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Single-particle degrees of freedom and the generator-coordinate method

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The generator-coordinate method which is usually used to describe collective degrees of freedom is extended to include two quasiparticle excitations and the coupling between these two different modes. As generating wave functions angular momentum and particle number projected Hartree-Fock-Bogoliubov states and quasiparticle excitations built on them are used. The Hartree-Fock-Bogoliubov functions are constrained to a given quadrupole moment, which serves as the generator coordinate. This method is applied to the *pf*-shell nuclei $^{46,50}\text{Ti}$, ^{52}Cr , and ^{54}Fe .

NUCLEAR STRUCTURE Generator coordinate method; Hartree-Fock-Bogoliubov approach; angular momentum projection; particle number projection; two-quasiparticle configurations; nuclear structure calculation in Ti, Cr, and Fe.

I. INTRODUCTION

For a completely microscopic description of nuclei which exhibit both collective and single-particle features shell model calculations in large model spaces are the obvious procedure. During the last years the nuclei of the *sd* shell have been studied extensively by means of complete diagonalizations of shell model Hamiltonians.^{1,2} For heavier nuclei, e.g., those of the *pf* shell, however, the number of configurations within the complete model space increases so rapidly owing to the larger number of active particles and valence shells that severe truncations of the space are necessary. For the nuclei with $20 \leq Z, N \leq 28$, for example, a shell model description has been attempted within the $f_{7/2}$ -shell model basis only.³ For such calculations one preferably extracts the matrix elements of the effective interaction from the excitation spectrum of some of these nuclei since a theoretical derivation of the effective interaction will be quite unstable for such a small model space. Moreover, several low-lying states cannot be reproduced within the model space. If, on the other hand, one adopts more valence shells but allows only certain types of *n*-particles-*n*-hole excitations, the truncation schemes employed are not yet well understood⁴ and yield often rather different results. Another indication that strong truncation will yield poor results is the fact that an expansion of the Hartree-Fock-Bogoliubov ground-state wave function already requires a large num-

ber of shell model configurations as basis states. Moreover, in the *pf* shell the Hartree-Fock-Bogoliubov solutions appear to be rather soft with respect to deformation. This collective property is also suggested by the experimental data.

A possible way out of these difficulties is the application of the generator-coordinate method (GCM).⁵⁻¹⁰ First, the GCM ansatz of the nuclear wave function is constructed to allow a microscopic description of phenomenological, collective motion assuming the final wave function to be a superposition of states with different values of the collective variable. Second, one can use a set of self-consistent wave functions obtained from Hartree-Fock (HF) or Hartree-Fock-Bogoliubov (HFB) calculations as generating functions, which in spite of their simplicity incorporate already many shell model configurations. By selecting in this way a set of appropriate self-consistent basis states, it hopefully turns out that a reliable description of some low-lying states can already be obtained within such a small subspace of the total shell model space. A comparison with exact shell model diagonalization for nuclei in the *sd* shell actually shows that such GCM calculations, using angular momentum and particle-number-projected HFB wave functions as basic states, yield a good approximation.⁸ Since it is one aim to keep the dimension of the model space as small as possible, it is important to estimate the degrees of freedom which are relevant for the states which one wishes to describe. The corresponding

collective variables may then be considered as generator coordinates. This choice of the generator coordinates may be supported theoretically by an investigation of the energy surface calculated for HF or HFB wave functions with different values of the collective parameters. In many cases the important coordinates can also be estimated from the experimental data with the help of some geometric understanding of the collective motion as it is manifested, e.g., in the phenomenological models. The excitation spectra of some nuclei, however, can hardly be understood in a purely collective model, since they also contain noncollective states which may be described as particle-hole or two-quasiparticle states. It is the aim of this contribution to present an extension of the GCM (GCM+QP) which allows the simultaneous consideration of collective and single-particle degrees of freedom, as well as their interference.

We would like to point out that the GCM+QP method provides a way to utilize a phenomenological interpretation of experimental data in a fully microscopic calculation. Therefore its aim is not an exact description of all states by a diagonalization in the entire shell model space, but an approximation for certain states that consists of a diagonalization in their relevant subspace. In some cases the GCM+QP method allows a microscopic foundation of phenomenological models due to the geometry associated with the generator coordinates.

Suitable examples for an application of such an extended GCM (GCM+QP) can be found among the *pf*-shell nuclei. In the mass region $A \approx 50$ especially, the excitation spectra of the $N=28$ isotones ^{50}Ti , ^{52}Cr , and ^{54}Fe display both collective and noncollective features. The excitation energies of the lowest 2^+ and 4^+ states of these nuclei resemble those of a vibrating system and the $E2$ transition probabilities are large. The lowest 6^+ states, however, are only slightly above the 4^+ states and the $6^+ \rightarrow 4^+$ transition probability is considerably smaller. From this behavior one can suggest that vibrational degrees of freedom may be important to describe the 2^+ and 4^+ states, while, e.g., the 6^+ states of these nuclei may be dominated by special two-quasiparticle components.

In Sec. II we present the formalism of the extended GCM which considers not only ground-state configurations but also two-quasiparticle components in the final wave function (GCM+QP). Since for the considered nuclei the pairing correlation turned out to be fairly large, we used HFB wave functions with different deformation as generating functions (Sec. IIB). To describe physical states the broken symmetries have to be restored

first by projecting the HFB wave functions on states with good angular momentum and particle number (Sec. IIC). Results of GCM+QP calculations on ^{46}Ti , ^{50}Ti , ^{52}Cr , and ^{54}Fe are discussed in Sec. III. The last section contains a short summary and conclusions.

II. GENERATOR-COORDINATE METHOD INCLUDING QUASIPARTICLE EXCITATIONS

A. Extension of the generator-coordinate method for bound states

The trial wave function for the GCM has the form⁵⁻⁷

$$|\Psi\rangle = \int dq f(q) \phi(q). \quad (1)$$

In this equation the parameter q denotes the parameters $q_1, \dots, q_m$ and $\phi(q)$ is a set of generating wave functions for different values of the generator coordinates q_i . When applied, for example, in describing the eigenstates of a shell model Hamiltonian, the general GCM ansatz (1) may always yield the exact solution if appropriate wave functions ϕ are chosen with a sufficient number of generator coordinates q_i . The reason for using the GCM, however, is to simplify the shell model calculation and to provide good approximations for the descriptions of some specific states by using only one or two generator coordinates with an appropriate geometrical meaning.⁸⁻¹⁰ For example, a deformation parameter may be used to describe vibrations. In this way the GCM has successfully been applied to the description of low-lying collective states employing angular momentum projected HF or HFB states for the generating wave functions $\phi(q)$.

If there is evidence, however, that besides collective degrees of freedom specific single-particle excitations also may be important, the GCM in its present form may not be very suitable. Then it may be necessary to choose a GCM wave function of the form

$$|\Psi\rangle = \int dq f(q) |\phi(q)\rangle + \sum_i \int dq f^i(q) |\phi^i(q)\rangle. \quad (2)$$

Here $|\phi(q)\rangle$ stands for a ground-state wave function like a constrained HF or HFB wave function, while $|\phi^i(q)\rangle$ represents a certain particle-hole or, more generally, a two-quasiparticle excitation on $|\phi(q)\rangle$. The variational principle $\delta\langle\Psi|\hat{H}-E|\Psi\rangle=0$ determines the unknown weight functions $f(q)$ and $f^i(q)$. This leads to a set of coupled integral equations:

$$\begin{aligned}
& \int dq f(q) \langle \phi(\tilde{q}) | \hat{H} - E | \phi(q) \rangle \\
& + \sum_i \int dq f^i(q) \langle \phi(\tilde{q}) | \hat{H} - E | \phi^i(q) \rangle = 0, \\
& \int dq f(q) \langle \phi^i(\tilde{q}) | \hat{H} - E | \phi(q) \rangle \\
& + \sum_i \int dq f^i(q) \langle \phi^i(\tilde{q}) | \hat{H} - E | \phi^i(q) \rangle = 0.
\end{aligned} \quad (3)$$

If one omits in these equations all the terms containing excited configurations ϕ^i , the usual Hill-Wheeler equation^{5,6} appears as a special case. In practice the integrals are discretized, so that a finite number of generating wave functions $|\phi(q_k)\rangle$ and $|\phi^i(q_k)\rangle$ are used.⁷ In this case the solution of the system of Eqs. (3) corresponds to a diagonalization of the Hamiltonian $\hat{H}$ in the space built up by the nonorthogonal basis $|\phi(q_k)\rangle$ and $|\phi^i(q_k)\rangle$. From this point of view it is evident that the GCM serves to select an appropriate subspace of the entire shell model space. The extension of the normal GCM by inclusion of excited configurations in the GCM+QP approach appears quite natural.

B. Choice of the generating wave functions

For a practical calculation it is essential to select suitable generating wave functions $|\phi(q)\rangle$ and $|\phi^i(q)\rangle$. Since these states are the basis for the final diagonalization of the Hamiltonian $\hat{H}$, they should contain as much information about the correlations of the nuclear system as possible, but they should also be easy to handle. Therefore in a first step we construct a set of HFB wave functions constrained to the different values for the collective parameters q .

If $c_\alpha^\dagger$ and c_α are creation and annihilation operators for nucleons in the single-particle states of the shell model basis, the effective shell model Hamiltonian $\hat{H}$ is defined by

$$\hat{H} = \sum_\alpha \epsilon_\alpha c_\alpha^\dagger c_\alpha + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma. \quad (4)$$

$$\begin{aligned}
& \sum_\alpha \left\{ \left[(\epsilon_\alpha - \lambda_{\tau\alpha}) \delta_{\beta\alpha} - \mu Q_{\beta\alpha} + \sum_{\gamma\delta} V_{\beta\gamma\alpha\delta} \rho_{\delta\gamma} \right] A_{\alpha k} + \left(\frac{1}{2} \sum_{\gamma\delta} V_{\beta\alpha\gamma\delta} \kappa_{\delta\gamma} \right) B_{\alpha k} \right\} = E_k A_{\beta k}, \\
& \sum_\alpha \left\{ - \left(\frac{1}{2} \sum_{\gamma\delta} V_{\beta\alpha\gamma\delta} \kappa_{\delta\gamma}^* \right) A_{\alpha k} - \left[(\epsilon_\alpha - \lambda_{\tau\alpha}) \delta_{\beta\alpha} - \mu Q_{\beta\alpha} + \sum_{\gamma\delta} V_{\beta\gamma\alpha\delta} \rho_{\delta\gamma} \right] B_{\alpha k} \right\} = E_k B_{\beta k}
\end{aligned} \quad (9)$$

with

$$\begin{aligned}
\rho_{\delta\gamma} &= \langle \text{HFB}(q) | c_\gamma^\dagger c_\delta | \text{HFB}(q) \rangle = (B^* B^T)_{\delta\gamma}, \\
\kappa_{\delta\gamma} &= \langle \text{HFB}(q) | c_\delta c_\gamma | \text{HFB}(q) \rangle = (A B^*)_{\delta\gamma}.
\end{aligned} \quad (10)$$

The system of nonlinear equations (9) is solved by

The effect of the inert core which is not included in the basis is represented by single-particle energies ϵ_α . $V_{\alpha\beta\gamma\delta}$ are the antisymmetrized two-body matrix elements of the effective interaction. The constrained HFB wave functions $|\text{HFB}(q)\rangle$ are obtained by solving the variational equation

$$\delta \frac{\langle \text{HFB}(q) | \hat{H} - \lambda_p \hat{N}_p - \lambda_n \hat{N}_n - \mu \hat{Q} | \text{HFB}(q) \rangle}{\langle \text{HFB}(q) | \text{HFB}(q) \rangle} = 0 \quad (5)$$

in the space of the trial functions

$$|\text{HFB}(q)\rangle = \left[\prod_k a_k(q) \right] |0\rangle. \quad (6)$$

Here $\hat{N}_p$ and $\hat{N}_n$ are the particle number operators for protons and neutrons, respectively, and $\hat{Q}$ stands for the operator which defines the collective coordinate q . The Lagrange parameters λ and μ are determined such that the expectation values of the particle numbers p and n and of the collective coordinates q for the HFB solution $|\text{HFB}(q)\rangle$ have the desired values

$$\begin{aligned}
\langle \text{HFB}(q) | \hat{N}_p | \text{HFB}(q) \rangle &= p, \\
\langle \text{HFB}(q) | \hat{N}_n | \text{HFB}(q) \rangle &= n, \\
\langle \text{HFB}(q) | \hat{Q} | \text{HFB}(q) \rangle &= q.
\end{aligned} \quad (7)$$

The state $|0\rangle$ in Eq. (6) denotes the vacuum of the shell model space and represents, therefore, the inert core. The quasiparticle operators a_k are constructed from the basis operators $c_\alpha^\dagger$ and c_α by the Bogoliubov transformation

$$a_k(q) = \sum_\alpha [A_{\alpha k}(q) c_\alpha^\dagger + B_{\alpha k}(q) c_\alpha]. \quad (8)$$

The transformation matrices $A(q)$ and $B(q)$ are the variational quantities in Eq. (5) and are determined with the help of the Euler-Lagrange equations of the variational problem (5). This leads to the following constrained HFB equations:

iteration. In each step of the iteration the Lagrange parameters μ , λ_p , and λ_n are adjusted to fulfill the conditions (7). Because a finite shell model basis is used to expand the HFB wave functions the expectation values of Q are bounded even for operators which are not bounded, e.g., in the

coordinate space. Therefore the solutions of the constrained HFB procedure have some meaning.¹¹

The simplest excited configurations built on these ground-state wave functions $|\text{HFB}(q)\rangle$ are the two-quasiparticle states

$$|\text{HFB}^i(q)\rangle = a_{i_1}^\dagger a_{i_2}^\dagger |\text{HFB}(q)\rangle. \quad (11)$$

Formally these quasiparticle states can be treated like a HFB wave function (6) as a vacuum for quasiparticle operators $\tilde{a}_k$ ¹²:

$$|\text{HFB}^i(q)\rangle \propto \left[\prod_k \tilde{a}_k(q) \right] |0\rangle. \quad (12)$$

For $k \neq i_1, i_2$ the quasiparticle operators $\tilde{a}_k$ are the same as the corresponding a_k for the HFB ground-state wave functions. For the states i_1 and i_2 the expansion matrices A and B of the Bogoliubov transformation (8) have to be interchanged

$$\tilde{a}_i^\dagger(q) = \sum_\alpha (B_{\alpha i}^{(q)} c_\alpha^\dagger + A_{\alpha i}^{(q)} c_\alpha). \quad (13)$$

It should be remarked that the excited configurations $|\text{HFB}^i(q)\rangle$ have expectation values for the particle number operators and the operator Q which differ from those of the corresponding ground-state configurations.

C. Symmetry conservation

Since in general the wave functions $|\text{HFB}(q)\rangle$ are eigenstates neither of the operator of the angular momentum squared $\hat{J}^2$ nor of the particle number operators $\hat{N}_p$ and $\hat{N}_n$, the states $|\text{HFB}(q)\rangle$ have to be projected on the subspace of states with good angular momentum and particle numbers:

$$|\phi_{J,p,n}(q)\rangle = \hat{P}_J \hat{P}_p \hat{P}_n |\text{HFB}(q)\rangle. \quad (14)$$

$$n_{12}(\Omega, \vartheta) = \langle \text{HFB}(q) | \hat{R}(\Omega) \hat{S}(\vartheta) | \text{HFB}(q') \rangle$$

$$= \{\det X(\Omega, \vartheta)\}^{1/2},$$

$$h_{12}(\Omega, \vartheta) = \langle \text{HFB}(q) | \hat{H} \hat{R}(\Omega) \hat{S}(\vartheta) | \text{HFB}(q') \rangle$$

$$= n_{12}(\Omega, \vartheta) \left[\sum_\alpha \epsilon_\alpha \rho_{\alpha\alpha}(\Omega, \vartheta) + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} V_{\alpha\gamma\beta\delta} \rho_{\beta\gamma}(\Omega, \vartheta) \rho_{\alpha\delta}(\Omega, \vartheta) + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} \kappa_{\beta\gamma}(\Omega, \vartheta) \sigma_{\beta\alpha}(\Omega, \vartheta) \right]. \quad (17)$$

Here the generalized density matrices $\rho(\Omega, \vartheta)$, the pairing tensors $\kappa(\Omega, \vartheta)$, $\sigma(\Omega, \vartheta)$, and the matrix X are given in terms of the transformation matrices A and B [Eq. (8)]:

$$X(\Omega, \vartheta) = A^T(q) R^*(\Omega) A^*(q') + B^T(q) R(\Omega) B^*(q') \exp(i\vartheta),$$

$$\rho(\Omega, \vartheta) = R(\Omega) B^*(q') \exp(i\vartheta) X^{-1}(\Omega, \vartheta) B^T(q), \quad (18)$$

$$\kappa(\Omega, \vartheta) = [R(\Omega) B^*(q') \exp(i\vartheta) X^{-1}(\Omega, \vartheta) A^T(q)]^T,$$

$$\sigma(\Omega, \vartheta) = R^*(\Omega) A^*(q') X^{-1}(\Omega, \vartheta) B^T(q).$$

Here $\hat{P}_J$, $\hat{P}_p$, and $\hat{P}_n$ are the corresponding projection operators.¹³ These projected wave functions $|\phi_{J,p,n}(q)\rangle$ serve as ground-state configurations in the generalized GCM ansatz of Eq. (2). This guarantees that the final wave functions have the proper quantum numbers. In a similar way the broken symmetries of the excited configurations are restored:

$$|\phi_{J,p,n}^i(q)\rangle = \hat{P}_J \hat{P}_p \hat{P}_n [a_{i_1}^\dagger(q) a_{i_2}^\dagger(q) |\text{HFB}(q)\rangle]. \quad (15)$$

With these generating wave functions [(14) and (15)] the generalized Hill-Wheeler equation (3) can be solved for each angular momentum J separately and expectation values and transition probabilities for the final wave functions can be calculated. Since also the two-quasiparticle states (11) can be written as a vacuum for a certain set of quasiparticle states [see Eq. (12)], the projection formulas for these states are, in principle, the same as for normal HFB states.¹³ Therefore, the expressions for the kernels of the integral equations (3) are

$$\begin{aligned} \langle \phi_{J,n}(q) | \hat{H} | \phi_{J,n}(q') \rangle \\ = \int d\Omega D_{KK}^{J*}(\Omega) \int d\vartheta \exp(-i\frac{1}{2}N\vartheta) h_{12}(\Omega, \vartheta), \end{aligned} \quad (16)$$

$$\begin{aligned} \langle \phi_{J,n}(q) | \phi_{J,n}(q') \rangle \\ = \int d\Omega D_{KK}^{J*}(\Omega) \int d\vartheta \exp(-i\frac{1}{2}N\vartheta) n_{12}(\Omega, \vartheta). \end{aligned}$$

For simplicity of notation the projection for one kind of particle only is considered in these equations. The generalization to a simultaneous particle number projection for protons and neutrons is straightforward. Also the indices M and K have been omitted. The overlap functions are

In these equations, (16)–(18) $D_{KK}^J(\Omega)$ is the Wigner D function, $\hat{R}(\Omega)$ is the rotation operator which depends on the three Euler angles Ω , and $\hat{S}(\vartheta)$ is the Gauge transformation for the particle number.¹³

III. APPLICATION TO pf SHELL NUCLEI

A. Details of the calculation

For the present calculation the whole pf shell is used as a basis assuming ^{40}Ca as an inert core.

For the residual interaction we used a modified version of the Kuo¹⁴ matrix elements. This modification has been proposed by McGrory¹⁵ who fitted the diagonal $f_{7/2}^2$ matrix elements to obtain agreement for his shell model calculations of $A \leq 44$ nuclei with experimental data. If, however, these matrix elements and the single-particle energies, derived from the experimental spectrum of ^{41}Ca , are used to calculate the single-particle spectra of ^{49}Ca , ^{49}Sc , and ^{57}Ni in a Hartree-Fock approximation, the agreement with experimental data is rather poor. This indicates that even the adjusted interaction is not appropriate for the description of heavier nuclei in the pf shell. Instead of readjusting the matrix elements of the interaction we improved the description of ^{49}Ca , ^{49}Sc , and ^{57}Ni without a careful fitting by increasing the gap between the single-particle energies of the $f_{7/2}$ state and the rest of the pf shell by 1 MeV. So we used as single-particle energies 0.0, 3.1, 4.9, and 7.5 MeV for the $f_{7/2}$, $1p_{3/2}$, $1p_{1/2}$, and $f_{5/2}$ shells, respectively.

To keep the computational effort within reasonable limits we restrict ourselves to axially symmetric HFB states with $K=0$. This approximation does not only simplify the HFB calculations but especially reduces the angular momentum projection integrals over the three Euler angles Ω in Eq. (16) to a one dimensional integral only. Furthermore, we select pairs of time conjugate quasiparticle operators $a_i^\dagger a_i^\dagger$ in Eq. (11). This restriction to only $K=0$ quasiparticle states may be justified, because the configuration with lowest excitation energy is of this form. In addition, the low-lying excitation spectrum should be dominated by $K=0$ configurations. With this selection of quasiparticle states also the excited configuration $a_i^\dagger a_i^\dagger | \text{HFB}(q) \rangle$ are symmetric under time reversal and the calculation of the matrix elements of Eq. (16) is again simplified.

For the generator coordinate q , we choose the quadrupole deformation of the intrinsic HFB functions. This choice is motivated by the vibration-like character of the lowest 0^+ , 2^+ , and 4^+ states in the considered pf -shell nuclei. In addition, the energy surfaces calculated with HFB wave functions for nuclei in this mass region are rather shallow with respect to β deformations and normally exhibit two minima with prolate and oblate deformations.

Since we are only interested in the low-energy spectrum, it is reasonable to neglect the two-quasiparticle state with large excitation energies. For the remaining configurations the energies of the angular momentum and particle number-projected components were calculated. If, at least for one of the considered angular momenta, this

energy was not too high above the corresponding energy originating from ground-state configurations, this two-quasiparticle state was included in the final GCM+QP calculation.

B. $N=28$ isotones

Due to the possible closure of the $f_{7/2}$ subshell for the neutrons, the $N=28$ isotones are distinguished from other pf -shell nuclei. A consequence of this subshell closure is shown in Fig. 1 for the typical example ^{50}Ti . The energies of the intrinsic HFB wave functions [Eq. (6)] with different deformations β are represented by a dashed line. The curve shows a shallow valley with a minimum for the spherical solution. This minimum, however, is very soft against small β deformation. This becomes obvious if one considers the solid curves in Fig. 1, which display the energies calculated for the angular momentum and particle number-projected component of the corresponding HFB wave function. For all angular momenta these curves show minima with small prolate and oblate deformations. This demonstrates that for these nuclei a variation of the deformation degrees of

FIG. 1. The energy surface of the intrinsic HFB state constrained to different deformations β (dashed line) and the energy surfaces of the states projected from it with good angular momentum J and particle number are given for the nucleus ^{50}Ti . The Hamiltonian is described in Sec. III A.

freedom *after* projection is indispensable. In addition, the two nearly degenerate minima for each angular momentum strongly support an application of the GCM with β as a generator coordinate, to allow a mixing of the wave function of these minima.

For the small deformations β , which are favored by the closed neutron shell, the excitation energies of the projected HFB states with $J \neq 0$ are fairly large. They even diverge for a spherical mass distribution ($\beta = 0$). Therefore the energies of states projected from two-quasiparticle excitations may be comparable to or even lower than those which originate from ground-state configurations. This means that already for these nuclei, the yrast states, the lowest states of each angular momentum, may be dominated by two-

quasiparticle components instead of configurations projected from ground-state HFB wave functions. This behavior can be seen in Figs. 2–4 for the nuclei ^{50}Ti , ^{52}Cr , and ^{54}Fe , respectively. These figures display the excitation spectra resulting from a pure β -GCM calculation and from a GCM + QP calculation and compare those calculated with experimental data.¹⁶ (The yrast states are plotted with thicker lines.) With the inclusion of more degrees of freedom in the GCM + QP calculations all energies are, of course, lowered more or less compared to the results of the bare GCM. Whereas the 0^+ and 2^+ yrast states are lowered by at most 0.3 MeV, the energy gain for the 4^+ states is 0.4, 0.5, and 1.7 MeV for the case of ^{50}Ti , ^{52}Cr , and ^{54}Fe , respectively. The 6^+ state of ^{50}Ti is modified by 1.2 MeV. In the case of ^{52}Cr and ^{54}Fe the inclusion of quasiparticle configurations leads to totally new 6^+ yrast states. The second excited 6^+ states have the same excitation energies as the yrast states of the bare GCM calculation and also a large overlap with these states. So for these states one may distinguish clearly between collective and quasiparticle excitations. The energies of the 8^+ and 10^+ yrast states remain unchanged except for the 8^+ in ^{52}Cr . This demonstrates that

FIG. 2. Excitation spectra for ^{50}Ti . The energies obtained by a bare GCM calculation and a GCM including two-quasiparticle excitations (GCM + QP) are compared with experimental data (Exp.). The calculated energies are normalized such, that the energy for the ground-state of the GCM + QP calculation is equal to zero. The energy levels of the yrast states are distinguished from the others by drawing a thicker line. The arrows stand for the transition with largest $B(E2)$ value obtained in GCM + QP calculation for each combination $J \rightarrow J - 2$ (see also Table I).

FIG. 3. Excitation spectra for ^{52}Cr . Further details see text below Fig. 2.

FIG. 4. Excitation spectra for ^{54}Fe . Further details see text below Fig. 2.

up to $J=6$, the importance of quasiparticle configurations for the description of the yrast state increases with increasing angular momentum, because the energies of the quasiparticle states with

$J=4$ and 6 are comparable to or lower than those of the projected HFB states. The states with angular momentum larger than 6 are hardly affected because only two-quasiparticle states up to $J=6$ can be obtained. From the present results and also from those obtained in Ref. 17 one can conclude that the excitation energies of the yrast states of the $N=28$ nuclei agree quite well with the experimental data, if one includes by the GCM+QP theory the modifications caused by the quasiparticle components.

Similar features can also be observed at $B(E2)$ transitions. Those values are given for GCM and GCM+QP in Table I using the rather little effective charges of 1.3 and 0.3 for protons and neutrons, respectively. In case of the $N=28$ nuclei the difference between GCM+QP and GCM appears to be as noticeable as for the excitation energies. In general, and in case of ^{50}Ti particularly, the comparison between the calculated values and the experimental data is in favor of the GCM+QP method. The experimental as well as the theoretical data demonstrate that the collective character of the yrast states decreases with increasing angular momentum.

Table I also displays for each $(J \rightarrow J-2)$ combination the largest calculated transition probabilities. These transitions are also plotted in the Figs. 2-4. It can be seen that for the calculation of all $N=28$ nuclei the first excited 0^+ state is a head of a collective band, which resembles a rotational band with decreasing moment of inertia. An investigation of the wave functions of the states belonging to these bands showed that they mainly originate from HFB wave functions with larger deformation than in the minima. Therefore this

TABLE I. Electromagnetic transitions in ^{50}Ti , ^{52}Cr , ^{54}Fe , and ^{46}Ti . The upper part of the table contains the transition probabilities for the yrast states, while the lower part displays for the $N=28$ isotones the largest calculated $B(E2)$ values for each combination $J \rightarrow J-2$. These collective transitions are represented in Fig. 2-4 by an arrow. The $B(E2)$ values are given in units of $e^2\text{fm}^4$. For the calculated values effective charges 1.3 and 0.3 for protons and neutrons, respectively, have been used. The lower part also contains the calculated branching ratios (b.r.) from the collective state $J_i(\text{coll})$ to $(J_i-2)(\text{coll})$ over the transition $J_i(\text{coll})$ to the lowest J_i-2 state, both calculated by GCM+QP.

$J_i \rightarrow J_f$	^{50}Ti			^{52}Cr			^{54}Fe			^{46}Ti		
	GCM	GCM+QP	Exp.	GCM	GCM+QP	Exp.	GCM	GCM+QP	Exp.	GCM	GCM+QP	Exp.
$2_1 \rightarrow 0_1$	61	63	66 ± 6	106	106	119 ± 7	94	88	102 ± 4	76	78	171 ± 8
$4_1 \rightarrow 2_1$	76	71	60 ± 14	136	112	83 ± 17	125	76	78 ± 16	106	102	...
$6_1 \rightarrow 4_1$	56	38	32.2 ± 1.2	40	86	59.5 ± 3.4	35	43	39.8 ± 0.5	110	103	...
$8_1 \rightarrow 6_1$	...	10	...	...	89	...	...	1	...	...	84	...
	$B(E2)$			b.r.			$B(E2)$			$B(E2)$		
$(2 \rightarrow 0)_{\text{coll}}$	73			0.7 ± 10^{-3}			189			192		
$(4 \rightarrow 2)_{\text{coll}}$	120			0.28			257			266		
$(6 \rightarrow 4)_{\text{coll}}$	78			0.01			271			278		

band can already be obtained in a bare GCM calculation. For a comparison with experiment one should keep in mind that this deformed band is obtained assuming ^{40}Ca as the inert core and therefore, e.g., the calculated moment of inertia of the deformed band may be somewhat too small. Our calculations show that for the nearly spherical $N=28$ nuclei such deformed bands may exist and can already be described within the pf -shell model basis.

In general the non-yrast states are not very much affected by the inclusion of quasiparticle states and, besides some exceptions, additional states which do not have a counterpart in the bare GCM calculation occur at high energies only. This does not mean that the low-lying states cannot be expressed in terms of quasiparticle excitation, but it shows that normally $K=0$ quasiparticle components, which are not contained in the space of the β -GCM calculation, lead to higher excited states. There are only a few but very interesting exceptions, like the 4^+ and 6^+ yrast states, for which the quasiparticle excitations are essential.

C. Application of the model to ^{46}Ti

The nucleus ^{46}Ti is different from the previous ones and more typical for nuclei in this mass region since it does not have a closed $N=28$ neutron shell. Therefore the energy surface for the intrinsic HFB wave function with different deformation already shows two minima with prolate and oblate deformation, whereas the spherical solution is about 1 MeV higher in energy (see Fig. 5). The minima of the energies for the projected states occur at nearly the same deformation as the intrinsic minima. Again due to the open shells for protons and neutrons, the intrinsic deformation of these minima is larger than for the $N=28$ nuclei. This corresponds to smaller excitation energies of the angular momentum projected state with $J>0$. In addition, the spectra projected from quasiparticle excitations are more rotational-like and their band heads are excited by several MeV. Thus the resulting yrast spectrum is quite regular up to the 10^+ and only little affected by two-quasiparticle excitations (see Fig. 6). The excitation energies of the calculated yrast state are in a very good agreement with the experimental data. The values for the $B(E2)$ transition probabilities calculated with the same, small effective charges as are used for the $N=28$ isotones, are too small compared to the experimental value. One can argue that for this more deformed nucleus larger effective charges should be used because the core is more affected than in the case of the nearly spherical $N=28$ isotones. Since in the case of ^{46}Ti

FIG. 5. Energy surfaces for the nucleus ^{46}Ti . Further details see text below Fig. 1.

FIG. 6. Excitation spectra for ^{46}Ti . Further details see text below Fig. 2.

the yrast band already is built up mainly by components with considerable intrinsic deformation, there is no excited collective band as there is for the $N=28$ isotones. The inclusion of quasiparticle components yields in comparison with the results of a β -GCM calculation a large number of additional excited states with excitation energies of 4–8 MeV.

IV. CONCLUSION

In this paper we presented an extension of the normal generator-coordinate method for a description of bound states of nuclei. In this GCM + QP method one considers as generating wave functions not only Hartree-Fock-Bogoliubov ground-state configurations with different values for the collective generator coordinate, but also two-quasiparticle excited states. The broken symmetries of the HFB as well as of the quasiparticle states are restored by projecting onto the components with good angular momentum J and onto the desired particle numbers for protons and neutrons. Although the numerical effort, especially to perform the projections, is quite large, this GCM + QP approach is feasible also on a larger basis for which a complete shell model diagonalization cannot be performed. The use of self-consistent HFB wave functions as a basis of the model space rather than simple shell model configurations gives rise to the hope that a small number of these basis states already is sufficient to describe the low energy spectrum of nuclei. Since also noncollective single-particle excitations are taken into account the GCM + QP approach can be considered as a useful tool to describe in a microscopic way the coupling of collective and single-particle degrees of freedom.

The GCM and GCM + QP method can, in principle, include any finite number of generator coordinates. We have restricted the calculation to the deformation parameter β (β -GCM). We tested

also the influence of the pairing correlation energy Δ as a generator coordinate (Müther *et al.*, Ref. 10). But we found no important modifications for the low-lying levels. The triaxial deformation degree of freedom γ may have some influence by producing states of a γ vibrational nature. But an inclusion of this degree of freedom is prohibitive owing to the tremendous amount of computer time connected with an angular momentum projection with $\gamma \neq 0$.

The model might easily be improved by including also four quasiparticle states. If the 2qp states of $(f_{7/2})^2$ nature form the yrast band already at angular momentum 6, one expects also a low-lying 8^+ of a $(f_{7/2})^4$ configuration.

Here we applied in Sec. III the GCM + QP method for $\gamma=0$ and quasiparticles to the $N=28$ isotones ^{50}Ti , ^{52}Cr , and ^{54}Fe , which may serve as a suitable example, for which the coupling between collective and single-particle degrees of freedom may be important. With the inclusion of quasiparticle configurations it appeared to be possible to describe the excitations of the yrast states as well as the $B(E2)$ transition probabilities. The calculated spectra also exhibit the possible existence of deformed excited bands for these nuclei. In the case of ^{46}Ti which was considered as a typical example of pf -shell nuclei with $N \neq 28$, the yrast states were not very much affected by the explicit inclusion of quasiparticle degrees of freedom, but some excited states were obtained around 5 MeV. Recently the GCM + QP method has also successfully been applied to describe the strange spectra of ^{72}Ge and neighbored nuclei¹⁸ and it gives also a microscopic description of the backbending phenomena in rare earth nuclei.¹⁹ Therefore we conclude that the GCM + QP approach is a useful tool to describe in a microscopic way certain phenomena, in excitation spectra of nuclei, which may originate from a coupling of collective and single-particle degrees of freedom.

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