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Non-thermal excited-state quantum phase transitions

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Abstract – We report a kind of phase transition which takes place in isolated quantum systems with a discrete symmetry. Different phases are separated by a critical energy and recognized by means of an order parameter, which can be experimentally measured. Below the critical energy, the symmetry is broken and the equilibrium state is non-thermal, keeping large amounts of memory of the initial condition. Above, the symmetry is restored and a thermal equilibrium state is reached. We identify two universality classes, one showing a second-order phase transition and represented by the Lipkin-Meshkov-Glick model, and another showing a first-order phase transition and represented by the Dicke model.

This work is dedicated to the memory of Joaquín Retamosa.

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Recent advances in experimental techniques allowing to keep mesoscopic systems well isolated from the environment have led to the observation of non-thermal equilibrium states [1–3]. This has spurred on the theoretical research on the fundamentals of statistical mechanics for this kind of systems [4]. It has been proved that almost any isolated quantum system reaches an equilibrium state ρ_{eq} after a sufficiently long-time evolution, meaning that the time-dependent expected value $\langle \Psi(t) | A | \Psi(t) \rangle$ for any operator A remains close to $\text{Tr}[\rho_{\text{eq}} A]$ for the majority of times, independently of the initial condition [5]. However, the nature of this equilibrium state is sometimes rather complicated and different from the usual thermodynamical behavior. In such occasions, large amounts of memory of the initial condition are stored in a set of extra constants of motion.

In this letter we report a kind of phase transition due to this non-thermal behavior. In a class of quantum systems with a global and discrete symmetry S , a transition from a non-thermal symmetry-breaking to a normal equilibrium state is observed at a certain critical energy E_c , if the system stays isolated. Below the critical energy, the properties of the equilibrium state $\rho_{\text{eq}}(E, \chi)$ depend on a number of extra constants of motion, denoted here by χ , in addition to the energy (or the microcanonical temperature). On the contrary, for $E > E_c$

the equilibrium state recovers the usual thermal behavior, and only depends on the energy of the system. We call this phenomenon a *non-thermal excited-state quantum phase transition* (NT-ESQPT), because its trademark is the non-thermal nature of the equilibrium state in one of the phases. It can be observed by measuring the expected values of certain observables, which act as order parameters of the transition—they are zero for $E < E_c$, and different from zero for $E > E_c$. We show that it takes place in two models, Lipkin-Meshkov-Glick and Dicke, that represent two different universality classes and can be experimentally tested [6–8].

Nature of the non-thermal excited-state quantum phase transition. – The requisites for this kind of phase transition are the following. First, a global and discrete symmetry S which commutes with the Hamiltonian for any values of the system parameters, $[H(\lambda), S] = 0$, $\forall \lambda$. And second, a singularity in the density of states at a certain critical energy E_c , called excited-state quantum phase transition (ESQPT), that divides the spectrum in two different regions, one where the eigenvalues are doubly degenerated and the symmetry S can be broken, and another where no degeneracies are present [9]. Although ESPQTs have been reported in a number of models covering quantum optics, molecular, atomic and nuclear

physics [10–15], their character as real phase transitions is controversial, since a clear and measurable signature that the critical energy separates two different phases is still unobserved.

In this letter we show that a real phase transition takes place at the critical energy E_c . Let us consider an isolated quantum system that fulfills the previous requisites. To label its eigenstates, we use the Hamiltonian H and the symmetry S , $H|E_i, \alpha\rangle = E_{i,\alpha}|E_i, \alpha\rangle$. Here α denotes the eigenvalues of S ; throughout this letter we consider that it has just two, $\alpha = \pm$. The index i runs over all the eigenstates of the Hamiltonian belonging to a subspace with definite value of S . With this notation and taking $\hbar = 1$, the time evolution of a certain initial condition $|\Psi(t=0)\rangle$ reads

$$|\Psi(t)\rangle = \sum_{i,\alpha} C_{i,\alpha} \exp(-iE_{i,\alpha}t) |E_i, \alpha\rangle, \quad (1)$$

where $C_{i,\alpha} = \langle E_i, \alpha | \Psi(t=0) \rangle$.

As is pointed in [5], any initial condition remains almost always close to an equilibrium state ρ_{eq} , given by the long-time average of the time-evolved pure state,

$$\begin{aligned} \rho_{\text{eq}} &= \sum_{i,j} \sum_{\alpha,\beta} \lim_{T \rightarrow \infty} \frac{1}{T} \\ &\times \int_0^T dt C_{i,\alpha} C_{j,\beta}^* \exp[-i(E_{i,\alpha} - E_{j,\beta})t] |E_i, \alpha\rangle \langle E_j, \beta|. \end{aligned} \quad (2)$$

The integral in the r.h.s of this equation is usually evaluated by means of the diagonal approximation [4]. It consists of removing all the terms for which $E_{i,\alpha} \neq E_{j,\beta}$, because they are modulated by a fastly-oscillating term and thus average to zero. To apply this approximation to the systems we are studying, is mandatory to put special attention on the degeneracies in the spectrum. Below the critical energy E_c , the eigenvalues of the Hamiltonian are degenerated by pairs $E_{i,+} = E_{i,-}$, and therefore the corresponding non-diagonal terms remain after performing the integral. On the contrary, above the critical energy $E_{i,+} \neq E_{i,-}$, and only diagonal terms contribute to the average. As a consequence, the equilibrium state is qualitatively different at both sides of the critical energy,

$$\begin{aligned} \rho_{\text{eq}}(E < E_c) &= \sum_{i,\alpha} |C_{i,\alpha}|^2 |E_i, \alpha\rangle \langle E_i, \alpha| \\ &+ \sum_i C_{i,+} C_{i,-}^* |E_i, +\rangle \langle E_i, -| + \text{h.c.}; \quad (3) \\ \rho_{\text{eq}}(E > E_c) &= \sum_{i,\alpha} |C_{i,\alpha}|^2 |E_i, \alpha\rangle \langle E_i, \alpha|. \quad (4) \end{aligned}$$

These equations constitute one of the main results of this letter. Below E_c , the equilibrium state stores a relevant piece of information about the initial condition in the coherences $C_{i,+} C_{i,-}^*$. This means that not only the expected value of the symmetry S is relevant, but also the

relative phases in the initial condition, and therefore the degree of symmetry breaking. As a paradigmatic example, an initial condition proportional to $|+\rangle + |-\rangle$ will give a different equilibrium state than another proportional to $|+\rangle - |-\rangle$, despite in both cases $\langle S \rangle = 0$. Therefore, the properties of the system after reaching the equilibrium cannot be described by the standard canonical or microcanonical ensembles, nor by the generalized Gibbs ensemble [16], which depends on the expected values of a number of relevant constants of motion. On the other hand, above the critical energy, ρ_{eq} is equal to the usual diagonal form, and reduces to the microcanonical or the canonical ensembles if the system fulfills certain generic conditions [17]. In the following, and relying in two paradigmatic models accessible to experiments, we show that this abrupt change gives rise to what we have called a non-thermal excited-state quantum phase transition.

Suppose that we let the system evolve from an initial condition which lies below the critical energy. As the system is isolated, energy is conserved and the equilibrium state reached after sufficiently long-time evolution is described by eq. (3). Therefore, a large piece of information is stored in the coherences $C_{i,+} C_{i,-}^*$; it can be inferred by measuring an adequate observable \mathcal{O} for which $\text{Tr}[\rho_{\text{eq}} \mathcal{O}] = f(C_{i,+} C_{i,-}^*)$, being $f(x)$ a certain function depending on the observable. If we then give the system a sufficient amount of energy, keeping it well isolated from the environment (changing an external parameter of the Hamiltonian, for example), the resulting equilibrium state will lie above E_c , and thus it will be described by eq. (4). In this situation, the equilibrium state does not depend on the coherences $C_{i,+} C_{i,-}^*$ anymore, and therefore $\text{Tr}[\rho_{\text{eq}} \mathcal{O}] = 0$. As a consequence, the observable \mathcal{O} behaves like an order parameter and can be used to characterize the NT-ESQPT.

It is worth to remark that the system must be isolated from the environment to experiment this transition. If the system is put in contact with a thermal bath, the information stored in the coherences is rapidly lost by dephasing, and a standard canonical equilibrium state $\rho = \exp(-\beta H)/Z$ arises, no matters if the system is below or above the critical energy E_c .

Physical models. – We study this NT-ESQPT in two different two-level systems, for which the symmetry S is linked to the parity of the occupation of one of the levels.

The Lipkin-Meshkov-Glick model (LMG) [18] describes the interaction between two kinds of scalar bosons s and t of opposite parity,

$$H = \lambda t^\dagger t + \frac{1-\lambda}{N} (s^\dagger t + t^\dagger s)^2, \quad (5)$$

where s^\dagger and s are the usual creator and annihilation operators for s bosons; t^\dagger and t , the same for t bosons, and $N = s^\dagger s + t^\dagger t$ is the total number of particles, which is conserved. S is the parity of the number of t bosons, $S = \exp(i\pi t^\dagger t)$.

The Dicke model (D) [19] describes the interaction between a set of two-level atoms and a single-mode radiation field,

$$H = \omega_0 J_z + \omega a^\dagger a + \frac{2\lambda}{\sqrt{N}} (a^\dagger + a) J_x, \quad (6)$$

where a^\dagger and a are the usual creation and annihilation operators of photons, $\vec{J} = (J_x, J_y, J_z)$ is the angular momentum, with a pseudo-spin length $J = N/2$, N is the conserved number of atoms, ω is the frequency of the cavity mode, ω_0 the transition frequency, and λ the coupling parameter. In this case, $S = \exp(i\pi [J + J_z + a^\dagger a])$ [20].

These models manifest both QPT and ESQPTs. The critical energy E_c can be estimated by means of a semiclassical approximation, and lies on $E_c = -J$ for D, taking $\omega_0 = \omega = 1$ [9,15], and $E_c = 0$ for LMG [13]. The main difference between them is that LMG has just one semiclassical degree of freedom, whereas D has two and exhibits quantum and semiclassical chaos [20–22]. As it is shown in the last part of this letter, this fact entails a relevant difference: the phase transition is second order in LMG, and first order in D. As a consequence, these models represent two different universality classes: LMG for systems which one semiclassical degree of freedom, and D for systems with two or more semiclassical degrees of freedom.

Equilibrium state and order parameters. – To characterize the NT-ESQPT, we select observables \mathcal{O} for which $\langle E_i, \alpha | \mathcal{O} | E_i, \alpha \rangle = 0$. So, non-diagonal contributions are required for $\text{Tr}[\rho_{\text{eq}} \mathcal{O}] \neq 0$, which entails that the symmetry S is broken in the equilibrium state. We choose $s^\dagger t + t^\dagger s$ for LMG, and J_x for D. In both cases, \mathcal{O} has been experimentally measured to show a QPT due to a classical bifurcation in LMG [6], and the symmetry breaking associated to the QPT in D [8]. So, measuring protocols for exploring the NT-ESQPT in these models are available within the current experimental facilities.

To study the behavior of the equilibrium states, we rely on the following protocol:

i) Start from the ground state of the Hamiltonian $H(\lambda_i)$ in the degenerated phase, at a certain initial value of the coupling constant λ_i . As ground states are doubly degenerated in this phase, any combination of $|E_0, +\rangle$ and $|E_0, -\rangle$ is also a ground state. So, we choose

$$|\Psi(t=0)\rangle = \cos(\chi) |E_0, +\rangle + \sin(\chi) |E_0, -\rangle, \quad (7)$$

where the angle χ determines how the two eigenstates of S are mixed. It is worth to mention that the experimental protocol followed in [8] starts with the same kind of initial state, with $\chi \approx \pi/4$ due to a tiny external perturbation. Also, the protocol in [6] starts with a symmetry-breaking initial condition.

ii) Carry out a quench $\lambda_i \rightarrow \lambda_f$. As it is a change in an external parameter of the Hamiltonian, it entails an energy cost $\Delta E(\lambda_i, \lambda_f) = E(\lambda_f) - E_0(\lambda_i)$, where $E(\lambda_f) = \langle \Psi(t=0) | H(\lambda_f) | \Psi(t=0) \rangle$, and $E_0(\lambda_i) = \langle \Psi(t=0) | H(\lambda_i) | \Psi(t=0) \rangle$. This energy change becomes

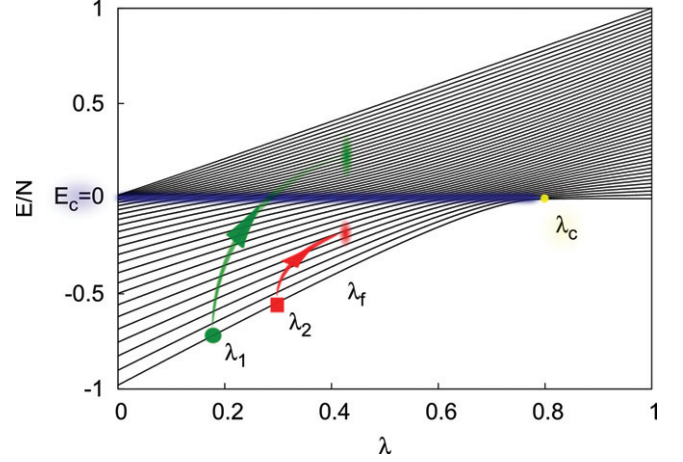


Fig. 1: (Colour on-line) Schematic representation of the protocol, illustrated using the LMG spectrum. The critical energy lies on $E_c = 0$ (blue); λ_c represents the critical point of the QPT (yellow). Two initial states are represented as the ground states at different values of the coupling constant, λ_1 and λ_2 ; after the quench both of them reach λ_f but with different energies. Quenching the initial state encoded by a circle (green) at λ_1 , the final state will lie above the critical energy $E_f > E_c$, whereas for the initial state encoded by a box (red) at λ_2 the quench gives an energy below the critical $E_f < E_c$.

the control parameter of the NT-ESQPT, since we can lead the system above or below the critical energy by adequately choosing λ_i and λ_f .

iii) Let the system evolve under the final Hamiltonian $H(\lambda_f)$ until it reaches the final equilibrium state ρ_{eq} .

iv) Finally, study the results for $\text{Tr}[\rho_{\text{eq}} \mathcal{O}]$ in terms of the energy E and the angle χ of the initial state.

A schematic diagram of this protocol is depicted in fig. 1. Starting from two different initial states, corresponding to the ground state at different coupling constants λ_1 and λ_2 , a quench to the same λ_f will provide different final energies, the larger jump $\Delta\lambda = \lambda_f - \lambda_i$ leading to the higher excited state.

In fig. 2 we plot $\text{Tr}[\rho_{\text{eq}} \mathcal{O}]$ for LMG with $\lambda_f = 0.7$ (upper panel), and D with $\lambda_f = 0.75$ (lower panel), in terms of the energy E normalized by N in LMG, and by J in D. Critical energies are $E/J = -1$ for D and $E/N = 0$ for LMG. Each curve corresponds to a different initial value of the angle χ . The maximum symmetry-breaking state is given by $\chi = \pi/4$ and is represented by solid lines (red online), while initial states with well-defined symmetry $\chi = 0$ are depicted by black dashed lines. Intermediate cases are depicted with different line styles (see caption of fig. 2 for details). The more broken the symmetry is in the initial state, the more change suffers the equilibrium state at the critical energy. In LMG we have considered $N = 2000$ bosons, while in D only $N = 64$ atoms, since it requires more computational resources.

The results plotted in fig. 2 recall the behavior of the order parameter of a standard phase transition, if the

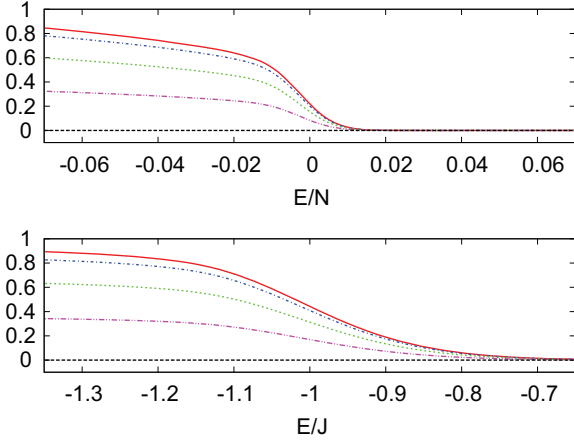


Fig. 2: (Colour on-line) Expected value of the order parameter \mathcal{O} in the equilibrium state for LMG (top) and D (bottom), in terms of the final energy and different angles χ of the initial state. In both cases the (red) solid line corresponds to $\chi = \pi/4$; the (blue) short-dash-dotted line to $\chi = 3\pi/16$; the (green) short-dashed line to $\pi/8$; the (magenta) long-dash-dotted line to $\pi/16$, and the (black) dashed line, to $\chi = 0$.

symmetry is not well defined in the initial state. The expected value of \mathcal{O} changes from a non-zero value in the degenerated phase, to zero in the normal one. But it is also important to remark the non-thermal nature of the symmetry-breaking phase: given a fixed energy E , the equilibrium expected value $\text{Tr}[\rho_{\text{eq}}\mathcal{O}]$ crucially depends on χ , and therefore the standard statistical ensembles cannot account for it. On the contrary, for initial states with well-defined symmetry, no transition is observed, since $\text{Tr}[\rho_{\text{eq}}\mathcal{O}] = 0$ for any value of E .

Thermodynamical limit and critical behavior. –

To study the behavior in the thermodynamical limit we profit from the fact that both LMG (in its spin version) and D are infinitely coordinated systems for which the mean-field approximation exactly holds [23]. So, we derive a classical analogue from a coherent state ansatz, which is expected to properly account for the thermodynamical limit

$$|\beta\rangle_{\text{LMG}} = e^{\sqrt{\frac{N}{1+\beta^2}}(s^\dagger + \beta t^\dagger)} |0\rangle, \quad (8a)$$

$$|\mu, \nu\rangle_D = \frac{e^{\nu^2/2}}{(1 + \mu^2)^J} e^{\mu J_+ + \nu a^\dagger} |J, -J\rangle \otimes |0\rangle, \quad (8b)$$

where μ , ν and β are complex numbers. To derive the classical equations of motion we perform a change of variables from these complex parameters to canonical positions and momenta. After this change, the Hamiltonian of both systems read (see, for example, [14,20]),

$$H_{\text{LMG}}(p, q) = (5\lambda - 4)p(1 - p) + \lambda p^2 - 4(\lambda - 1)p(1 - p)\sin^2 q, \quad (9)$$

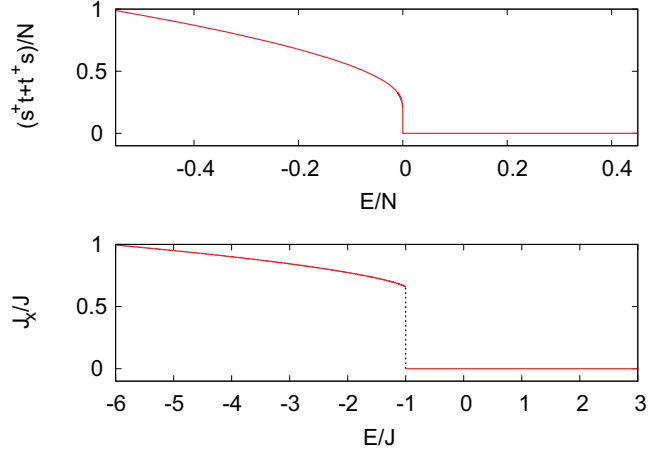


Fig. 3: (Colour on-line) Expected value of the order parameter \mathcal{O} for LMG (top) and D (bottom) in the thermodynamical limit as a function of the energy E . The results show a second-order NT-ESQPT in LMG, and a first-order NT-ESQPT in D.

$$H_D(\vec{p}, \vec{q}) = -J\omega_0 + 2\lambda\sqrt{\omega\omega_0}q_1q_2\eta + \frac{1}{2}\left(\omega^2q_1^2 + \omega_0^2q_2^2 + |\vec{p}|^2 - \omega - \omega_0\right), \quad (10)$$

$$\eta = \sqrt{1 - \frac{\omega_0^2q_2^2 + p_2^2 - \omega_0}{4J\omega_0}}.$$

We use vectorial notation (\vec{p}, \vec{q}) for D to indicate that two positions and two momenta are considered. We keep this notation in the following paragraph to indicate that the same reasoning is valid for a system with any number of degrees of freedom.

The expected values of observables within this approximation are obtained by performing a long-time average over the trajectory of the system

$$\langle \mathcal{O} \rangle = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \mathcal{O}(\vec{p}[t], \vec{q}[t]). \quad (11)$$

The statistical method to calculate this average is to assume that the trajectories are ergodic and to replace this integral by an average over the whole energy surface. However, for the systems we are studying, the phase space is divided in two disjoint regions that we denote γ_+ and γ_- below E_c [9,14]. This fact entails that every initial condition $(\vec{p}[0], \vec{q}[0])$ with $E < E_c$ remains in the same region throughout the whole time evolution, and therefore the corresponding trajectories do not explore the whole energy surface. As a consequence, to develop a statistical description is mandatory to restrict phase-space averages to the region in which the trajectories lie. Therefore, assuming that the dynamic is ergodic within each region, that is, the trajectories explore the whole γ_+ (or γ_-) region (see [20,22] for a discussion in D), the expected value of the observable \mathcal{O} can be calculated as follows:

$$\langle \mathcal{O} \rangle = \frac{\int_{\gamma_+} d\vec{p}d\vec{q} \mathcal{O}(\vec{p}, \vec{q}) \delta(H(\vec{p}, \vec{q}) - E)}{\int_{\gamma_+} d\vec{p}d\vec{q} \delta(H(\vec{p}, \vec{q}) - E)}. \quad (12)$$

On the contrary, for $E > E_c$ trajectories are expected to cover all the energy surface, and therefore one has to rely on the standard microcanonical average, instead of eq. (12).

Following this procedure, one can extract the behavior of the observables in the thermodynamical limit as a function of the energy. Notwithstanding, it is important to have in mind that this is a semiclassical approximation, and thus it cannot account for the cases resulting of quantum superpositions. For both LMG and D models, the coherent state ansatz eq. (8) represent a maximum symmetry-breaking state $\chi = \pm\pi/4$, where the positive sign stands for the positive branch of \mathcal{O} (the one plotted in fig. 2), and the negative sign, for the negative branch (not plotted in fig. 2). The intermediate cases cannot be directly calculated by this procedure, but can be estimated by averaging the results for these two branches with adequate weights.

We show the results in fig. 3. The main outcome is that a second-order NT-ESPQT is obtained for LMG, whereas for D a finite-step jump occurs at the critical energy, raising a first-order NT-ESPQT. This fact is closely related to the behavior of the density of states (DOS), appearing at the denominator of eq. (12). In LMG there is a logarithmic divergence in DOS at $E_c = 0$ [24], hence the expected value of the observable goes to zero as the energy approaches to E_c as $\langle\mathcal{O}\rangle \sim \log^{-1}|E - E_c|$. On the contrary, as the DOS does not diverge at $E = E_c$ for D [25], the expected value of J_x keeps different from zero as $E \rightarrow E_c^-$, and then abruptly jumps to zero at $E = E_c$, the point at which the semiclassical trajectories start to explore the whole phase space and thus the standard microcanonical average is recovered. These simple and qualitative differences between LMG and D lead us to postulate that they represent two different universality classes. One, for systems in which the DOS diverges at the critical energy, giving rise to a continuous second-order NT-ESPQT. The other, for systems in which the divergence takes place in the derivatives of the DOS, giving rise to a first-order NT-ESPQT. The first one is expected to happen in quantum systems with just one semiclassical degree of freedom; the second one, in quantum systems with more semiclassical degrees of freedom. So, the kind of phase transition reported in this letter is expected to occur in other quantum systems, like two-site Bose Hubbard, vibron model, Interacting Boson Model, etc. All of them are expected to belong to one of these universality classes, depending on their number of semiclassical degrees of freedom.

Conclusions. – In this letter we report a phase transition from non-thermal symmetry-breaking to normal equilibrium states, happening at a critical energy E_c . This phase transition takes place at that critical energy when, changing external parameters, energy is transferred to a system with a global symmetry S , provided that the system remains isolated from the environment and the

symmetry is broken in the initial state. It entails an abrupt change in the equilibrium state, as a consequence of the extra conserved quantities of the Hamiltonian; so, it does not happen if the system is put in contact with a thermal bath. We have shown this phenomenon in two quantum systems: the Lipkin-Meshkov-Glick and the Dicke models, which can be tested in experiments making use of the current technology. We have found good order parameters which characterize the different phases —their expected values in the equilibrium states are zero in normal phase, and non-zero in the non-thermal symmetry-breaking phase. We have also shown that these order parameters become non-analytic at the critical energy in the thermodynamical limit. Furthermore, we have identified two different universality classes, represented by the Lipkin-Meshkov-Glick and the Dicke models. The former displays a second-order phase transition, due to the logarithmic divergence of the density of states at the critical energy E_c —the order parameter goes to zero continuously, following a logarithmic law. The second universality class is characterized by a first-order phase transition. This occurs when the divergence at the critical energy does not appear in the density of states, but in its derivatives, giving rise to an abrupt jump in the expected value of the order parameter.

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