Phonon and multi-phonon excitations in rotational nuclei by exact diagonalization of the Bohr Hamiltonian

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Abstract

Exact numerical diagonalization of the Bohr Hamiltonian by SU(1, 1) × SO(5) methods is used to obtain detailed quantitative predictions for single-phonon and multi-phonon excitations in well-deformed rotor nuclei. Dynamical γ deformation is found to significantly influence the predictions through its coupling to the rotational motion. Basic signatures for the onset of rigid triaxial deformation are obtained.

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The Bohr collective Hamiltonian has served as a conceptual benchmark for the interpretation of quadrupole collective dynamics in nuclei for several decades [1, 2]. A tractable scheme for numerical diagonalization of the Bohr Hamiltonian, the algebraic collective model (ACM) [3–7], has recently been proposed, based on SU(1, 1) × SO(5) algebraic methods. The need for such an approach arises since the conventional approach to numerical diagonalization of the Bohr Hamiltonian, in a five-dimensional oscillator basis [8–10], is slowly convergent and requires a large number of basis states to describe a general deformed rotor-vibrator nucleus. Consequently, it has been necessary to apply varying degrees of approximation in addressing the dynamics of transitional and deformed nuclei, as in the classical rotation-vibration model [11] and rigid triaxial rotor [12] treatments of the Bohr Hamiltonian, or in more recent studies of critical phenomena [13–16].

The ACM scheme, in conjunction with recent progress in construction of the relevant SO(5) ⊃ SO(3) Clebsch-Gordan coefficients [7], now permits the diagonalization of the Bohr Hamiltonian for potentials of essentially arbitrary stiffness, as considered in this letter. The Bohr Hamiltonian can consequently be applied, without approximation, to the full range of nuclear quadrupole rotational-vibrational structure, from spherical oscillator to axial rotor to triaxial rotor. Specifically, the direct product basis obtained from an optimally chosen set of SU(1, 1) β wave functions [17] and the SO(5) ⊃ SO(3) spherical harmonics $\Psi_{\text{SO}(3)}(\gamma, \Omega)$ [4] provides an exceedingly efficient basis for numerical solution of the Bohr Hamiltonian [5]. For application to transitional and deformed nuclei, the method yields order-of-magnitude reductions in the basis size needed for convergence, as compared to diagonalization in a five-dimensional oscillator basis. The SU(1, 1) × SO(5) algebraic structure of the basis facilitates construction of matrix elements for a wide variety of potential and kinetic energy operators.

In this letter, detailed quantitative predictions for single-phonon and multi-phonon excitations in deformed rotor nuclei are established by exact numerical diagonalization of the Bohr Hamiltonian, making use of newly-calculated SO(5) ⊃ SO(3) Clebsch-Gordan coefficients [7]. In the past, interpretation of rotational phonon states within the Bohr description has largely been at a schematic level (e.g., Refs. [18–22]): adiabatic separation of the rotational and vibrational degrees of freedom is assumed, the β and γ excitations are taken to be harmonic, and phonon selection rules are assumed for electric quadrupole transitions. These predictions are then adjusted by spin-dependent band mixing [23] with ad hoc mixing parameters. Here, instead, we explore the actual predictions of the Bohr Hamiltonian. The signatures for the onset of rigid triaxial deformation within the Bohr framework are also considered. Preliminary results were presented in Ref. [24].

The Bohr Hamiltonian [2] is given, in terms of the quadrupole deformation variables β and γ and Euler angles Ω, by

$$H = \frac{\hbar^2}{2B} \left[ \frac{1}{\beta^2} \frac{\partial^2}{\partial \beta^2} + \frac{1}{\gamma^2} \frac{\partial^2}{\partial \gamma^2} + \frac{\hat{\Lambda}^2}{\beta^2} \right] + V(\beta, \gamma),$$

(1)

where $\hat{\Lambda}^2$ is the angular ($\gamma, \Omega$) part of the Laplacian in five dimensions. The essential aspect of the present ACM solutions is that the angular degrees of freedom are treated in full, including dynamical γ deformation and its coupling to the rotational motion. In the context of small-oscillation approximations for γ (e.g., Ref. [2, 13]), the γ dependence of the potential is simply taken as $\propto \gamma^2$, but for solution of the full problem the γ dependence must be defined more completely. From the symmetry properties of a quadrupole-deformed nucleus [10], the potential energy $V(\beta, \gamma)$ must be periodic in γ (with period 120°), and it must be symmetric about $\gamma = 0°$ and $\gamma = 60°$. The simplest potential of this form, with minimum at $\gamma = 0°$, is $V(\gamma) \propto (1 - \cos 3\gamma)$ [3], as shown in Fig. 1(a,inset).

Let us first consider a problem proposed by Iachello [14], with Hamiltonian

$$H = \hat{\Lambda}^2 + \chi ((1 - \cos 3\gamma) + \xi \cos^2 3\gamma).$$

(2)
Only the angular variables $(\gamma, \Omega)$ are considered, with $\beta$ held fixed [25]. The possible forms of the potential $V(\gamma)$ and the results of illustrative calculations are shown in Fig. 1. For $\xi = 0$, a simple $(1 - \cos 3\gamma)$ potential is obtained [Fig. 1(a)], approximately harmonic (locally $\propto \gamma^2$) around $\gamma = 0^\circ$. For $\xi = 1/2$, the potential is more softly confining in $\gamma$, with a quartic minimum ($\propto \gamma^4$) at $\gamma = 0^\circ$ [Fig. 1(b)]. This case is termed “critical” in Ref. [14]. For $\xi > 1/2$, the potential has a minimum at some nonzero value of $\gamma$, given by $\cos 3\gamma_0 = 1/(2\xi)$ [Fig. 1(c)]. The basis functions for the diagonalization consist simply of the $SO(5) \supset SO(3)$ spherical harmonics $\Psi_{\alpha L \mu \nu}(\gamma, \Omega)$. The matrix elements of physical operators with respect to this basis, both for the Hamiltonian and for electromagnetic transitions, can be computed directly from the $SO(5) \supset SO(3)$ Clebsch-Gordan coefficients [4, 7, 26]. Seniority quantum numbers $v \leq 50$ amply suffice for convergence of the calculations shown.

The nature of the spectrum obtained depends both on the shape of the potential (determined by $\xi$) and on the depth of the potential (determined by $\chi$). The low-lying states form quasi-bands which may be roughly identified with the $\gamma$ vibrational excitation ($K = 2$) and two-phonon $\gamma$ excitations ($K = 0$ and 4). For each calculation in Fig. 1, $\chi$ is chosen to give $E(2^+_\gamma)/E(2^+_1) \approx 10$, appropriate to the well-deformed rare earth nuclei. Principal spectroscopic properties considered here include the band energies, the detailed level spacings within the bands, and the interband electric quadrupole transition strengths.

With the onset of triaxiality (increasing $\xi$), the two-phonon energy anharmonicities evolve from slightly negative ($E_{\gamma\gamma}/E_\gamma < 2$) for $\xi = 0$ [Fig. 1(a)] to positive ($E_{\gamma\gamma}/E_\gamma > 2$) [Fig. 1(c)]. The anharmonicity of the excited $K = 0$ quasi-band rises more rapidly than that of the $K = 4$ quasi-band. Qualitatively, this is consistent with evolution towards a $\gamma$-stiff, adiabatic triaxial rotor [26, 27], for which the $K = 4$ quasi-band is a triaxial rotational excitation and the $K = 0$ quasi-band is a $\gamma$ vibrational excitation.

It is essential to observe that the stiffness of the potential around its minimum in $\gamma$ determines not only the $\gamma$ vibrational energy scale but also how well confined the wave function is with respect to $\gamma$. Thus, within the framework of the Bohr Hamiltonian, the $\gamma$ band energy [more specifically, the energy ratio $E(2^+_\gamma)/E(2^+_1)$, or separation of vibrational and rotational energy scales] and the $\gamma$ softness of the wave function are inextricably linked. From Fig. 1(a,inset), it is seen that for $E(2^+_\gamma)/E(2^+_1) \approx 10$ the $\gamma$ confinement is weak, and that the range of energetically accessible $\gamma$ values increases significantly for successive phonon excitations. Confinement is almost nonexistent at the energy of the two-phonon excitations.

Consequently, dynamical $\gamma$ deformation plays a major role in the calculated structure, as reflected in significant deviations from ideal rotational behavior in the spectroscopic predictions. Level energies within the $\gamma$ quasi-band [Fig. 1(a)] follow a gently $\gamma$-soft staggering pattern $[2(34)(56) \ldots]$. (The relation between the $\gamma$ excitation energy and residual level energy staggering was noted for transitional nuclei in Ref. [28].) The deviations are even more pronounced for the two-phonon quasi-bands. Note especially the near doubling of the rotational constant, or rotational energy spacing scale, for the two-phonon excitations.
bands relative to the ground state band.

With increasing $\xi$, the level energies within the $\gamma$ band progress from $\gamma$-soft staggering to the pattern associated with triaxial rotation [(23)(45)…] [12]. This may be seen most clearly from plots of the level energy second difference $S(L) \equiv [(E(L) - E(L-1)) - (E(L-1) - E(L-2))]/E(2^+_1)$ [Fig. 1(d-f)], which has minima at even $L$ for $\gamma$-soft staggering and at odd $L$ for triaxial staggering. As surveyed in Ref. [29], the data for most rotational nuclei yield $S(L)$ plots which are either $\gamma$-soft [Fig. 1(d)] or near-constant [Fig. 1(e)].

The relation between $\gamma$ softness and spectroscopic properties is more systematically and quantitatively examined in Fig. 2. For Hamiltonian (2), at fixed $\xi$, the parameter $\chi$ controls the depth and hence $\gamma$ softness of the potential. The evolution of energy and transition strength prediction with respect to $\chi$ is shown in Fig. 2 for the pure $V(\gamma) \propto (1 - \cos 3\gamma)$ potential ($\xi = 0$). Note especially the correlation between the $\gamma$ band energy [Fig. 2(b)] and the ground state band energy ratio $E(4^+_1)/E(2^+_1)$ [Fig. 2(a)], which varies from 2.5 for $\gamma$-soft rotation to 3.33 for rigid axial rotation. This ratio is commonly taken as an indicator of rotational adiabaticity. (The quantitative details are affected also by the $B$ degree of freedom.) The evolution of $\gamma$-soft band energies, approaching harmonicity for large $\gamma$, can also be traced in Fig. 2. The electric quadrupole branching ratios, shown for the $2^+_1$ state in Fig. 2(c), approach the Alaga rule ratios [30] of the adiabatic axial rotor, but only slowly, as the $\gamma$ softness increases.

The phenomenological analysis of electromagnetic transition strengths in rotational nuclei is founded upon the reduction of these strengths to a single intrinsic electromagnetic matrix element and single mixing parameter between each pair of bands, according to the Mikhailov mixing formalism [23]. Within this framework, all transition amplitudes fall on a straight line on an appropriate (Mikhailov) plot, and the intrinsic matrix elements and mixing parameter are identified from the slope and intercept [2, Sec. 4-4]. The electric quadrupole transition strengths for the fully-converged Bohr Hamiltonian calculations described above (Fig. 1) are shown in Mikhailov form in Fig. 3. Deviations from linearity are significant for transitions involving the two-phonon excitations in the $\xi = 0$ calculation [Fig. 3(d)], as might be expected from the substantial $\gamma$ softness already noted. Otherwise the transition amplitudes at least approximately follow an essentially linear pattern. It is therefore meaningful to extract effective intrinsic matrix elements and mixing parameters for comparison with experiment. The matrix elements for the $\gamma \rightarrow g$ transitions and for the $\gamma \gamma \rightarrow \gamma$ transitions (relative to $\gamma \rightarrow g$) are listed in Table 1. The adiabatic harmonic values [27] and a previous estimate [Y(5)] for the “critical” ($\xi = 0.5$) case [14] are shown for comparison.

![Figure 2: Evolution of spectroscopic properties with $\gamma$ softness for the angular Hamiltonian (2), for a purely axial potential ($\xi = 0$). Quantities shown are (a) the energy ratio $E(4^+_1)/E(2^+_1)$, (b) excitation energies of low-lying levels, normalized to $E(2^+_1)$, and (c) electric quadrupole transition strengths from the quasi-$\gamma$ band head to the ground band members, normalized to $B(E2; 2^+_1 \rightarrow 0^+_1)$.](image)

![Figure 3: Intersband transition amplitudes, from the $\gamma$ quasi-band to the ground state band (top) and from the $K = 4$ $\gamma \gamma$ quasi-band to the $\gamma$ quasi-band (bottom), in Mikhailov form. Values are shown for the calculations of Fig. 1, with $\xi = 0$ ($\chi = 50$) (left), $\xi = 0.5$ ($\chi = 100$) (middle), and $\xi = 0.8$ ($\chi = 500$) (right). The values shown are for transitions between levels with $L \leq 6$, normalized to $B(E2; 2^+_1 \rightarrow 0^+_1) \equiv 1$.](image)

| Harmonic | $\xi = 0$ ($\chi = 50$) | $\xi = 0.5$ ($\chi = 100$) | $\xi = 0.8$ ($\chi = 500$) |
|----------|------------------------|------------------------|------------------------|
| $^{162}$Dy | 0.241(3) | 0.99(3) | 0.54(3)* |

*For the $K^\pi = 0^+$ excitation at 1400 keV excitation energy.

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Table 1: Effective intersband intrinsic matrix elements, as extracted from the calculations of Fig. 3. The harmonic axial [27] and Y(5) triaxial [14] estimates are included for comparison, along with the experimental values for $^{162}$Dy [31].

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For the $K^\pi = 0^+$ excitation at 1400 keV excitation energy.
The nucleus $^{162}$Dy has recently been the subject of detailed spectroscopic study by Aprahamian et al. [31], yielding extensive sets of experimental values for interband electric transition strengths. The experimental intrinsic matrix elements are given in Table 1. The $\gamma$ band and candidate two-phonon $\gamma$ band energies for $^{162}$Dy closely match those of the $\xi = 0$ ($\chi = 50$) calculation of Fig. 1(a). The measured $\gamma \rightarrow g$ strength is about a factor of two lower than the Bohr Hamiltonian predictions, and the $K = 4 \gamma \gamma \rightarrow \gamma$ strength is yet a factor of two lower again, i.e., even taken relative to this already reduced $\gamma \rightarrow g$ strength. Moreover, the observed level energies in $^{162}$Dy [31] conform much more closely to adiabatic rotational $L(L + 1)$ spacings than expected from the Bohr Hamiltonian calculation [Fig. 1(a)]. Although we do not include a detailed quantitative analysis here, for the $\gamma$ band staggering, compare Fig. 3(d) of Ref. [29] with the present Fig. 1(d). The excited bands in $^{162}$Dy are actually observed to exhibit decreased rotational constants, relative to the ground state band, in stark contrast to the present calculation (a similar discrepancy is noted [20] in comparison of interacting boson model [32] predictions with data). A more detailed comparison requires exploration of the interaction of the $\beta$ and $\gamma$ degrees of freedom.

Let us briefly examine the results of a calculation involving the full dynamics of the Bohr Hamiltonian (1), including the $\beta$ degree of freedom. An essentially unlimited variety of combined $\beta$ and $\gamma$ dependences (e.g., $\beta^n \cos^m 3\gamma$) may be used in the ACM potential [26]. For illustration, we consider a Davidson potential for $\beta$ [Fig. 4(a, inset)], together with the simplest ax-

$E_{\text{b}}(l) = (l^2 + l)^{1/2} \frac{\hbar^2}{2B}$

$E_{\text{b}}(l) \propto (\beta_0/\beta - \beta/\beta_0)^2 + \chi(1 - \cos 3\gamma)$. Without loss of generality, we may take the proportionality constant and the inertial constant $\hbar^2/(2B)$ to be unity, if only energy and $E_2$ strength ratios are to be considered [33]. This leaves freedom only in the $\beta$ stiffness ($\beta_0$) and $\gamma$ stiffness ($\chi$). A fully converged ACM calculation, for $\beta_0 = 3$ and $\chi = 5$, is shown in Fig. 4(a), with quasi-band assignments indicated. Fewer than five SU(1, 1) basis functions are required for convergence. Electric quadrupole transitions connecting the ground, $\beta$, and $\gamma$ bands are shown in Fig. 4(b–d). The zero in the Mikhailov plot for the $\beta \rightarrow \gamma$ transitions [Fig. 4(d)] reflects the zero expected [at $L_2(L_2 + 1) - L_1(L_1 + 1) = 4$] if simple phonon selection rules hold on the intrinsic matrix elements (see Fig. 12 of Ref. [34]).

The possibility of exact diagonalization of the Bohr Hamiltonian for essentially arbitrary $\beta$ and $\gamma$ stiffness, by means of the algebraic collective model, opens the door for direct comparison of the Bohr Hamiltonian predictions with experiment throughout the range of possible dynamics for the nuclear quadrupole degree of freedom. At a phenomenological level, this permits meaningful tests of the Bohr Hamiltonian for general rotor-vibrator nuclei. More fundamentally, in the context of nuclear many-body theory, it is essential to know the limitations and necessary modifications to the Bohr framework, since microscopic descriptions of nuclear collectivity rely upon a reduction of the many-body problem to one involving effective collective degrees of freedom, typically those of the Bohr description [35, 36] or its symplectic generalization [37].

Notably, these preliminary results suggest that the Bohr description quantitatively overpredicts and even qualitatively mispredicts the nature of deviations from adiabatic rotational structure, and that these deviations result from dynamical $\gamma$ softness inherently incorporated into the description. The Bohr description also strongly overpredicts $\gamma$ phonon interband transition strengths (although this could already be anticipated from, e.g., rotation-vibration model estimates). A basic question is therefore the extent to which the discrepancies lie in the details of the description (e.g., restriction of the kinetic energy operator to quadratic order in the momenta) or in a fundamental failure of the collective quadrupole degree of freedom to account for the observed phenomena.

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