''}(-V_{hh'h''p'} + V_{hp'h''h'})]/\sqrt{2}, \tag{B12}$$

$$Z^{p''h''}_{php'h'} = -[\mathcal{H}_{h'p}\delta_{p'p''}\delta_{hh''} + \mathcal{H}_{hp'}\delta_{pp''}\delta_{h'h''}]/(2\sqrt{2}). \tag{B13}$$

APPENDIX C: SYMMETRIES AND REQUANTIZATION

When requantizing a system with ellipsoidal symmetry, one must be careful to implement the symmetry with respect to the group D_2, consisting of the identity operator and the rotation about 180° with respect to each intrinsic symmetry axis. The boundary conditions for such a situation were first evaluated by Bohr.[1] We here follow the discussion of these results by Kumar and Baranger,[17] but would like to point out the discussion in Ref. 12.

The idea starts from reconstructing a wavefunction from the intrinsic frame. We thus decompose the rotationally invariant wave function as (e.g., Appendix A in Ref. 13)

$$\phi_{IM}(Q,\Omega) = \sum_K \phi_K(Q)\langle\Omega|IMK\rangle, \tag{C1}$$

where the properly symmetrized angular functions are given as a sum of Wigner D functions,

$$\langle\Omega|IMKr_1\rangle = [2(1+\delta_{K0})]^{-1/2}\sqrt{\frac{2I+1}{8\pi^2}} \times(D^I_{MK}(\Omega)^* + (-1)^I D^I_{M-K}(\Omega)^*). \tag{C2}$$

the usual conditions for reflection about $\gamma = 0$ and $\gamma = 2\pi/3$ can be related to a symmetry about $Q = 0$ and $Q = Q_P$, where Q_P is the value for Q at the point of prolate symmetry, which lead to the following boundary conditions. First we find $\phi_K(\epsilon) = (-1)^{K/2}\phi_K(-\epsilon)$, which leads to the conditions:

$$\begin{aligned} &K \text{ fourfold}: \quad d\phi_K(Q)/dQ|_{Q=0} = 0 \\ &K \text{ not fourfold}: \quad \phi_K(0) = 0. \end{aligned} \tag{C3}$$

The boundary conditions at the other end are more complicated, reflecting the fact that we have similar relations as given above, but the symmetry axis is no longer the z axis. The relations are of the form

$$\phi_K(Q_p - \epsilon) = M^I_{KK'}\phi_{K'}(Q_p + \epsilon), \tag{C4}$$

with

$$M^I_{KK'} = \frac{(-1)^{K'/2}2^{-I+1}}{[(1+\delta_{K0})(1+\delta_{K'0})]^{1/2}}\sum_S (-1)^{(I-S)}\frac{[(I+K)!(I-K)!(I+K')!(I-K')!]^{1/2}}{S!(K+K'+S)!(I-K-S)!(I-K'-S)!}. \tag{C5}$$

We now seek to find a finite difference approximation to the Hamiltonian. We shall not impose the boundary conditions given above, but instead shall use the boundary condition to check the eigenfunctions after diagonalization.

If we evaluate $\langle\phi|H-E|\phi\rangle$ we find

$$I = \langle\phi|H-E|\phi\rangle = \int dQ \tfrac{1}{2}\sum_{KK'j}\left\langle IK\left|\frac{J_j^2}{2\mathcal{I}_j}\right|IK'\right\rangle\phi_K(Q)\phi_{K'}(Q) + \sum_K \tfrac{1}{2}\left(\frac{d\phi_K}{dQ}\right)^2 + \sum_K [V(Q)-E]\phi_K(Q)^2. \tag{C6}$$

Now let the potential and moments of inertia be known at the points $Q_1, \ldots, Q_N$, chosen such that Q_1 corresponds to the prolate state and Q_N to the oblate state, and let the index i label a quantity at such a point. The functional I can then approximately be evaluated as

$$\begin{aligned} I = {} & \tfrac{1}{2}\sum_{KK'j}\langle IK|J_j^2|IK'\rangle\sum_{i=1}^{N-1}\tfrac{1}{2}\left(\frac{\phi_{Ki}\phi_{K'i}}{2\mathcal{I}_{ji}} + \frac{\phi_{Ki+1}\phi_{K'i+1}}{2\mathcal{I}_{ji+1}}\right)(Q_{i+1}-Q_i) \\ & + \sum_K\sum_{i=1}^{N-1}\tfrac{1}{2}\left(\frac{\phi_{Ki+1}-\phi_{Ki}}{Q_{i+1}-Q_i}\right)^2(Q_{i+1}-Q_i) + \sum_K\sum_{i=1}^{N-1}\tfrac{1}{2}[(V_i-E)\phi_{Ki}^2 + (V_{i+1}-E)\phi_{Ki+1}^2](Q_{i+1}-Q_i). \end{aligned} \tag{C7}$$

If we vary with respect to ϕ_{Ki} and put $\partial I/\partial\phi_{Ki} = 0$, we obtain the generalized eigenvalue equation

$$0 = \sum_{K'j}\langle IK|J_j^2|IK'\rangle\frac{\phi_{K'i}}{2\mathcal{I}_{ji}}g_i + \frac{\phi_{Ki}}{(Q_{i+1}-Q_i)(Q_i-Q_{i-1})}g_i - \frac{\phi_{Ki+1}}{Q_{i+1}-Q_i} - \frac{\phi_{Ki-1}}{Q_i-Q_{i-1}} + (V_i-E)\phi_{Ki}g_i\ , \tag{C8}$$

where

$$g_i = Q_{i+1} - Q_{i-1}, \quad g_1 = Q_2 - Q_1, \quad g_N = Q_N - Q_{N-1}. \tag{C9}$$

If we now redefine $\tilde{\phi}_{Ki} = g_i^{1/2}\phi_{Ki}$, we obtain the ordinary eigenvalue equation (where we have dropped the tildes)

$$\frac{\phi_{Ki}}{(Q_{i+1}-Q_i)(Q_i-Q_{i-1})} - \frac{\phi_{Ki+1}}{Q_{i+1}-Q_i}(g_i g_{i+1})^{-1/2} - \frac{\phi_{Ki-1}}{Q_i-Q_{i-1}}(g_i g_{i-1})^{-1/2} + \sum_{K'j}\langle IK|J_j^2|IK'\rangle\frac{\phi_{K'i}}{2\mathcal{I}_{ji}} + V_i\phi_{Ki} = E\phi_{Ki}. \tag{C10}$$

Since this is a very sparse matrix problem, we solve this by the iterative Lanczos method.[18]

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