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LETTER TO THE EDITOR

Monodromy and excited-state quantum phase transitions in integrable systems: collective vibrations of nuclei

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Abstract

Quantum phase transitions affecting the structure of ground and excited states of integrable systems with the Mexican-hat type potential are shown to be related to a singular torus of classical orbits passing the point of unstable equilibrium. As a specific example, we consider nuclear collective vibrations described by the $O(6)$ – $U(5)$ transitional Hamiltonian of the interacting boson model. While all states with zero values of the $O(5)$ invariant undergo a continuous phase transition when crossing the energy of unstable equilibrium, the other states evolve in an analytic way.

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Motions of a classical integrable system with n degrees of freedom in the phase space stick onto surfaces that are topologically equivalent to $2n$ -dimensional tori. It is generally thought that this feature results in a fully analytic expressibility of observables for integrable systems. However, in some cases the analyticity cannot be maintained in the global sense. A common obstacle for $n = 2$ is monodromy [1], related to the existence of an anomalous, so-called pinched torus of orbits. Most usually, the pinched torus originates from a singular point of unstable equilibrium of the focus–focus type and is connected with a class of trajectories with period $\tau \rightarrow \infty$ if the energy crosses a certain critical value E_{mon} . The presence of such orbits in the phase space also affects the quantum spectrum, producing a ‘crystal defect’ in the joint spectrum of commuting operators [2].

One of the systems with monodromy is the spherical pendulum [3]. Here, the pinched torus is formed by orbits passing the upper point with just the energy needed for equilibration. Classical motions with zero value of the conserved angular momentum L_z undergo a qualitative

change and the corresponding quantum lattice in the joint spectrum has a defect at $E = E_{\text{mon}}$ and the L_z quantum number $m = 0$. The parts of the lattice below and above E_{mon} are characterized by nearly degenerate multiplets of states with the same vibrational and rotational quantum numbers, respectively, and both types of multiplets fail to smoothly extend across the monodromy point to the other domain.

Another example of monodromy follows from the Mexican-hat potential $V \propto r^4 - r^2$ with $r^2 = x^2 + y^2$ [4]. The local maximum at $r = 0$ corresponds to an unstable equilibrium with $E_{\text{mon}} = 0$, which results in a pinched torus of $L_z = 0$ orbits. Crossing the critical energy induces a transition between two types of $L_z = 0$ motions, the first type confined within the annulus $r \in [r_{\text{min}}, r_{\text{max}}]$, and the second one traversing across a compact region $r \in [0, r_{\text{max}}]$. Also the joint spectrum shows a crossover between multiplets characterized by the radial quantum number n_{rad} (below E_{mon}) and those labelled by the principal quantum number $2n_{\text{rad}} + m$ (above E_{mon}) [4].

These effects are reminiscent of another interesting class of phenomena—quantum phase transitions (QPTs). These are usually introduced as nonanalytic (in the thermodynamic limit) changes of system's ground-state properties with external parameters [5, 6]. Here, the concept will be extended also to excited states. The first-order or a continuous QPT, respectively, for the i th state is defined as the discontinuity of the first derivative or a more subtle nonanalyticity in the dependence of excitation energy E_i on a control parameter η . It is related to a nonanalytic evolution of the respective wavefunction $|\psi_i\rangle$. The aim of this letter is to show that monodromy and excited-state QPTs in integrable systems are closely related. This is exemplified by quadrupole vibrations of atomic nuclei in the so-called γ -soft regime [7, 8].

Recall that simplified models of nuclear collective motions take into account only the degrees of freedom corresponding to quadrupole deformations [7]. The quadrupole tensor α is characterized by five parameters, two of them describing the deformed shape and the other three its orientation. A pair of deformation parameters can be constructed from the only two independent scalar combinations of α , namely $[\alpha \times \alpha]^{(0)} = \beta^2/\sqrt{5}$ and $[[\alpha \times \alpha]^{(2)} \times \alpha]^{(0)} = -\sqrt{2/35}\beta^3 \cos 3\gamma$, where $[\bullet \times \bullet]^{(\lambda)}$ stands for coupling of the quantities involved to angular momentum λ . Variables $\beta \in [0, \infty)$ and $\gamma \in [0, 2\pi)$ represent Bohr deformation parameters [7], which can be visualized as polar coordinates in the plane $x \times y$. The radius β measures the overall deformation, while the angle γ characterizes the deformed shape type, orientation in the principal frame, and the degree of triaxiality.

The collective Hamiltonian can be written as

$$H = T_{\text{rot}} + T_{\text{vib}} + A\beta^2 + B\beta^3 \cos 3\gamma + C\beta^4 + \dots, \quad (1)$$

where T_{rot} and $T_{\text{vib}} = K\pi^2 + \dots$ [with $\pi^2 = \pi_x^2 + \pi_y^2 = \pi_\beta^2 + (\pi_\gamma/\beta)^2$] stand for the rotational and vibrational kinetic energies (π_i denotes the momentum canonically conjugated to coordinate i). $\{K, A, B, C, \dots\}$ is a set of external parameters ($K, C > 0$). Here, we included only the lowest order vibrational kinetic terms and the potential energy up to the quartic term.

If Hamiltonian (1) does not depend on γ (i.e., is ' γ -soft'), it is integrable. In the following, we will deal with motions at zero angular momentum J , thus $T_{\text{rot}} = 0$, when the system has just two vibrational degrees of freedom and in the γ -soft case yields two commuting integrals of motions—energy E and momentum $\pi_\gamma = x\pi_y - y\pi_x$ (analogue of L_z). Without the higher order terms and for $B = 0$, $A < 0$ the potential energy in equation (1) represents the Mexican-hat potential that leads to monodromy at $E = \pi_\gamma = 0$.

It is known [9] that Hamiltonian (1) exhibits the ground-state QPT from deformed ($\beta_0 > 0$) to spherical ($\beta_0 = 0$) equilibrium shape at $A_c = B^2/4C$. For $B = 0$ we have $A_c = 0$ and the transition is continuous (of second order in the Ehrenfest classification). In this case, the

QPT is realized within an integrable domain with monodromy. Note that the $B = 0$, $A < 0$ half-line itself demarcates the first-order QPT between prolate ($\gamma_0 = 0$, $B < 0$) and oblate ($\gamma_0 = \pi/3$, $B > 0$) shapes, so the second-order transition lies in the intersection of three first-order phase separatrices [10].

Specific realization of Hamiltonian (1) can be achieved within the interacting boson model (IBM) [11]. The model, formulated in terms of s and d -bosons (with angular momenta 0 and 2), exploits the decompositions of dynamical algebra $U(6)$ into chains of subalgebras terminating at the symmetry algebra $O(3)$. Three such chains, called after the highest subalgebra $U(5)$, $O(6)$ and $SU(3)$ define dynamical symmetry limits (if the Hamiltonian is composed of invariants of the respective chain), while transitional Hamiltonians are located within a ‘triangle’ between these limits. In the dynamical-symmetry cases the model is integrable, and this property is preserved also along the transition between $O(6)$ and $U(5)$, where the underlying $O(5)$ symmetry results in conserved quantum number ν called seniority [12].

In the following, we will consider a simplified $O(6)$ – $U(5)$ transitional Hamiltonian given by

$$H^{(\eta)} = \eta \frac{n_d}{N} - (1 - \eta) \frac{Q \cdot Q}{N^2}, \quad (2)$$

where N stands for the total number of bosons, $n_d = d^\dagger \cdot \tilde{d}$ for the d -boson number operator and $Q = d^\dagger s + s^\dagger \tilde{d}$ for the quadrupole operator. Note that the dot represents scalar coupling and $\tilde{d}_\mu = (-)^\mu d_{-\mu}$. For Hamiltonian (2) the $O(6)$ dynamical symmetry is located at $\eta = 0$ and $U(5)$ at $\eta = 1$. Using Glauber coherent states $|\alpha\rangle \propto \exp(\alpha_s s^\dagger + \sum_\mu \alpha_\mu d_\mu^\dagger)|0\rangle$ (where α_s can be eliminated by fixing the average of N and the global phase) [13], one can rewrite Hamiltonian (2) in the form (1) with $B = 0$:

$$H_{\text{clas}}^{(\eta)} = T_{\text{rot}}^{(\eta)} + \frac{\eta}{2} \pi^2 + (1 - \eta) \beta^2 \pi^2 + \frac{5\eta - 4}{2} \beta^2 + (1 - \eta) \beta^4. \quad (3)$$

Since the role of \hbar is played by N^{-1} , the classical limit is attained for $N \rightarrow \infty$. Moreover, in the $J = 0$ case ($T_{\text{rot}} = 0$), due to the coherent-state relation $C_2^{O(5)}/N^2 \mapsto \pi_\gamma^2$, where $C_2^{O(5)} = n_d(n_d + 3) - (d^\dagger \cdot d^\dagger)(\tilde{d} \cdot \tilde{d})$ is the $O(5)$ invariant with eigenvalues $\nu(\nu + 3)$, the momentum π_γ can be (for $N \rightarrow \infty$) associated with relative seniority $\delta = \nu/N$ (where $\nu = 0, 3, 6, \dots \leq N$ for $J = 0$).

It is clear from equation (3) that a continuous QPT between $O(6)$ - and $U(5)$ -like ground-state configurations happens at $\eta_c = 4/5$, where the potential changes from the Mexican-hat shape to a quartic oscillator. Note, however, that the IBM shows some specific differences from these standard potential systems: first, due to boundedness of Hamiltonian (2) the physical domain is restricted to $\beta \in [0, \sqrt{2}]$, $\pi_\beta \in [0, \sqrt{2}]$ and $\pi_\gamma \in [0, 1]$. Second, equation (3) also contains an unusual kinetic term $\propto \beta^2 \pi^2$. Third, for $J = 0$ the quantum grid of states in E versus ν differs from the standard E versus m grid associated with the given potential; this results from inherent differences between the $O(5)$ - and $O(2)$ -based angular momenta.

Figure 1 illustrates classical monodromy of Hamiltonian (3) at absolute energy $E_{\text{mon}} = 0$ for $\eta < 4/5$. The Poincaré phase-space section shows crossings of 30 orbits of $\pi_\gamma > 0$ with the plane $\beta \times \pi_\beta$. The $\pi_\gamma = 0$ orbits passing asymptotically the point $\beta = 0$ form the pinched torus, whose section corresponds to the cusped enveloping curve of the filled area. The surface of the pinched torus, nonanalytic at $\beta = 0$, interpolates between two distinct types of analytic $\pi_\gamma = 0$ tori at lower and higher energies. This results in a nonanalytic growth of the available phase-space volume $\Omega(E) = \int \delta(H - E) d\pi_x d\pi_y dx dy$ at $E = E_{\text{mon}}$. In particular,

$$\Omega(E) = 4\pi \int_{\beta_{\text{min}}(E)}^{\beta_{\text{max}}(E)} \pi_\beta(E, \beta, \pi_\gamma = 0) \beta d\beta, \quad (4)$$

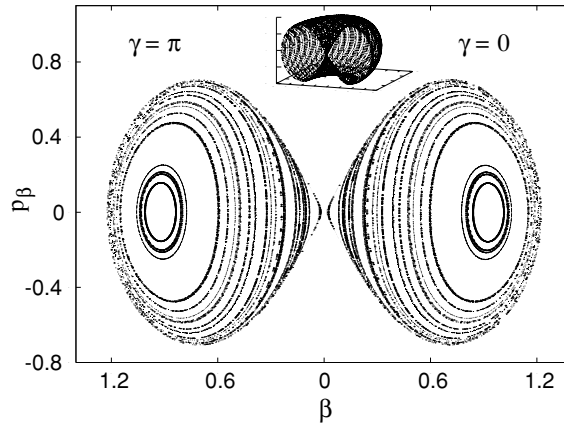


Figure 1. Poincaré phase-space section associated with Hamiltonian (3) at $E = 0$ and $\eta = 0.6$ and the enveloping pinched torus of $\pi_\gamma = 0$ orbits (inset).

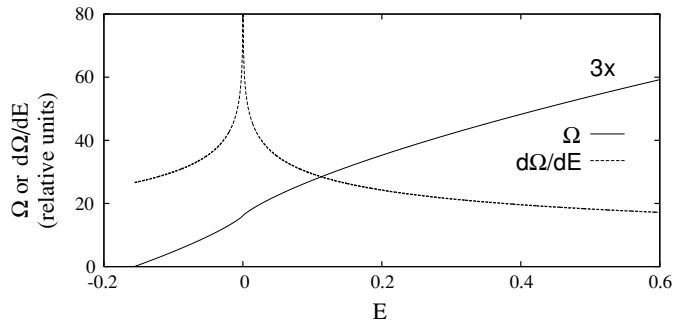


Figure 2. The available phase-space volume (4) and its first derivative at $\eta = 0.6$.

where π_β as well as β_{\min} and β_{\max} are evaluated from equation (3), has a singular tangent at zero energy, as shown in figure 2. Note that $\Omega(E)$ is related to the smooth part of the quantum density of states $\rho(E) = \text{Tr} \delta(H - E)$; the oscillatory part depends on properties of periodic orbits (also singular at E_{mon} [8]) and is not discussed here.

Features of Hamiltonians (2) and (3) related to the anomalous behaviour at E_{mon} were recently analysed in [8]. It was shown that monodromy is correlated with two important dynamical effects: (i) on the classical level, trajectories with predominantly large values of the ratio $R = \tau_\gamma/\tau_\beta$ of β - and γ -vibration periods transform to those within a narrow band above $R = 2$. While values $R \gg 2$ observed for $E < E_{\text{mon}}$ correspond to zig-zag orbits inside the accessible annular region in the $x \times y$ plane, the value $R \approx 2$ valid for $E > E_{\text{mon}}$ is connected with ‘bouncing-ball’ orbits traversing through the central region. In particular, the $\pi_\gamma = 0$ trajectories undergo a discontinuous change from $R = \infty$ to $R = 2$. (ii) On the quantum level it was shown that $O(6)$ - and $U(5)$ -like types of elementary cells in the E versus ν lattice of $J = 0$ quantum states exist in energy domains below and above E_{mon} , respectively, i.e., interchange at about the monodromy energy. This is accompanied by degeneracy of levels with different seniorities and by coherent patterns of avoided crossings of levels with the same seniority, both at energy $E \approx E_{\text{mon}}$.

To show that these structures correspond to QPT evolutions of excited states with zero seniority, we invoke an oscillator approximation recently discussed by Rowe [14]. The method is valid on the $O(6)$ side of the transition for finite seniorities and asymptotic boson numbers, when $x = 2n_d/N - 1$ can be treated as a continuous variable. Eigenstates $|\psi_i\rangle$ are expressed as conventional wavefunctions $\psi_i(x) \equiv \langle n_d | \psi_i \rangle$ and the scaled Hamiltonian $H^{(\eta)}/(1 - \eta)$ from equation (2) turns into a differential operator

$$-\frac{4}{N^2} \frac{d}{dx} (1 - x^2) \frac{d}{dx} + \left[x - \frac{\eta}{4(\eta - 1)} \right]^2 - \left[\frac{5\eta - 4}{4(1 - \eta)} \right]^2, \quad (5)$$

where the use is made [14] of the fact that Hamiltonian (2) only connects states with $\Delta n_d = 0 \pm 2$ and is therefore local in x for $N \rightarrow \infty$. The last expression, after neglecting $\mathcal{O}(N^{-1})$ and higher terms, reduces to a quantum oscillator with variable centroid position and energy shift, and with an x -dependent mass. (The latter feature was not discussed in [14] and can be neglected for $x \approx 0$.) Therefore, the $O(6)$ quasi-dynamical symmetry extends away from $\eta = 0$ through an analytic transformation of eigensolutions.

However, the analytic extension is limited to the range of η where the semiclassical wavefunction is located within the physical domain $n_d \in [0, N]$, thus $x \in [-1, +1] \equiv [x_{\min}, x_{\max}]$. Once the classical turning points of the oscillator particle reach these bounds, expression (5) is no longer applicable for the given state. This happens when the actual level energy E_i crosses the value of the oscillator potential energy at the lower edge, $V_{\text{osc}}^{(\eta)}(x_{\min}) = 0$, i.e., just when $E_i = E_{\text{mon}}$. At this point, the probability distribution $P(x) \propto \dot{x}^{-1}$ (where \dot{x} stands for the velocity of the oscillator particle) becomes singular since the mass diverges for $x = \pm 1$ and the particle spends infinite time in an infinitesimal vicinity of x_{\min} . An equivalent conclusion follows from the classical Hamiltonian (3), which for $E = E_{\text{mon}}$ yields a singular concentration of the probability distribution $P(\beta) \propto \dot{\beta}^{-1}$ at $\beta = 0$. As the analytic extension of $\eta = 0$ semiclassical wavefunction cannot pass over the singularity, the parameter range is split into two disconnected branches, which can be named quasi- $O(6)$ and quasi- $U(5)$.

The ground-state energy E_0 crosses E_{mon} at $\eta_c = 4/5$. For the other $v = 0$ states with increasing excitation energy, the crossings form a descending sequence of points within the interval $\eta \in (0, \eta_c)$. These are positions of excited-state QPTs where individual eigenfunctions $|\psi_i\rangle$ and energies E_i evolve in a nonanalytic way. Note that for Hamiltonian (2), which has the form $H^{(0)} + \eta V$, the relation $dE_i/d\eta = \langle \psi_i | V | \psi_i \rangle$ transmits nonanalytic behaviours of wavefunctions to level energies. Since $\langle \psi_i | V | \psi_i \rangle$ itself changes in a continuous way, the QPT for excited states is—like the one for the ground state—continuous. The present analysis, however, does not allow one to specify the type of nonanalyticity for $i > 0$.

Finite- N precursors of excited-state QPTs are shown in figure 3, where we display $J = v = 0$ level dynamics and two examples of wavefunctions (n_d -distributions) for $N = 80$. Wavefunctions for $E_i < 0$ are approximate eigenstates of the oscillator Hamiltonian (5). They reach the $n_d = 0$ edge just when passing $E = 0$ (the region with multiple avoided crossings) where the validity of the quasi- $O(6)$ description for the given level ends. At the transition, the slope of individual energy curves tends to vanish, in agreement with the fact that $\langle \psi_i | V | \psi_i \rangle = 0$ at $E_i = E_{\text{mon}}$ for $N \rightarrow \infty$. The $E_i > 0$ branch of wavefunction is analytically connected to the $U(5)$ limit.

Formula (5) is valid only if $\delta = v/N \rightarrow 0$ in the classical limit, i.e., for $v \approx 0$ in finite- N approximations. Therefore, a question appears what happens to states with $\delta \in [0, 1]$. The answer can be obtained from equation (3) that allows one to extract an effective potential corresponding to the fixed value $\pi_\gamma = \delta$:

$$V_{\text{eff}}^{(\eta, \delta)}(\beta) = \frac{\eta \delta^2}{2} \frac{1}{\beta^2} + (1 - \eta) \delta^2 + \frac{5\eta - 4}{2} \beta^2 + (1 - \eta) \beta^4. \quad (6)$$

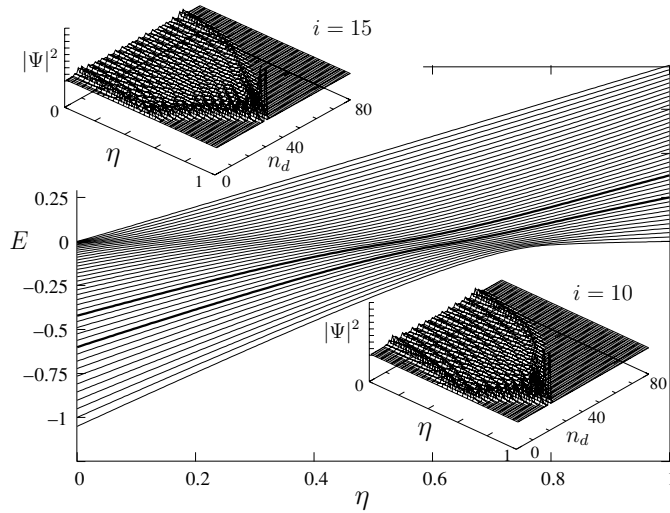


Figure 3. The evolution of $v = 0$ level energies between $O(6)$ and $U(5)$ limits and the n_d -distributions for the 10th and 15th excited states (thicker curves); $N = 80$.

This expression contains, besides the standard potential terms of Hamiltonian (3), also a constant shift and a centrifugal term $\propto \beta^{-2}$ resulting from the fixed value of π_γ . The centrifugal term keeps the solutions with $\delta \neq 0$ away from $\beta = 0$ (in agreement with the fact that minimal n_d for a given v is equal to v [11]) and destroys the Mexican-hat shape of the potential for states with nonzero seniority. Does the phase-transitional evolution survive under these circumstances?

The minimum β_0 of V_{eff} interpolates between $\beta_0 = 1$ at $\eta = 0$ and $\beta_0 = \sqrt{\delta}$ at $\eta = 1$. As we know, for $\delta = 0$ the minimum has a discontinuous derivative $d\beta_0/d\eta$ at $\eta_c = 4/5$ which leads to a jump in the second derivative of the V_{eff} minimal value. On the other hand, for $\delta \neq 0$ the minimum evolves in a fully analytic way, as can be seen from the fact that within $\eta \in [0, 1]$ it does not cross the border where the sign of $\partial^2 V_{\text{eff}}/\partial \beta^2$ changes (for $v = 0$ this happens at η_c). Therefore, $V_{\text{eff}}(\beta_0)$ is analytic for $\delta \neq 0$ implying that no phase transition occurs in the behaviour of the *lowest* state with $v \neq 0$. Although potential (6) itself does not allow us to predict properties of individual excited states, the above result and the absence of the central maximum in the $\delta \neq 0$ effective potential make one assume that critical behaviour dies out for *all* states with nonzero seniority. This conforms with numerical calculations of finite- N spectral properties [8] and also with classical considerations showing that only the $\pi_\gamma = 0$ trajectories change the form abruptly (at the monodromy point) as η and/or E vary. Of course, for very small v 's one still obtains rapid, though analytic structural rearrangement in the $E \approx 0$ region.

In summary, we gave an example of integrable system where monodromy triggers continuous QPT evolutions of excited-state energies and wavefunctions. It shows that the critical value of interaction parameter may depend on the excitation and that some subsets of states may not undergo the phase transition at all. In the derivation, the key role was played by the oscillator approximation (5) (for $v = 0$ states) and by the effective potential (6) (for $v \neq 0$). Links of QPT phenomena to specific motions on the classical level were found crucial. It would be interesting to learn how the above-discussed properties extend to the nonintegrable regime with $B \neq 0$.

It can be anticipated that our conclusions, apart from having particular consequences for $J = 0$ collective states in γ -soft nuclei between deformed and spherical shapes, are generic for all quantum systems with the Mexican-hat potential. In particular, recent studies [15] of the Lipkin model disclosed very similar nonanalytic structures of quantum properties correlated with the top of a double-well potential. Since the fundamental Ginzburg–Landau model [16] of spontaneous symmetry breaking is based on the same type of potential, the present results might be relevant in rather broad context.

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