Applicability of truncation schemes in the cranked deformed shell model

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Two truncation schemes for cranking the many-particle states of a deformed potential (including monopole pairing) are compared with some exact results. A truncation emphasizing alignment properties proves much better than a truncation which includes only the low-lying many-particle configurations at zero rotational frequency.

In recent years there has been some effort[1,2] to perform cranked deformed shell-model calculations in a many-particle configuration space. These approaches have certain advantages over the usual cranked-quasiparticle methods. For example, the problem of number nonconservation,[3] which leads to the unphysical disappearance of pairing correlations at the band crossing, does not arise and some other errors (e.g., interaction strengths) due to the use of the Hartree-Fock-Bogoliubov (HFB) approach are also absent.[4]

The problem, of course, is that in a full cranked deformed shell-model calculation, the many-particle configuration space is very large compared with the quasiparticle space, which is just twice the size of the single-particle basis. For example, even for only 6 particles in a single $i_{13/2}$ shell, the dimension of the Hamiltonian matrix is 3003. In a more realistic situation, where several angular momentum orbitals need to be considered, these matrices may easily run into millions, and a truncation scheme is obviously needed if a quantitative comparison with experiment is to made. This truncation should be such that it faithfully reproduces the basic features of at least the lowest few states of the full space. It is thus important to ask what the dominant components of the near-yrast configurations are.

In Refs. 5, a truncation scheme (hereafter referred to as *A*) was formulated on alignment considerations (see later). It was demonstrated that it reproduces the lowest few states reasonably well, and the overlap between the exact and truncated wavefunctions was found to be more than 90% for the lowest five states. Recently, a different truncation scheme based on energy considerations (hereafter referred to as *B*) was proposed in Ref. 6. The purpose of this Brief Report is to make a comparison of the two truncations with the exact calculations carried out in the present work.

We study a model Hamiltonian (as in Refs. 2–6)

$$H' = h_{\rm def} + V_2 - \omega J_x \ , \tag{1}$$

where $h_{\rm def}$ is the quadrupole-deformed mean field:

$$h_{\rm def} = \kappa \sum_m \left[\frac{3m^2}{j(j+1)} - 1 \right] C_m^\dagger C_m \ , \tag{2}$$

where $C_m^\dagger$ and C_m are the creation and destruction operators for the state $|jm\rangle$ and V_2 is the two-body nucleon-nucleon interaction which is chosen here (and in Ref. 6) to be of the monopole pairing type, i.e.,

$$V_2 = -G \sum_{mm'>0} C_m^\dagger \tilde{C}^\dagger_m \tilde{C}_{m'} C_{m'} \ , \tag{3}$$

with

$$\tilde{C}^\dagger_m = (-1)^{j-m} C^\dagger_{-m} \ . \tag{4}$$

In Eq. (1), J_x is the component of the total angular momentum along the cranking axis (x). The eigenstates of the system have good signature exponent α, defined by $\exp(-i\pi J_x)\Psi = \exp(-i\pi\alpha)\Psi$.

The truncation scheme *A* (Ref. 5) is essentially based on the alignment properties of the undeformed system [$\kappa = 0$ in Eq. (1)]. In this spherical problem, the states have a well-defined angular momentum J and projection M_x along the x axis. For the monopole pair force they also have good seniority v (Ref. 7) which may be thought of as the number of nucleons not paired to $J = 0$. In Fig. 1 the routhians E' (energies in the rotating frame) are presented for the nondeformed case with $G = 0.15$. [The figure scales simply for other values of G (Ref. 4).] We show in Fig. 1 only the maximally aligning state for each seniority v and have labeled the states $(v, J = M_x)$. For an even particle number, the maximum number of states in this shell occurs for $n = 6$ when states up to $v = 6$ are necessary. The maximum number is 3003. The reason for choosing the particular states shown in Fig. 1 is that they successively become yrast, i.e., the fully paired state ($v = 0$) is yrast up to $\omega = 0.0875$, where it is crossed by an aligned two-particle state with $J = M_x = 12$; this is in turn crossed by a four-aligned-particle state at $\omega = 0.0938$ ($J = M_x = 20$), the final crossing brings in the six-aligned-particle configuration ($J = M_x = 24$) at $\omega = 0.1125$. The first and second of these crossings are conventionally labeled *AB* and *CD* as in Fig. 1.

We see from the above considerations that the yrast state has sudden increases in angular momentum through the breaking of $J = 0$ pairs. With the deformation switched on ($\kappa \neq 0$) this will happen more gradually, though for small $|\kappa|$ the crossings will still be rather sharp.[8] The reason for this is that the quadrupole field, which is proportional to

$$Y^{(z)}_{20} = -\tfrac{1}{2} Y^{(x)}_{20} + (\tfrac{3}{8})^{1/2} (Y^{(x)}_{22} + Y^{(x)}_{2-2}) \ , \tag{5}$$

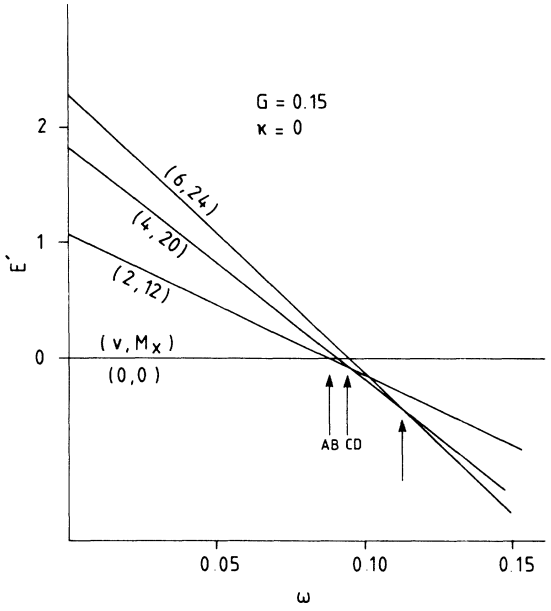

FIG. 1. The most aligning states ($M_x = J_{max}$) for even-particle-number systems in the $i_{13/2}$ shell. The levels are labeled (v, M_x). Results are shown for $G = 0.15$ but scale simply for other G values. The frequencies at which successively higher seniority (and alignment) states become yrast are indicated.

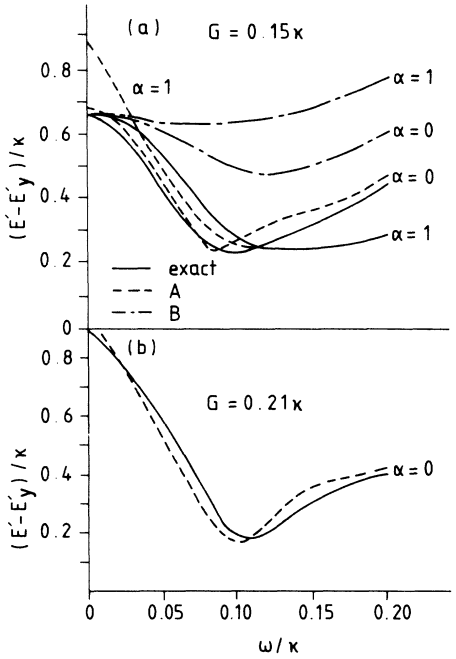

FIG. 2. (a) The results of truncations A (— — —) and B (— · — · —) are compared with exact calculations (——) for $G = 0.15\kappa$. The cranked energies for the lowest $\alpha = 0$ and $\alpha = 1$ states are shown relative to the yrast state ($\alpha = 0$). Energies and the rotational frequency are shown in units of κ. (b) Same as in (a) for the lowest $\alpha = 0$ state with $G = 0.21\kappa$ (truncation A only).

has to act several times to mix the crossing states. For example at the AB crossing the angular momentum J and M_x change by 12 units. The AB crossing strength is, therefore, sixth order in κ since to mix the states ($v = 0$, $J = M_x = 0$) and ($v = 2$, $J = M_x = 12$), $Y_{20}^{(z)}$ must act at least six times. (Specifically, in lowest order $Y_{22}^{(x)}$ must act six times.) Thus many intermediate states are involved in the band mixing, with the "stretched" configurations $J = M_x$ playing a dominant role. For this reason truncation A takes *all* the many-particle basis states with $M_x = J$ and $J - 2$, since each time the deformation acts it is possible to change v by two units and thus even in the AB crossing, where v goes from 0 to 2, intermediate states with $v = 6$ are involved.[8]

The truncation scheme B of Ref. 6 simply takes the many-particle states calculated in the deformed field and truncates at an energy of 3.5κ to obtain a basis. In some respects this will have similar effects to truncation A, since the states which lie low in energy in the deformed field will tend to have low-K values [$K = \Sigma m$, see Eq. (2)]. When expressed with respect to the x axis rather than the z axis,

$$|JM'\rangle_z = \sum_M d^J_{M'M}(\tfrac{1}{2}\pi)|JM\rangle_x \ , \tag{6}$$

these states will contain some of the large M_x components and thus may align strongly. However, not all the strengths of these states will be kept if one makes the truncation in energy. One will almost certainly lose some of the components of the intermediate states of high M_x specifically retained in the former truncation. Thus the interaction between bands may not be so well reproduced.

Evidence for this may be seen in Fig. 2(a) which shows, relative to the yrast state ($\alpha = 0$), the energies of the first excited states with $\alpha = 0$ and 1. (We have followed the format of Ref. 6 for Fig. 2 so that we can directly compare our results with those of that reference, and we have also used κ as an energy unit for the same reason.) The solid curves are our exact results, while the dashed and dotted-dashed lines show truncations A and B, respectively. Since B emphasizes the effects of deformation we see that it is rather better than A at $\omega = 0$. However, as ω increases, A rapidly becomes the better approximation, giving the cross frequency, interaction strength, and alignments (slopes) rather well. Although the slope of approximation B is reasonable after the crossing (showing that the configuration has the correct alignment), the interaction is rather poor, presumably due to the absence of the intermediate states discussed earlier. The crossing of the $\alpha = 0$ and $\alpha = 1$ excited states is also correctly reproduced by A and not by B.

The dimensions of the aforementioned truncations are (for $\alpha = 0$) 245 for A and 273 for B, compared with 1519 for the exact calculation. Thus the better results of A are produced with fewer basis states! The deformation used in the aforementioned calculations is rather large relative to the pairing force, and has been taken in order to compare our results with those of Ref. 6. We have also performed our calculations for a more reasonable[3] ratio of

pairing to deformation forces, corresponding to $G/\kappa=0.21$. The results for the first $\alpha=0$ excited states are shown in Fig. 2(b) and are seen to be equally as good as those in Fig. 2(a).

In conclusion, we note that it is essential to retain some high-energy stretched configurations in order to describe correctly the interactions between crossing bands. It should also be noted that the vanishing of this interaction for certain diabolic points[9] should cause the pair transfer matrix elements $\langle n+2|A^{+}|n\rangle$ to oscillate.[10,11] It was shown in Ref. 8 that for small deformations the interaction strength is well described in the J_x scheme by the inclusion of very few stretched basis states. It was further shown that the diabolic points and oscillating transfer matrix elements existed for all deformations. The absence of such oscillations in the results of Ref. 6 is further evidence that interactions are not being correctly treated in that approach.

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