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Rotational motion in nuclei

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A new method is presented for treating rotational motion up to very high spin in deformed nuclei. Going beyond the mean field approach by the generator coordinate method, we take into account additional corelations, in particular, the interaction between the yrast and the two quasiparticle bands.

[NUCLEAR STRUCTURE Rotational motion; heavy nuclei; generator coordinate method.]

In recent years, much work has been done on the high spin region of deformed nuclei, theoretically as well as experimentally (see Refs. 1 and 2, respectively, for recent reports).

The most successful theory explaining data has probably been the cranking technique combined with the Hartree-Fock-Bogoliubov (HFB) approximation in its different versions: full self-consistent determination of the mean field [the so-called self-consistent cranking (SCC)],[3] with constant deformation β, γ, and Δ, or only β and γ [the so-called cranked shell model (CSM)],[4] and the generalizations of these approximations to the particle number projection case.[5,6]

Nevertheless, all these calculations suffer from more or less important deficiences. In order to analyze some of these, let us consider separately the two approximations involved in the SCC (CSM): first, the restriction of the wave functions to those of product type and second, the cranking procedure to restore the angular momentum on the average. The combination of both approximations gives, as is known, a mean field theory in the rotating system. Though the second one is a consequence of the first, both are independent in the sense that we could, for instance, maintain the HFB ansatz and project out exactly the angular momentum. We could, on the contrary, improve the wave functions, remaining nonrotationally invariant and keeping the cranking technique.

We can now consider both approximations as a function of the angular momentum (cranking velocity). It is known[7] that the cranking technique is a good approximation for well deformed heavy nuclei with large fluctuations in the angular momentum, and that it becomes an even better approximation for large values of the angular momentum because it corresponds to the classical limit. Nevertheless, as we shall see below, the neglect of the fluctuations in the angular momentum, as implied in the cranking approach, is not justified in the band crossing region. For the mean field theory in the rotating system, we have well defined minima at low angular velocity with the first excited states lying at about 1 MeV high. By increasing the angular velocity, the minima become flatter and flatter due to the high level density near the yrast band, the increment in the level density being caused by the two quasiparticle states coming down because of the Coriolis force. As a consequence of this, the mean field theory will, probably, be worse.

Another source of deficiency is the fact that the SCC (CSM) wave functions usually show too much alignment[5,6,8] at low angular momentum in comparison with the experiment, which is also connected with the band crossing problem.[9–16] We can understand with the following schematic arguments the reasons why the mean field approximation cannot describe correctly these facts: To describe the band crossing region properly we have to combine both bands at a given value of the angular momentum I_0. We should therefore allow wave functions of the type

$$|\Phi\rangle = c_1|\Phi\rangle_{\omega_1} + c_2|\Phi\rangle_{\omega_2} ,$$

where $|\Phi\rangle_{\omega_1}$ and $\alpha_1^\dagger\alpha_2^\dagger|\Phi\rangle_{\omega_2}$ are the wave functions of the yrast and the two quasiparticle band, respectively; $\alpha_1^\dagger$, $\alpha_2^\dagger$ are the two low lying quasiparticles with respect to $|\Phi\rangle_{\omega_1}$. Taking into account the aligned nature of $\alpha_1^\dagger\alpha_2^\dagger|\Phi\rangle_{\omega_2}$ before the band crossing and the fact that both components of $|\Phi\rangle$ above have approximately the same expectation value of $\hat{J}_x$, we conclude that $\omega_2 < \omega_1$. On the other hand, in the region after the band crossing, due to the aligned character of the yrast band, we have $\omega_2 > \omega_1$.

The linear combinations considered above are not, in general, of the HFB type. Only for the case $\omega_1 = \omega_2 = \omega$ can we write

$$|\Phi\rangle = e^{\alpha_1^\dagger\alpha_2^\dagger}|\Phi\rangle_\omega = |\Phi\rangle_\omega + \alpha_1^\dagger\alpha_2^\dagger|\Phi\rangle_\omega ,$$

which means that we have too much alignment before the band crossing and too little after.

All these facts point out the necessity of considering more correlations in the wave functions or to restore the angular momentum symmetry in a better approach. Some steps have already been taken in this direction. Several authors[10,17] have proposed using the random phase approximation (RPA) in the rotating system (CRPA) to describe the yrast band and the excited states. Realistic calculations[11] have been done in the rare earth region for ^{164}Er. The theoretical results for the excited states were in good agreement with the experiment for angular momentum I up to $22\hbar$. With respect to the yrast band, not too much can be said because the coupling constants were fitted for the SCC approach. Nevertheless, if the mean field (HFB) is not a good approximation at very high spins or in the band crossing region, obviously, neither is the RPA.

A very powerful theory that goes beyond the mean field approximation and allows the introduction of correlations in a simple way is the generator coordinate method (GCM); one has only to be careful in the choice of the generating coordinates and in the number of these, otherwise the dimensions rise tremendously.

In the spirit of this method we consider the following wave function:

$$|\Psi\rangle = \int_{-\infty}^{\infty} |\Phi(\omega)\rangle \, d\omega \ , \tag{1}$$

with

$$|\Phi(\omega)\rangle = f_{00}(\omega)|\Phi\rangle_\omega + \sum f_{\mu\nu}(\omega)\alpha_\mu^\dagger(\omega)\alpha_\nu^\dagger(\omega)|\Phi\rangle_\omega \ , \tag{2}$$

where $|\Phi\rangle_\omega$ is a wave function of the HFB type, eigenfunction of $\hat{H}_0' = \hat{H}_0 - \omega\hat{J}_x$, $\hat{H}_0$ being the one-body approximation to the Hamiltonian $\hat{H}$, and $\hat{J}_x$ the x component of the total angular momentum operator. In other words, $|\Phi\rangle_\omega$ are the wave functions used in the SCC (or CSM) to describe the yrast states; $\alpha_\mu^\dagger(\omega)$ are the corresponding quasiparticle operators to $|\Phi\rangle_\omega$, and $f_{\rho\sigma}(\omega)$ are coefficients to be determined by minimization of the energy. The velocity ω has been used as generator coordinate by Thouless and Peierls.[12] However, these authors were restricted to low spins because of the linear response approximation in ω.

Since the wave functions $|\Phi(\omega)\rangle$ are not eigenstates of the angular momentum, nor are the $|\Psi\rangle$ (the same happens with the particle number; to simplify the discussion we shall concentrate only on $\hat{J}_x$); this means we have to minimize

$$E^I = \langle\Psi|\hat{H}P^I\Psi\rangle / \langle\Psi|P^I|\Psi\rangle \ , \tag{3}$$

with P^I an operator which projects on angular momentum I. Another possibility is to treat the projection approximately. This can be done under the assumption of large deformation when we can develop the Hamilton overlap as a function of the derivatives of the norm overlap (Kamlah expansion). In this case we get,[7] up to second order,

$$E^I = \langle\Psi|H|\Psi\rangle + \Omega[\sqrt{I(I+1)} - \langle\Psi|\hat{J}_x|\Psi\rangle] + \frac{1}{2\mathcal{I}_Y}[\sqrt{I(I+1)} - \langle\Psi|\hat{J}_x|\Psi\rangle]^2 - \frac{\langle\Psi|\Delta\hat{J}^2|\Psi\rangle}{2\mathcal{I}_Y} \ , \tag{4}$$

with the moment of inertia of Yoccoz $\mathcal{I}_Y$ and Ω given by

$$\frac{1}{2\mathcal{I}_Y} = \frac{\langle\Psi|(H-\langle H\rangle)\Delta\hat{J}^2|\Psi\rangle}{2(\langle\Delta J_x^2\rangle^2 + \langle J_y^2\rangle^2 + \langle J_z^2\rangle^2)} \ ; \ \Omega = \frac{\langle\Psi|\hat{H}\Delta\hat{J}_x|\Psi\rangle}{\langle\Psi|\Delta J_x^2|\Psi\rangle}$$

If we assume that $\langle\Delta J^2\rangle/2\mathcal{I}_Y$ is constant, we obtain the cranking model; i.e., we have to minimize

$$E = \langle\Psi|\hat{H}|\Psi\rangle / \langle\Psi|\Psi\rangle \tag{5}$$

with the constraint

$$\sqrt{I(I+1)} = \langle\Psi|\hat{J}_x|\Psi\rangle / \langle\Psi|\Psi\rangle \ . \tag{5a}$$

We see therefore that we can restore the angular momentum symmetry in three ways: exactly, i.e., by (3); by minimization of (4), which contains the fluctuation term; or by the cranking descriptions (5) and (5a). At this point we can comment on the neglect of the term $\langle\Delta J^2\rangle 2\mathcal{I}_Y$ in the cranking approach: Using the commutation relations for the pairing plus quadrupole Hamiltonian we can get,[16] in a good approximation, an analytical expression for this term:

$$\Delta E_Y = -\frac{\langle\Delta J^2\rangle}{2\mathcal{I}_Y} = -K\frac{\beta^2}{\langle\Delta J^2\rangle} \ ,$$

with K a positive constant and β the deformation parameter. From this expression we can see clearly that this term will be very important in the band crossing region where $\langle\Delta\hat{J}^2\rangle$ changes very much and β remains approximately constant. If we do not neglect this term, but vary expression (4), the condition of minimum will attempt to make ΔE_Y as large as possible, i.e., $\langle\Delta J^2\rangle$ as small as possible; and therefore the bands (ground and aligned) will mix as little as possible, causing a sharper band crossing then in the usual cranking model. In conclusion, we feel that to get a right description of the band crossing we cannot neglect the fluctuation term. In the rest of the spectrum it will probably not be as important because $\langle\Delta J^2\rangle$ shows a smooth behavior which could be renormalized in the force constants.

We think that the wave function (1), being a superposition of many specially chosen generalized Slater determinants, contains enough correlations to give the right alignment. Also, the two quasiparticle parts in (2) will contribute toward a better description of the band crossing region and of the very high spin region. Furthermore, we think that some failures imputed to the cranking procedure will not appear if

we have a better wave function than in the mean field approximation. It is also important to note that the fluctuation term in (4) is at least a two-body operator, which means that a mean field treatment of this term may not be appropriate.

The purpose of this Communication is to show the applicability of this method to the calculation of yrast and excited states in well-deformed nuclei. In particular, we shall restrict ourselves to the approximate methods to restore the angular momentum because of its simplicity to contrast with the exact projection (3).

We shall see that with the wave function (1), the problems (5) and (5a), we could call the cranked generator coordinate method (CGCM), as well as the minimization of (4) which includes the fluctuation term, can be solved with a relatively small effort. The second method, though somewhat more complicated, will be much more accurate.

To gain some insight into the method let us discuss it in some detail. For practical reasons it is more convenient to write the integral (1) as a sum:

$$|\Psi\rangle = \sum_{\omega_a=-\omega_M}^{+\omega_M} |\Phi(\omega_a)\rangle \ , \tag{6}$$

where we have also restricted the values of ω from $-\omega_M$ to some maximum value ω_M which will be properly chosen; we will treat this point subsequently. We denote by

$$|i\rangle \quad (i=1,2,\ldots,N) \ , \tag{7}$$

the basis states

$$\begin{aligned}
&|\Phi\rangle_{-\omega_M}, \alpha_1^\dagger(-\omega_M)\alpha_2^\dagger(-\omega_M)|\Phi\rangle_{-\omega_M}, \ldots, \alpha_{K-1}^\dagger(-\omega_M)\alpha_K^\dagger(-\omega_M)|\Phi\rangle_{-\omega_M}, \ldots, \\
&|\Phi\rangle_{\omega_0}, \alpha_1^\dagger(\omega_0)\alpha_2^\dagger(\omega_0)|\phi\rangle_{\omega_0}, \ldots, \alpha_{K-1}^\dagger(\omega_0)\alpha_K^\dagger(\omega_0)|\Phi\rangle_{\omega_0}, \ldots, \\
&|\Phi\rangle_{\omega_M}, \alpha_1^\dagger(\omega_M)\alpha_2^\dagger(\omega_M)|\Phi\rangle_{\omega_M}, \ldots, \alpha_{K-1}^\dagger(\omega_M)\alpha_K^\dagger(\omega_M)|\Phi\rangle_{\omega_M} \ ,
\end{aligned} \tag{8}$$

appearing in (2). N in (7) is the dimension of the configuration space and depends on the number of ω values introduced in the discretization of (1) and on the amount of two quasiparticle states we allow in (2); K in (8) numbers the quasiparticles. In this notation (1) takes the form

$$|\Psi\rangle = \sum_j f_j |j\rangle \ , \tag{9}$$

with f_j instead of $f_{\rho\sigma}$ in (2). The basis states $|i\rangle$, as frequently happens in the GCM, are nonorthogonal, not complete and linearly dependent.

We turn now to the problem of the minimization of the energy. We shall concentrate for the moment on the minimization without considering the constraint; later on we shall discuss how to incorporate it. The variation of $E = \langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle$ leads to the Hill-Wheeler equation

$$\mathcal{H}f = E\mathcal{N}f \ , \tag{10}$$

with the matrix overlaps

$$\mathcal{H}_{ij} = \langle i|\hat{H}|j\rangle, \quad \mathcal{N}_{ij} = \langle i|j\rangle \ . \tag{11}$$

As already known from the above-mentioned properties of the basis state $|i\rangle$, the usual methods of diagonalization cannot be applied directly. What is usually done to remedy these problems, i.e., to go to an orthonormalized set (see, for instance, Ref. 13), is the so-called symmetric orthogonalization which corresponds to a diagonalization of the Hermitian operator $\mathcal{N}$. That is,

$$\sum_j \mathcal{N}_{ij} u_j^L = n_L u_i^L \ . \tag{12}$$

Since $\mathcal{N}$ is a norm, the eigenvalues n_L are greater or equal to zero. The functions u_i^L form a complete orthonormalized set in the space of the weight functions f_j.

If a zero eigenvalue n_L exists, this has to be suppressed, otherwise the weight functions f_j corresponding to a state $|\Psi\rangle$ are not determined uniquely. To find a unique correspondence between $|\Psi\rangle$ and f we should restrict f_j to weight functions that are linear combinations of functions u_i^L with $n_L \neq 0$. For each of these functions there exists a normalized vector in the Hilbert space

$$|L\rangle = (n_L)^{-1/2} \sum_i u_i^L |i\rangle \ . \tag{13}$$

These states are orthonormal and the Hilbert space that they span is the smallest Hilbert space which contains all the generating states. If we now write

$$|\Psi\rangle = \sum_L g_L |L\rangle \tag{14}$$

instead of (10), we have to diagonalize

$$\sum_K \langle L|\hat{H}|K\rangle g_L = E g_L \ . \tag{15}$$

The matrix elements which are needed for this expression can be calculated by the techniques exposed in Ref. 5.

If we did not have a constraint on $\hat{J}_x$ [or we did not want to vary expression (4)] the problem would finish here. Though (15) is a linear problem the consideration of the constraint (5a) or the second-order term in (4) introduces some nonlinearities. To bypass this difficulty, one can use the steepest des-

cent method[14] which has been used, with great success, for HFB wave functions. Because of the iterative character of this method, its applicability depends very strongly on the complexity of the gradient of the involved operators. We will now see that these gradients are very easy to calculate with our wave functions. The wave function (14) can be written as

$$|\Psi\rangle = \left[1 + \sum_{K=2} g_K^2\right]^{-1/2} \left[|1\rangle + \sum_{K=2} g_K |K\rangle\right] ,$$

in each step of the iteration. The gradient of the expectation value of any operator $\hat{0}$ is then given by

$$\frac{\partial}{\partial g_K} \langle \Psi|\hat{0}|\Psi\rangle_{g_K=0} = 2\langle 1|\hat{0}|K\rangle ,$$

and this expression is simply the first row of the representation of $\hat{0}$.

Once we have found the yrast state $|\Psi_1\rangle$ corresponding to angular momentum I, we can apply the same method to calculate excited states of the same I by excluding $|\Psi_1\rangle$ from the basis states.

Some points must still be remarked concerning the wave function (1), such as the discretization of the integral, the two quasiparticle states to be considered in (2), and the maximum value of ω to be used in (6). As a general comment on these points one can say[15] that, since we are working on a linearly dependent basis, the increase of this does not necessarily mean a better approximation. With respect to the two quasiparticle states, as we know, the main role is played by the intruder orbitals, in the rare-earth region, the $ni_{13/2}$ and the $\pi h_{11/2}$. The maximum value of ω will depend obviously on the maximum value of I, which we want to calculate.

It is important to note that for the whole spectrum the full basis (8) is needed *only once* to diagonalize the matrix $\mathfrak{N}$ in (12) and to find the representations of $\hat{H}$ and $\hat{J}_x$ [eventually of the operators appearing in (4)]. The posterior calculation of all states will require much less dimension because of the omission of the linearly dependent states.

In conclusion, for treating rotational motion in nuclei, we propose the use of a linear superposition of the yrast wave functions of the SCC (CSM of any similar theory) and the two quasiparticle states based on those, in the spirit of GCM. The coefficients of this superposition are determined by minimization of the energy. If a projection technique is not used to restore the angular momentum (particle number) symmetry, approximative projection methods which may or may not include the fluctuations in the angular momentum can be applied to this GCM wave function.

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