

Thermodynamic analogy for quantum phase transitions at zero temperature

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We propose a relationship between thermodynamic phase transitions and ground-state quantum phase transitions in systems with variable Hamiltonian parameters. It is based on a link between zeros of the canonical partition function at complex temperatures and branch points of a quantum Hamiltonian in the complex-extended parameter space. This approach is applied in the interacting boson model, where it is shown to properly distinguish the first- and second-order phase transitions.

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Quantum phase transitions (QPTs) are now a well-documented phenomenon in both lattice [1] and many-body systems [2–19]. A QPT Hamiltonian usually reads as a superposition of two incompatible terms,

$$H(\lambda) = H_0 + \lambda V = (1 - \lambda)H(0) + \lambda H(1), \quad (1)$$

$[H_0, V] \neq 0$, where $\lambda \in [0,1]$ is a dimensionless control parameter that drives the system between two limiting modes of motions. It can be shown that the ground-state (g.s.) average $\langle V \rangle_0 \equiv \langle \Psi_0(\lambda) | V | \Psi_0(\lambda) \rangle$ is a nonincreasing function of λ . In the QPT situation it evolves in such a way that either $\langle V \rangle_0$ itself or some of its derivatives change discontinuously (for systems of infinite size) at a certain critical value λ_c .

Of particular interest are the cases when $\langle V \rangle_0$ drops to zero and, simultaneously, also $\langle V^2 \rangle_0 = 0$ at the critical point. Typically, this may happen if V is semi-positively definite. Then zero of $\langle V \rangle_0$ at an arbitrary point λ_c implies that $\langle V \rangle_0 = 0$ for all $\lambda \geq \lambda_c$ and if the ground state is nondegenerate, its wave function gets fixed. In these cases, $\langle V \rangle_0$ plays a role of an “order parameter” whose value (zero or nonzero) distinguishes two quantum “phases” of the model. Such a scenario is realized in various many-body models, mostly known from nuclear physics. Limits $H(0)$ and $H(1)$ are usually connected with collective or single-particle motions corresponding to spherical and deformed nuclear shapes [2–6,10–15,18,19] but they can also represent paired and unpaired fermionic phases of nuclei [4,5,7,16], or normal and super-radiant modes of interacting atom-field systems [17]. Quantum phase transitions were also studied in open quantum systems [8,9].

Questions often arise concerning the depth to which the term “phase transition” can be followed toward standard thermodynamics. The g.s. QPTs happen at zero temperature and thus have no real thermal attributes. Nevertheless, as discussed, for example, in Refs. [12,15,16,20], counterparts of some thermodynamic terms can often be derived from standard quantum-mechanical expressions. A unified thermodynamic-like approach to characterize the QPT situation is, however, missing.

In this Rapid Communication, we present a method capable of establishing the thermodynamic analogy for QPTs on a new, general ground. The method is based on a *surmise* that there

exists a similarity between the distribution of zeros of the canonical partition function $Z(T)$ at complex temperatures T for systems undergoing classical phase transitions [21–23] and the distribution of branch points of QPT Hamiltonians (1) in the complex-extended λ plane (these are points of unavoided crossings of the Hamiltonian eigenvalues) [5,8,24–28]. This link is not artificial. Whereas in generic finite systems neither zeros nor branch points occur on the real T or λ axes (here and in the whole paper we consider branch points that characterize subsets of states with the same symmetry quantum numbers), it is known that their distribution in the complex plane determines the key features of the system in the physical (real) domain. Zeros and branch points thus play crucial roles also in the fundamental theory of classical and quantum phase transitions. Indeed, places where in the thermodynamic limit complex zeros of $Z(T)$ approach infinitely close to the real T -axis can be identified with points of classical phase transitions [21–23], whereas similar convergence of branch points to real λ induces singular evolution of energies and wave functions, as observed in $T = 0$ QPTs [5,8,11].

An obvious way to quantitatively exploit the thermodynamic analogy for QPTs relies on connecting the g.s. energy $E_0(\lambda)$ as a function of the interaction parameter λ , with the equilibrium value of a thermodynamic potential $F_0(T)$ as a function of temperature T (or inverse temperature β). This method leads to the standard QPT classification, known from the literature [3]. From the relation $\langle V \rangle_0 = dE_0/d\lambda$ it follows that if the $(l - 1)$ th derivative of $\langle V \rangle_0$ is discontinuous at λ_c , then derivatives of the g.s. energy are discontinuous (singular) starting from $d^l E_0/d\lambda^l$ so that the QPT is of the l th order. The “specific heat” defined [15] through the second derivative of E_0 in such a transition (in analogy to the standard definition $C = -T \partial^2 F_0 / \partial T^2$),

$$C_1 = -\lambda \frac{d^2 E_0}{d\lambda^2} = -\lambda \frac{d\langle V \rangle_0}{d\lambda} = 2\lambda \sum_{i>0} \frac{|\langle \Psi_i | V | \Psi_0 \rangle|^2}{E_i - E_0}, \quad (2)$$

behaves exactly as expected for a thermodynamic phase transition of the same order. Here, $E_i(\lambda)$ and $|\Psi_i(\lambda)\rangle$ are the i th energy and eigenvector, respectively.

This relation can be easily verified [15] in the interacting boson model (IBM) [29], where both first- and second-order

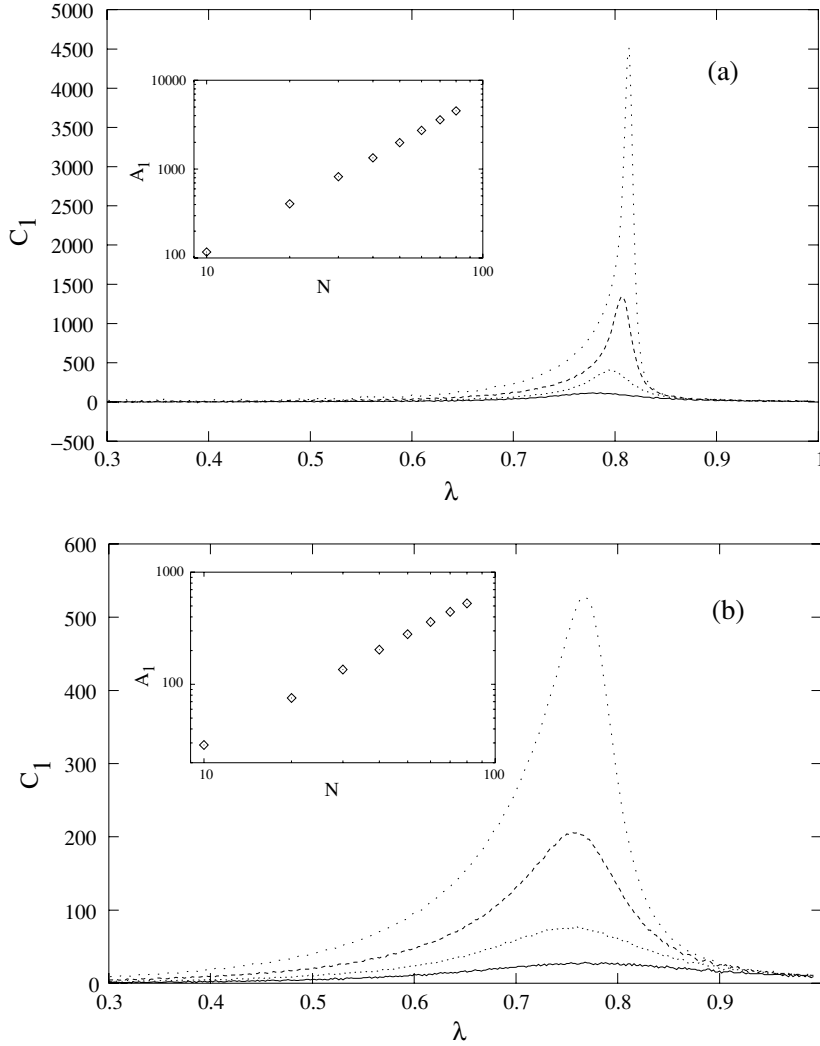


FIG. 1. “Specific heat” (2) in the (a) first-order and (b) second-order QPT of the interacting boson model [Hamiltonian (3) with (a) $\chi = -\sqrt{7}/2$ and (b) $\chi = 0$]. The curves, in order from the lowest to the highest, correspond to $N = 10, 20, 40$, and 80 , respectively; the insets show the increase of the maximal value with N .

QPTs between spherical and deformed g.s. shapes are present in the parameter space [2,3,6,10–15,18]. The model describes shapes and collective motions of atomic nuclei in terms of an ensemble of N interacting s and d bosons with angular momenta 0 and 2, respectively. We use the Hamiltonian [10–15]

$$H(\lambda) = (1 - \lambda) \left[-\frac{q_\chi \cdot q_\chi}{N} \right] + \lambda n_d, \quad (3)$$

where $n_d = d^\dagger \cdot \tilde{d}$ is the d -boson number operator, and $q_\chi = d^\dagger \tilde{s} + s^\dagger \tilde{d} + \chi (d^\dagger \tilde{d})^{(2)}$ is the quadrupole operator. Clearly, $V = n_d + q_\chi \cdot q_\chi / N$ is semi-positive. In the $N \rightarrow \infty$ limit, the order parameter $\langle V \rangle_0 / N$ (where normalization per boson is necessary to deal with effects of varying N) can be expressed in terms of the g.s. deformation parameter β_0 [2]:

$$\lim_{N \rightarrow \infty} \frac{\langle V \rangle_0}{N} = \frac{5\beta_0^2 - 4\sqrt{\frac{2}{7}}\chi\beta_0^3 + (\frac{2}{7}\chi^2 + 1)\beta_0^4}{(1 + \beta_0^2)^2}. \quad (4)$$

For $\chi \neq 0$, the value of β_0 drops from a nonzero value β_{0c} to 0 at $\lambda = \lambda_c(\chi) = (4 + 2\chi^2/7)/(5 + 2\chi^2/7)$, indicating a first-order deformed-spherical QPT. For $\chi = 0$, the value $\beta_0 \propto \sqrt{\lambda_c - \lambda}$ valid in the left vicinity of the critical point $\lambda_c(0)$ continuously joins with $\beta_0 = 0$ valid above λ_c ; the

corresponding QPT is of second order (with the critical exponent for $\langle V \rangle_0 / N$ equal to 1). The dependence of C_1 on λ in the first- and second-order QPT regions is shown in Fig. 1 for various boson numbers N .

In the following, we will focus on the thermodynamic analogy based on the distribution of branch points. These are points in the complex plane of parameter λ where various pairs of eigenvalues of the complex-extended Hamiltonian (1) coalesce [24]. They are simultaneous solutions of equations $\det[E - H(\lambda)] = 0$ and $(\partial/\partial E)\det[E - H(\lambda)] = 0$, which after elimination yield the following condition [25,27]:

$$D(\lambda) = \prod_k D_k(\lambda) = (-)^{\frac{n(n-1)}{2}} \prod_{i < j} [E_j(\lambda) - E_i(\lambda)]^2 = 0, \quad (5)$$

$$D_k(\lambda) = \prod_{i(\neq k)} [E_i(\lambda) - E_k(\lambda)]. \quad (6)$$

The discriminant $D(\lambda)$ is a polynomial of order $n(n-1)$ in λ (where n is the dimension of the Hilbert space, which is assumed to be finite) with real coefficients and its roots thus occur as $n(n-1)/2$ complex conjugate pairs. Except at these points, the complex eigenvalue $E(\lambda)$ obtained from the characteristic polynomial of Hamiltonian (1) is a single analytic function defined on n Riemann sheets. The energy

labels in Eqs. (5) and (6) enumerate the respective Riemann sheet according to the ordering of energies at real λ . The degeneracy points are square-root branch points where the Riemann sheets are pairwise (in generic cases) connected. The leading-order behavior on the two connected sheets close to the branch point λ_0 is given by $E(\lambda) - E(\lambda_0) \approx a\sqrt{\lambda - \lambda_0}$ (as a doubly valued function), with a being a complex constant [5,26,27].

The relation of branch points to QPTs has been declared several times—see, for example, Refs. [5,8,11]. Clearly, a branch point located close to the real λ axis affects the local evolution of the corresponding pair of real energies so that the two levels undergo an avoided crossing with accompanying rapid changes of wave functions. A cumulation of branch points close to some real point λ_c thus can give rise to massive structural changes of eigenstates, as observed in QPTs. Although this mechanism was illustrated by several model examples [5,8,11], quantitative determination of the arrangement and density of branch points needed to trigger a phase-transitional behavior is still missing.

We will argue that such a criterion can be derived from the above-mentioned surmise concerning branch points and zeros of partition functions. Namely, a link will be established between the l th-order QPT distribution of the g.s.-related branch points and a distribution of complex zeros of the classical partition function $Z(T)$ characterizing an l th-order thermodynamic phase transition. To this end, we assume the correspondence $Z(T) \leftrightarrow D_0(\lambda)$, where D_0 stands for the $k = 0$ partial discriminant (6). This means that (in a QPT case) the partial discriminant $D_0(\lambda)$ is to be treated in the same way as if it were a partition function $Z(T)$ of a fictitious classical system undergoing classical phase transition (so $Z(T)$ is *not* the actual partition function of the QPT system). Recall that the square D_k^2 of any partial discriminant is a polynomial with $n - 1$ complex conjugate pairs of roots, each of them being simultaneously assigned to one other D_k^2 . These roots correspond to the branch points located on the k th Riemann sheet. Thus zeros of D_0 represent singularities on the g.s. Riemann sheet that are now assumed to play a role similar to zeros of $Z(T)$ in standard phase transitions.

This correspondence allows us to find a quantum counterpart of the thermodynamic potential $F_0 = -T \ln Z$. It is proportional to the g.s. “potential energy,” $U = -\sum_{i>0} \ln |E_i - E_0|$, as obtained in the static Coulomb-gas description of quantal spectra [30]. For the “specific heat” one obtains

$$\begin{aligned} C_2 &= -S\lambda \frac{d^2(\lambda U)}{d\lambda^2} \\ &= S \sum_{i>0} \left[\lambda^2 \left\{ \frac{\frac{d^2 E_i}{d\lambda^2} - \frac{d^2 E_0}{d\lambda^2}}{E_i - E_0} - \left(\frac{\frac{dE_i}{d\lambda} - \frac{dE_0}{d\lambda}}{E_i - E_0} \right)^2 \right\} \right. \\ &\quad \left. + 2\lambda \left(\frac{\frac{dE_i}{d\lambda} - \frac{dE_0}{d\lambda}}{E_i - E_0} \right) \right]. \end{aligned} \quad (7)$$

The first expression here is analogous to Eq. (2), but with E_0 replaced by λU . The second formula in Eq. (7) can be further decomposed, using the Pechukas-Yukawa method [31] as in Eq. (2), into a double sum of terms containing matrix

elements of V and energy differences. (The result is not shown here.) Note that any power of D_0 used in this thermodynamic correspondence (the power is, in fact, arbitrary) would modify just the scaling factor S . This factor must also depend on the size of the system and will be discussed later.

A direct numerical determination of the g.s. branch points is prohibitively difficult for large dimensions. (IBM results for $N = 20$ are shown in Ref. [32], but with no distinction between branch points lying on different Riemann sheets.) However, the quantity C_2 , which is easily computable and depends solely on real- λ observables, represents an *indirect measure* of the density of branch points on the g.s. Riemann sheet near the real axis. Consider, as a simplified example, a chain $\lambda_{\pm m} = \lambda_c \pm i\tilde{\lambda}_m$ (with $\tilde{\lambda}_m \leq \tilde{\lambda}_{m+1}$) of complex-conjugate pairs of zeros of D_0 along a line perpendicular to the real axis. If $\tilde{\lambda}_1 \rightarrow 0$ when the system’s size (N) increases to infinity, a QPT will most probably occur at λ_c (with little space being left for an unlikely nonanalytic but still smooth behavior of $E_0(\lambda)$ at λ_c). Let $\rho(\tilde{\lambda})$ be a density of branch points along the $\lambda_c + i\tilde{\lambda}$ line for $N \rightarrow \infty$. The D_0^2 polynomial is determined (up to a multiplicative constant) by the roots, and specific heat (7) is for real λ given by

$$C_2 \propto \lambda^2 \int_0^\infty \frac{\rho(\tilde{\lambda})(\tilde{\lambda}^2 - \Delta^2)}{(\tilde{\lambda}^2 + \Delta^2)^2} d\tilde{\lambda} + 2\lambda\Delta \int_0^\infty \frac{\rho(\tilde{\lambda})}{\tilde{\lambda}^2 + \Delta^2} d\tilde{\lambda}, \quad (8)$$

where $\Delta = \lambda - \lambda_c$. This implies that the “latent heat” $Q = \lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{+\epsilon} C_2(\Delta) d\Delta$ is zero if $\rho(\tilde{\lambda})$ decreases sufficiently fast when approaching the real axis. A rate of the $\rho(\tilde{\lambda})$ decrease can, in fact, help us to classify the corresponding QPT.

In particular, if in this example $\rho(\tilde{\lambda}) \sim \tilde{\lambda}^\alpha$ for $\tilde{\lambda}$ close to zero, we obtain the following possibilities: (i) a “first-order” QPT, with $C_2 \rightarrow \infty$ at $\Delta = 0$ and Q finite, for $\alpha = 0$, (ii) a “second-order” QPT, with $C_2 \rightarrow \infty$ but $Q = 0$, for $\alpha \in (0, 1]$, and (iii) a “higher order” QPT, with C_2 finite and $Q = 0$, for $\alpha > 1$. This relation is the same as in standard thermodynamics, where the order of a phase transition reflects the density of the $Z(T)$ zeros close to a critical temperature T_c [22]. In the QPT case, however, there is no direct connection between C_2 and the form of $E_0(\lambda)$, so it must be stressed that the “order” deduced from C_2 cannot be *a priori* expected to coincide with the order determined via C_1 . In the following we focus on this problem showing that the IBM first- and second-order QPTs (in the sense of C_1) are correctly distinguished by C_2 if the scaling factor S involves a natural dependence on the relevant dimension n .

The specific heat C_2 in the IBM first- and second-order QPT for $S = 1$ is shown in Fig. 2, where panels (a) and (b) again correspond to $\chi = -\sqrt{7}/2$ and 0, respectively. All the levels with $J = 0$ were included in the sum (7). We know that for $\chi = 0$ some pairs of levels actually cross at real λ (owing to the seniority quantum number ν that survives all the way across the transition [33]). This implies discontinuities and singularities of some first and second derivatives in Eq. (7), which however cancel out exactly and do not affect the C_2 shape in Fig. 2(b) [32]. Let us stress that since the g.s. branch points in the IBM are not aligned perpendicularly to the real axis, formula (8) does not apply here.

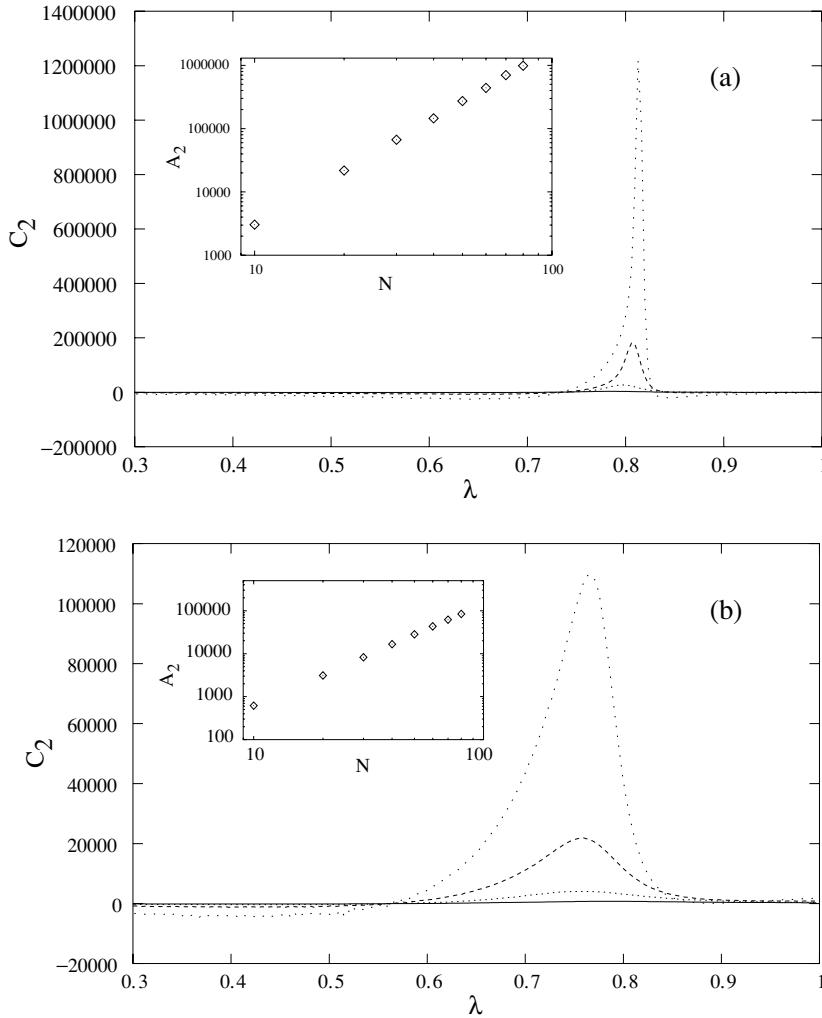


FIG. 2. The same as in Fig. 1 but for “specific heat” (7) including all $J = 0$ states.

It is clear that the peaks in panels (a) of both Figs. 1 and 2 are sharper and higher than those in panels (b), as indeed expected in the first- and second-order phase transitions. The log-log insets in these figures indicate that maximal values— A_1 and A_2 —in the C_1 and C_2 peaks exhibit roughly an algebraic increase with the boson number. The increase is faster for the first-order QPT than for the second-order one.

With a proper normalization to the system’s size, the values of A_1 and A_2 corresponding to the second-order QPT have finite $N \rightarrow \infty$ asymptotics, whereas these values for the first-order QPT, normalized in the same way, diverge. To prove this, we show in Fig. 3 the dependence of A_1/N and A_2/N^2 for the second-order QPT on the boson number up to $N = 1000$. The calculation for such high dimensions was enabled by the underlying $O(5)$ symmetry for $\chi = 0$ [33]. Clearly, the curves in Fig. 3 have finite asymptotics. The behavior of A_1 is consistent with the analytic result $A_1/N \rightarrow 12.5$ that can be derived from the $N \rightarrow \infty$ limit of the g.s. energy per boson [2]. Similar analytic calculation for $\chi \neq 0$ shows a divergence of C_1/N at $\lambda_c(\chi)$ in the first-order QPT.

Specific heat C_2 in Fig. 2 behaves in a similar way, but—as follows from Fig. 3—in this case the correct normalization is by $1/N^2$. This factor reflects the dimension of the subspace of states with $J = 0$, which grows roughly as $n \sim N^2/12$ for very

large boson numbers (whereas the total number of IBM states is $\sim N^5/120$). Since there are $n - 1$ pairs of branch points on each Riemann sheet, the choice of $S = 1/(n - 1) \propto 1/N^2$ in Eq. (7) normalizes the density $\rho(\tilde{\lambda})$ [cf. Eq. (8)] in the finite- n case to a unit integral. Again, the faster increase of A_2 for $\chi = \sqrt{7}/2$ [see Fig. 2(a)] indicates a divergence of C_2/N^2 in the first-order transitions.

Therefore, we can conclude that the quantity C_2 , which was derived directly from the initial surmise introducing the thermodynamic analogy discussed here, with $S \sim 1/n$, yields a plausible analog of specific heat in the IBM. It can be seen as a mere alternative of C_1 , but more appropriately it should be recognized as a direct reflection of the mechanism underlying QPT behavior, which is based on specific arrangements of branch points, similar to arrangements of a partition function’s complex zeros. It is also possible to further test the validity of this description by restricting the sum in Eq. (7) for $\chi = 0$ only to $J = 0$ states with seniority $v = 0$. In this case, the dimension increases as $n \sim N/2$, so that $S \propto 1/N$ should represent the proper normalization. Unfortunately, the convergence of A_2/N to a postulated finite asymptotic value (if any) is very slow in this case and the results (although compatible with the aforementioned assumption) are not fully conclusive; see Ref. [32] for details.

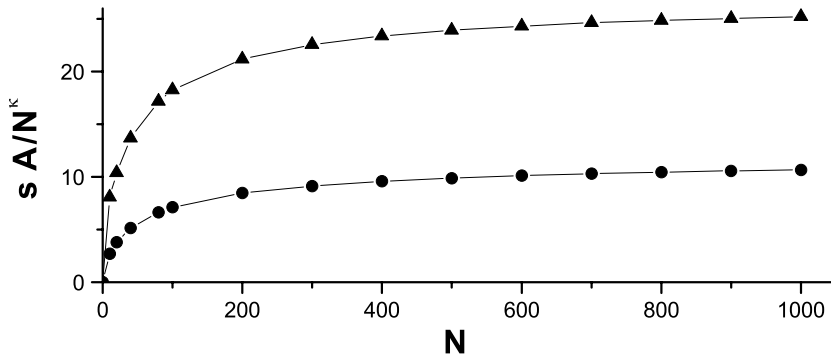


FIG. 3. Normalized maximal values A_1/N (dots) and $10A_2/N^2$ (triangles) of “specific heat” (2) and (7) in the IBM second-order QPT ($\chi = 0$) for very large boson numbers.

In summary, we proposed a method capable of indirectly measuring the distribution of branch points of the Hamiltonian (1) on the g.s. Riemann sheet near the real- λ axis. This distribution is of great importance in the fundamental theory of quantum phase transitions. The method is based on the analogy between generic QPT arrangements of branch points and similar behaviors of complex zeros of the canonical partition function in thermodynamic phase transitions. Our approach was tested in the first- and second-order QPTs of the interacting boson model, where the “specific heat” C_2 from Eq. (7), normalized with respect to the relevant

dimension, turned out to behave in the same way as standard specific heat in typical thermodynamic phase transitions of the respective orders. We expect that the method is applicable also in other QPT systems. It discloses a surprising analogy between standard thermodynamics and quantum mechanics of parameter-dependent systems.

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