Quantum phase transitions in finite algebraic systems

Pavel Cejnar
Institute of Particle and Nuclear Physics, Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, 180000 Prague, Czech Republic
E-mail: cejnar@ipnp.troja.mff.cuni.cz

Abstract. We discuss features of quantum phase transitions affecting collective dynamics of many-body systems. Due to a finite number of collective degrees of freedom, the infinite-size limit of the corresponding models coincides with the classical limit and quantum critical phenomena for both the ground and excited states are determined by the structure of the classical phase space. An example of an excited-state phase transition for the interacting boson model in its SU(3) limit is presented.

1. Introduction
Quantum phase transitions (QPTs) belong to the most interesting topics in modern quantum physics [1]. They were recognized in the 1970’s [2, 3] as abrupt changes of the ground state of some condensed-matter systems with a varying non-thermal control parameter \( \lambda \) (typically an interaction strength in the Hamiltonian). The ground-state wave functions on the two sides of the quantum critical point \( \lambda = \lambda_c \) constitute two qualitatively different types of solution which—for the system’s size increased to infinity—cannot be smoothly connected. This shows up also in a non-analytic change of the ground-state energy at the critical point.

Various types of QPT have been theoretically described and in numerous cases also experimentally realized in diverse solid-state and optical systems [1, 4, 5]. QPTs are also discussed in connection with the equilibrium shapes of atomic nuclei [3, 6] (for recent reviews see Refs. [7, 8]) and with the form of molecules and various mesoscopic systems [9]. Although nuclei and molecules as strictly finite objects can only show some faint precursors of the ideal QPT behavior, they play an important role in the development of the concept. In particular, since the models describing these systems are often formulated in an algebraic way [10, 11, 12, 13], they bring to the field descriptions based on exact symmetries and their various effective approximations [14].

In this article, we focus on QPTs in the systems with finite (moderate) numbers of degrees of freedom. In many-body physics, such finite systems (or, more precisely, finite models) are mostly used for the description of collective dynamics. The number of collective degrees of freedom of a given type (e.g., those describing quadrupole deformation of nuclei) is fixed and does not depend on the number of constituents of the many-body system (the number of nucleons). As argued below, such models and their QPTs have some specific features.

2. Finite versus infinite systems
Let us consider an algebraically based quantum model for some collective degrees of freedom. The Hilbert space of state vectors coincides with one of the irreps of a finite dynamical (spectrum
generating) algebra $\mathcal{G}$. The generators of $\mathcal{G}$, satisfying the closure relation $[G_i, G_j] = c_{ijk}G_k$ (where $c_{ijk}$ stand for structure constants), serve as building blocks for all relevant physical operators, including the Hamiltonian $H = H(G_i)$.

Assume that the model includes a parameter $\mathcal{N}$ measuring the size of the system. For instance, in the interacting boson model of nuclei as well as in the related vibron models of molecules [10, 11, 12] the size parameter can be naturally identified with the total number of bosons $N_B$. In general, it is convenient if the thermal dispersion $\langle (E^2) \rangle \equiv \langle E^2 \rangle - \langle E \rangle^2$ of the total energy grows linearly with $\mathcal{N}$ (note that $\langle (E^2) \rangle$ is proportional the total specific heat of the system). Then thermal fluctuations of the scaled energy $\mathcal{E} \equiv E/\mathcal{N}$ vanish for $\mathcal{N} \to \infty$, allowing one to properly define the thermodynamic limit with a crossover from canonical to microcanonical description.

Due to the finiteness of the dynamical group $\mathcal{G}$, the system has a finite number of degrees of freedom $f$. This number coincides with the size of a complete set of not fully degenerate commuting operators characterizing $\mathcal{G}$ [15]. The fact that $f$ does not change with $\mathcal{N}$ implies an important difference from ordinary many-body systems, in which the number of degrees of freedom grows proportionally to the number of constituents. In particular, for finite algebraic models the infinite-size limit is synonymous with the classical limit. This can be deduced from the use of scaled generators $g_i = G_i/\mathcal{N}^\kappa$ with $\kappa > 0$ defined through a consistent scaling of the Hamiltonian $H/\mathcal{N} = H(G_i/\mathcal{N}^\kappa)$. The closure relation for $G_i$ leads for $\mathcal{N} \to \infty$ to $[g_i, g_j] \to 0$. Since vanishing commutators of scaled observables constitute a classical description, we are here in a radically different situation than with a truly many-body model, for which the infinite-size limit leads to a quantum-field description.

3. Ground-state and excited-state phase transitions

The classical limit of finite collective models is standardly obtained by the coherent-state formalism [16]. There is a plethora of ways how the coherent states can be constructed for the dynamical algebra $\mathcal{G}$, the resulting classical Hamiltonians being equivalent up to some canonical transformations. One possibility is to employ a bosonic representation of $\mathcal{G}$ (Holstein-Primakoff or Schwinger type) and then use either Glauber coherent states with indefinite total boson number $N_B$, or their projection to a fixed $N_B$ (boson condensate states). It turns out that every independent boson operator $b^\dagger_k$ that appears in the representation adds one degree of freedom, the resulting number being reduced by one due to the conservation of $N_B$. The corresponding coordinate $q_k$ and momentum $p_k$ are associated with the complex coefficient in front of $b^\dagger_k$ in the respective coherent-state expression. Denoting the coherent state as $|\{p_k, q_k\}\rangle \equiv |p, q\rangle$, the classical Hamiltonian is given by

$$H_{cl}(\lambda; p, q) = \mathcal{N}^{-1}(p, q)|H(\lambda)|p, q\rangle,$$

where the scaling ensures convenient properties of $H_{cl}$ in the asymptotic domain of $\mathcal{N}$.

Any critical behavior of the ground-state energy can only be observed for $\mathcal{N} \to \infty$. It results from a non-analytic dependence of the energy minimum $E_0(\lambda) = \min_{p,q} H_{cl}(\lambda; p, q)$ on the control parameter $\lambda$ at a certain critical value $\lambda = \lambda_{cl}$. Note that the minimization of $H_{cl}$ in $p$ and $q$ can be reduced to minimization of the classical potential $V_{cl}(\lambda; q) \equiv H_{cl}(\lambda; p = 0, q)$ in $q$. Within the coherent-state formalism, $V_{cl}$ can be expressed as a power series in both $q$ and $\lambda$. This makes it possible, in finite models, to describe the ground-state QPTs analytically, using either the Landau theory of thermal phase transitions [17] or the catastrophe theory of structurally unstable systems [4].

Non-analytic dependences can also affect individual excited states [18, 19, 20]. The critical value $\lambda_{cl}$ associated with a given energy level $E_i(\lambda) = E_i(\lambda)/\mathcal{N}$ depends on the excitation index $i \geq 0$ counting the states increasingly with energy. It should be stresses that these so-called excited-state quantum phase transitions (ESQPTs) do not affect only the states in a close vicinity
of the ground state \( i = 0 \), but can be observed across the whole spectrum of quantum states or its considerable fraction. In finite models, the ESQPTs are rooted in non-analyticities connected with dynamical features of the classical Hamiltonian \( H_{cl} \). This is in contrast to the ground-state QPTs, which reflect properties of the static equilibrium.

The ESQPTs were so far mostly studied \([18, 19, 20]\) in systems with just one effective degree of freedom \((f = 1)\). Such systems provide a straightforward algorithm to analyze properties of the scaled energies \( \mathcal{E}_i(\lambda) \) as functions of the control parameter \( \lambda \) for \( \aleph \to \infty \). It follows from the familiar semiclassical quantization formula \( S(\lambda, \mathcal{E}_i) = \text{const}_i \), where \( S = \oint p \, dq \) represents the action along a closed orbit. The constant on the right-hand side is the \((i + m/4)\)th multiple of the Planck constant \( h \), where the integer \( m \) (called Maslov index) depends on the particular orbit type.

Consider as an example a Hamiltonian

\[
H_{cl} = \frac{1}{2M} p^2 + (\lambda c_0 - \lambda) q^2 + q^4
\]

where \( M \) is an arbitrary mass and \( \lambda c_0 \) a critical value of the control parameter \( \lambda \). Hamiltonians of this form (with a quartic potential, but usually with a more complicated kinetic terms) appear in the classical limit of some finite bosonic systems with two-body interactions. The contour curves \( S = \text{const} \) in the plane \( \lambda \times \mathcal{E} \) are shown in Fig. 1 for \( \lambda \in [0, 2\lambda c_0] \). According to the semiclassical quantization, the contours of \( S \) represent spectral “flow lines” moving in parallel with actual energy levels in the limit \( \aleph \to \infty \). Note that the Hamiltonian (2) implies a ground-state QPT in the corresponding quantum system at \( \lambda = \lambda c_0 \), where the second derivative of \( \mathcal{E}_0(\lambda) \) changes discontinuously. This can be anticipated from the trajectory of the lowest contour in Fig. 1. For \( \lambda \) increasing above \( \lambda c_0 \), a chain of ESQPTs is observed for excited states with consecutively
increasing values of $i = 1, 2, 3, \ldots$. This can be seen from the coherent bending of contours around $\mathcal{E} = 0$. The semiclassical analysis shows [18] that the second derivative of each $\mathcal{E}_i(\lambda)$ diverges logarithmically (while the first derivative drops to zero) at the point $\lambda_c$, where the level crosses a critical energy $\mathcal{E}_c = 0$. This energy corresponds to the local maximum ($q = 0$) of the double-well potential in Eq. (2) for $\lambda > \lambda_c$. The classical trajectory in the phase space at $\mathcal{E} = \mathcal{E}_c$ has an infinite period and forms a separatrix between two different types of orbits—“bounded” (i.e., located within one of the minima) for $\mathcal{E} < \mathcal{E}_c$, and “unbounded” (flying over both minima) for $\mathcal{E} > \mathcal{E}_c$.

For non-separable systems with $f > 1$ the determination of the $\mathcal{E}_i(\lambda)$ curves by a simple semiclassical formula fails. In fact, if an ESQPT affects a bunch of excited states in a non-integrable system, only an ensemble-averaged dependence $\langle \mathcal{E}_i(\lambda) \rangle$ is relevant since individual levels often show rather different responses [20]. In these cases, the phase-space volume criterion becomes more useful. It is based on the integral

$$\Gamma(\lambda, \mathcal{E}) = \int \delta(\mathcal{E} - H_{cl}) \, d\lambda \rho$$

with $\Gamma \, d\mathcal{E}$ standing for the phase-space volume available in a $d\mathcal{E}$ interval around energy $\mathcal{E}$. A non-analytic dependence of $\Gamma$ on $\mathcal{E}$ at a certain value $\mathcal{E}_c(\lambda)$ for a fixed $\lambda$ indicates an ESQPT at this critical energy. Note that $\Gamma$ is proportional to the smooth part $\tilde{\rho}$ of the total level density $\rho(\lambda, E)$ (the oscillatory part $\check{\rho}$ yielding infinitely rapid fluctuations in the $N \to \infty$ limit). Since $\ln \rho$ represents the microcanonical entropy, the non-analyticities of the phase-space volume (3) can be translated into the language analogous to that used in the description of thermal phase transitions. It should be stressed, however, that systems with moderate phase-space dimensions can generate phase transitions of different types than those known for $f \to \infty$ systems. For instance, a local maximum of a one-dimensional potential, such as the one in Eq. (2), yields an infinite peak in $\Gamma$ and $\rho$ (cf. the $\mathcal{E} = 0$ bunching of contours in Fig. 1), which from the thermodynamic viewpoint is a rather nongeneric type of dependence.

4. Example: IBM in the SU(3) limit

Ground-state QPTs were thoroughly investigated in several models describing collective dynamics—see Refs. [7, 8] for recent reviews focused mostly on nuclear physics. On the other hand, the excited-state QPTs have been so far described only in the simplest situations. The existing studies refer mostly to systems with an effective number of degrees of freedom $f = 1$, like the Lipkin model [21], the two- and three-dimensional vibron models for a subset of states with angular momentum $l = 0$ [22], the interacting boson model along its O(6)-U(5) transition for a subset of states with angular momentum and seniority $l = v = 0$ [18], a so-called cusp Hamiltonian [20], or schematic pairing models [19, 23, 24]. New results concern the Jaynes-Cummings model of quantum optics and a related model based on the SU(1,1) dynamical algebra [25]. In majority of cases, a singularity of the type shown in Fig. 1 was reported. It is connected with a local maximum (or a saddle point) of one-dimensional classical potential.

Here we present another example of an ESQPT, which we derive for the SU(3) limit of the interacting boson model (IBM) [10]. The Hamiltonian is taken in the simple form

$$H = -N_B^{-1}(Q \cdot Q), \quad Q = s^3d + d^3s - \frac{\sqrt{7}}{2}[d^1d]^{(2)},$$

where $Q$ is the SU(3) quadrupole operator. The energy eigenvalues are given in terms of the SU(3) quantum numbers ($\lambda, \mu$) [10]. The scaled energy $\mathcal{E} = E/N_B$ (an additional scaling to the one in $H$) satisfies $-2 \lesssim \mathcal{E} \lesssim 0$ and is an intensive quantity with respect to $N_B$. In the following,
Figure 2. The $\lambda \times \mu$ plane of the SU(3) quantum numbers. Right: Allowed $(\lambda, \mu)$ combinations for the IBM states with $l = 0$ and $N_B = 20$. Left: Contours of constant energy $\mathcal{E}$ (step $\Delta \mathcal{E} = 0.1$) from Eq. (5) for $N_B \to \infty$. The thick curve represents the critical ESQPT contour $\mathcal{E}_c = -0.5$.

we only consider states with angular momentum $l = 0$. For these states, the formula for $\mathcal{E}$ reads as

$$\mathcal{E} = \frac{1}{2} \left( \frac{\lambda}{N_B} \right)^2 + \left( \frac{\mu}{N_B} \right)^2 + \frac{\lambda}{N_B} \frac{\mu}{N_B} + \frac{3}{N_B} \left( \frac{\lambda}{N_B} + \frac{\mu}{N_B} \right)$$

(5)

where the allowed values of $\lambda \in [0, 2N_B]$ and $\mu \in [0, N_B]$ are given by the known selection rules [10]. These values form a triangle in the $\lambda \times \mu$ plane, which is for $N_B = 20$ shown in the right-hand panel of Fig. 2. The contours of constant $\mathcal{E}$ in this plane are for $N_B \to \infty$ depicted in the left-hand panel.

Each of the $(\lambda, \mu)$ points in Fig. 2 (right) represents a single eigenstate with $l = 0$. The ground state corresponds to the rightmost point, while the states with an increasing excitation energy fill the interior areas of the triangle towards the vertical side on the left. Note that the points in the triangle have a uniform density $\propto N_B^2$. It means that the number of states between energies $\mathcal{E}_1$ and $\mathcal{E}_2$ is proportional to the area of the segment of the triangle located between the respective contours of Eq. (5). The proportionality is exact for $N_B \to \infty$. Therefore, the energy dependence of the $l = 0$ state density for large $N_B$ can be calculated analytically as $\rho \propto dA/d\mathcal{E}$, where $A(\mathcal{E})$ is the area within the triangle located on the right-hand side of the contour with energy $\mathcal{E}$.

This function is depicted in the left-hand panel of Fig. 3. One observes a nonanalyticity (a place of the vertical-to-horizontal turnover of the tangent), which corresponds to a critical contour with $\mathcal{E} = -0.5$ crossing the upper corner of the triangle (the thick curve in Fig. 2; the infinite derivative of $\rho$ is due to a locally parallel direction of the critical contour with the upper edge of the triangle). The right-hand panel of Fig. 3 shows a finite $N_B$-realization of this dependence. The curve, which oscillates around the average predicted in the left-hand panel, represents a smoothened state density obtained from the actual $l = 0$ spectrum for $N_B = 60$ (shown on the rightmost edge of the figure).

The classical potential assigned to the above-given SU(3) Hamiltonian by the coherent-state technique is

$$V = -\left( 4\beta^2 + 2\sqrt{2}\beta^3 \cos \gamma + \frac{1}{2} \beta^4 \right) (1 + \beta^2)^{-2},$$

(6)

where $\beta \in [0, \infty)$ and $\gamma \in [0, 2\pi]$ are the quadrupole shape variables present in the coherent-state parametrization [10]. These variables are the only active degrees of freedom associated with the IBM for $l = 0$ since in the non-rotational case the three Euler angles are frozen. The potential takes values between $V_{\text{min}} = -2$ and $V_{\text{max}} = 0$ coinciding with the boundaries of the scaled
Figure 3. The density of $l = 0$ states in the SU(3) limit of the IBM. Left: The $N_B \to \infty$ density calculated from the area between contours in Fig. 2. Right: Numerical (smoothened) density for $N_B = 60$ (the discrete spectrum shown on the right). Both axes in arbitrary units.

spectrum for $\aleph \to \infty$. The critical energy $E_c = -0.5$ coincides with the saddle point $V_{\text{sad}} = -0.5$ of the potential, demarcating the energy where "unbounded" trajectories ranging over all three potential wells (around minima at $\gamma = 0, 2\pi/3, 4\pi/3$) emerge in the classical dynamics. (Note that the same energy is also associated with the $\beta \to \infty$ asymptote of $V$.)

Therefore, like in the above-discussed case of Hamiltonian (2), a stationary point of the IBM potential (6) is again connected with an ESQPT phenomenon. The analysis of the phase-space volume (3) confirms that a saddle point of a general two-dimensional potential results in a singular growth of $\Gamma(E)$ with an infinite derivative at the corresponding energy $E_c$. This is clearly manifested in the quantum spectrum of Fig. 3.

Similar considerations can be extended to higher-dimensional models, where however the ESQPT signatures (types of non-analyticities) get softer with an increasing dimension. An interesting question is also connected with the influence of chaotic spectral correlations away from the dynamical symmetries. For example, the IBM coherent-state potential exhibits local maxima and saddle points within the whole Casten triangle, but the associated ESQPTs are less apparent than in the dynamical-symmetry cases (at least in the available spectra with moderate $N_B$ values).

5. Conclusions
We have discussed quantum phase transitions in some simple models related to collective dynamics of many-body systems. Specific features of critical phenomena in these models follow from a rather limited number of degrees of freedom $f$, which does not grow with the size parameter $\aleph$ of the system. As a consequence, all non-analytic dependences of the ground state and excited states on the control parameter $\lambda$ for $\aleph \to \infty$ originate in some singular properties of the corresponding classical Hamiltonians.

Apart from the ground-state phase transitions, connected with non-analytic changes of the classical point of static equilibrium, we have seen some examples of excited-state phase transitions, which are rooted in abrupt changes of classical dynamics. For atomic nuclei, the ESQPTs predicted by the collective models (such as the IBM) seem to be located in too high energy domains, where the collective states are already strongly mixed with the others and the low-energy models lose their relevance. However, the critical phenomena for excited states may be available to experimental study in molecular, mesoscopic and quantum optical systems, which are often described up to very high relative excitations by similar models as those applied
in nuclei at low energies. As proposed recently [25], ESQPTs in such systems may show up through a strongly anomalous dynamical response to some specific external manipulations.

Acknowledgments
This work was supported by the Czech Science Foundation (202/09/0084) and by the Czech Ministry of Education (MSM 0021620859).

References
[1] Carr L D (editor) 2010, Understanding Quantum Phase Transitions (Boca Raton, Taylor & Francis).
[2] Hertz J 1976, Phys. Rev. B 14, 1165
[3] Gilmore R and Feng D H 1978, Nucl. Phys. A 301, 189
   Gilmore R 1979, J. Math. Phys. 20, 891
[4] Gilmore R 1981, Catastrophe Theory for Scientists and Engineers (New York, Wiley)
[5] Sachdev S 1999, Quantum Phase Transitions (Cambridge University Press)
   Vojta M 2003, Rep. Prog. Phys. 66, 2060
[6] Dieperink A E L, Scholten O and Iachello F 1980, Phys. Rev. Lett. 44, 1747
   Feng D H, Gilmore R and Deans S R 1981, Phys. Rev. C 23, 1254
[7] Casten R F 2009, Prog. Part. Nucl. Phys. 62, 183
   Cejnar P and Jolie J 2009, ibid. 62, 210
[8] Cejnar P, Jolie J and Casten R F 2010, Rev. Mod. Phys. 82, 2155
[9] Iachello F and Oss S 2002, Eur. Phys. J. D 19, 307
   Dusuel S, Vidal J, Arias J M, Dukelsky J and García-Ramos J E 2005, Phys. Rev. C 72, 011301(R)
   Vidal J, Arias J M, Dukelsky J and García-Ramos J E 2006, Phys. Rev. C 73, 054305
   Cejnar P and Iachello F 2007, J. Phys. A 40, 581
[10] Iachello F and Arima A 1987, The Interacting Boson Model (Cambridge University Press)
[11] Iachello F and Levine R D 1995, Algebraic Theory of Molecules, (Oxford University Press)
[12] Frank A and Van Isacker P 2005, Symmetry Methods in Molecules and Nuclei (México D.F., S y G editores)
[13] Rowe D J and Wood J L 2010, Fundamentals of Nuclear Models (Singapore, World Scientific)
[14] Rowe D J, Bahri C and Wijesundera W 1998, Phys. Rev. Lett. 80, 4394
   Iachello F 2000, ibid. 85, 3580
   Iachello F 2001, ibid. 87, 052502
   Rowe D J 2004, ibid. 93, 122502
[15] Zhang W-M and Feng D H 1995, Phys. Rep. 252, 1
[16] Zhang W-M, Feng D H and Gilmore R 1990, Rev. Mod. Phys. 62, 867
[17] Landau L 1937, Phys. Z. Sowjet. 11, 26; 545
[18] Cejnar P, Macek M, Heinze S, Jolie J and Dobeš J 2006, J. Phys. A 39, L515
[19] Caprio M A, Cejnar P and Iachello F 2008, Ann. Phys. (N.Y.) 323, 1106
[20] Cejnar P and Stránský P 2008, Phys. Rev. E 78, 031130
[21] Leyvraz F and Heiss W D 2005, Phys. Rev. Lett. 95, 050402
[22] Pérez-Bernal F and Iachello F 2008, Phys. Rev. A 77, 032115
[23] Reis M, Terra Cunha M O, Oliviera A C and Nemes M C 2005, Phys. Lett. A 344, 164
[24] Caprio M A, Skrabacz J H and Iachello F 2011, J. Phys. A 44, 075303
[25] Pérez-Fernández P, Cejnar P, Arias J M, Dukelsky J, García-Ramos J E and Relaño A 2011, Phys. Rev. A 83, 033802