Thermal Critical Dynamics from Equilibrium Quantum Fluctuations

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We show that quantum fluctuations display a singularity at thermal critical points, involving the dynamical z exponent. Quantum fluctuations, captured by the quantum variance [Frérot *et al.*, Phys. Rev. B **94**, 075121 (2016)], can be expressed via purely static quantities; this in turn allows us to extract the z exponent related to the intrinsic Hamiltonian dynamics via *equilibrium* unbiased numerical calculations, without invoking any effective classical model for the critical dynamics. These findings illustrate that, unlike classical systems, in quantum systems static and dynamic properties remain inextricably linked even at finite-temperature transitions, provided that one focuses on static quantities that do not bear any classical analog—namely, on quantum fluctuations.

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Characterizing the dynamical behavior of systems close to symmetry-breaking phase transitions [1] has far-reaching implications, ranging from our understanding of the early Universe to the behavior of interacting systems in laboratory experiments [2–4]. Indeed, close to a critical point, the fluctuations of the order parameter become correlated over a characteristic distance (the correlation length ξ) which can exceed arbitrarily the microscopic length (namely, the distance between the elementary constituents); as a consequence, such fluctuations build up over a characteristic timescale (the relaxation time t_c) much larger than microscopic timescales. In particular, in the vicinity of a thermal critical point at temperature T_c, ξ and t_c are expected to be related to the temperature T via

$$t_c \sim \xi^z \sim |T - T_c|^{-\nu z}, \tag{1}$$

where ν governs the divergence of ξ: and z is the dynamical exponent [1,5] governing the so-called critical slowing down of the order-parameter dynamics. A central goal of the study of critical phenomena is the evaluation of the various critical exponents for a given universality class.

A fundamental paradigm in classical physics is that, in order to extract the dynamical exponent z at a thermal phase transition, it is necessary to go beyond static thermodynamic observables, and to investigate instead the dynamics at criticality. Indeed, all static quantities can be obtained from the knowledge of the free energy $F = -k_B T \log Z$ (where Z is the partition function) and of its derivatives; and, for classical systems, F is completely independent of the dynamics. As a matter of fact, quantities such as position and momentum enter independently in the statistical sum over phase space, and, as an example, the partition function of a system of classical particles is fully independent of whether these particles have a ballistic dynamics, a stochastic dynamics, etc.; therefore the dynamical exponent z cannot be obtained from the knowledge of the free energy. On the other hand, the z exponent governs the singular behavior of dynamics, in accordance with dynamical scaling theory [1], which has been confirmed either directly by measuring the dynamical response functions in the vicinity of a critical point [6–9]; indirectly via signatures of the Kibble-Zurek mechanism [10,11]; and in numerical simulations of the dynamics of (classical) microscopic models or classical field theories [12–18].

In the case of quantum systems, extracting *ab initio* the z exponent at thermal transitions for a given quantum Hamiltonian represents a notoriously difficult task. On the theory side, the effective coarse-grained dynamics to be studied can severely depend on the approximations made (e.g., how collective modes are effectively included), see, for instance, Refs. [19–21]; in numerical simulations, computing the fully quantum real-time dynamics, or performing the analytical continuation of imaginary-time correlators [22], are prohibitive tasks for many-body quantum systems.

Yet, in spite of the above cited difficulties to investigate their dynamics, quantum systems differ fundamentally from classical ones in that, in quantum mechanics, static and dynamic properties remain inextricably intertwined. As a striking illustration, at zero-temperature (quantum) phase transitions the corresponding dynamical exponent does govern the scaling of the (free) energy [23]. The link between statics and dynamics must remain true at finite-temperature transitions as well, given that the quantum-mechanical partition function is the trace of the imaginary-time evolution operator. In this Letter we probe this connection by considering microscopic quantum models possessing a thermal phase transition, and whose order parameter is not a conserved quantity; namely, it does not commute with the Hamiltonian. As a consequence, the order parameter has quantum fluctuations in addition to thermal fluctuations [24,25]. We show that these quantum fluctuations exhibit a weak singularity at thermal transitions, governed by a combination of critical exponents involving the dynamical z exponent.

Our prediction for the singularity of quantum fluctuations stems from the dynamical scaling hypothesis, the fluctuation-dissipation theorem and Kramers-Kronig relations; and it is rigorously verified using several exactly solvable quantum models of thermal phase transitions. As quantum fluctuations can be obtained from the partition function, this singularity establishes a fundamental link between the thermal critical dynamics of a quantum system and its statistical properties. Our results are not in contradiction with the notion that thermal criticality is fundamentally of classical origin, as the leading singular behavior of the order-parameter fluctuations coincides with that of the classical limit of the models of interest; yet quantum fluctuations of the order parameter introduce a *subleading* singular behavior (containing the exponent z) which can be analytically singled out, and which disappears in the classical limit. At the practical level, this insight allows one to extract the thermal z exponent of microscopic quantum Hamiltonians without simulating the many-body dynamics at all. We demonstrate that our approach can be carried out successfully via numerically exact quantum Monte Carlo (QMC) calculations on paradigmatic quantum spin models exhibiting thermal transitions.

To avoid any confusion, it should be stressed that the behavior of quantum fluctuations at thermal critical points, as studied in this Letter, is completely independent of their behavior at (zero-temperature) quantum critical points [23,26–28], which are of no relevance to the present study. We also stress that the thermal singularity of quantum fluctuations is different from that of entanglement estimators, such as negativity, whose thermal critical behavior still lacks a general understanding [29–32].

Dynamical scaling hypothesis, and thermal singularity of the quantum variance.—The linear response of a system at thermal equilibrium to a weak time-dependent perturbation is characterized by its dynamical susceptibility [1,33]. If O denotes the order parameter of a symmetry-breaking phase transition, and if a weak time-dependent perturbation in the form $-f(t)O$ is added to the Hamiltonian $\mathcal{H}$ of the system, the dynamical susceptibility is defined as $\chi_O(\omega) = \delta\langle O\rangle(\omega)/\delta f(\omega)|_{f=0}$, where $\langle O\rangle(\omega)$ and $f(\omega)$ are the Fourier transforms of $\langle O\rangle(t)$ and $f(t)$, respectively. Here, $\langle O\rangle(t) = Z^{-1}\mathrm{Tr}[O(t)\exp(-\beta\mathcal{H})]$ denotes an average over the equilibrium distribution at inverse temperature $\beta = (k_B T)^{-1}$, with k_B the Boltzmann constant, and $O(t) = e^{i\mathcal{H}t/\hbar}Oe^{-i\mathcal{H}t/\hbar}$ is the time-evolved operator in the Heisenberg picture. According to the dynamical scaling hypothesis [1,5], close to the critical point, the singular part of the spectral function $\chi''_O(t) = (1/2\hbar)\langle[O(t), O(0)]\rangle$ (the imaginary part of $\chi_O(t)$) obeys in Fourier space the scaling form

$$[\chi''_O(\omega)]_s = [\chi^{(0)}_O]_s\, g\left(\frac{\omega}{\omega_c}\right), \qquad (2)$$

where $\omega_c \sim t_c^{-1} \sim |T - T_c|^{\nu z}$; $g(x)$ is a scaling function such that $\int dx g(x)/x = \pi$; and $[\chi^{(0)}_O]_s \sim |T - T_c|^{-\gamma}$ is the singular part of the static susceptibility of the order parameter with critical exponent γ.

In classical systems the variance of the order parameter $\mathrm{Var}(O) = \langle O^2\rangle - \langle O\rangle^2$ is related to the susceptibility via the fluctuation-response relation $\mathrm{Var}(O) = k_B T\chi^{(0)}_O$, and therefore it exhibits the same power-law singularity. In quantum systems, the above relation holds only if O is a conserved quantity, namely, if $[\mathcal{H}, O] = 0$; otherwise quantum fluctuations are responsible for an extra contribution to the variance, the quantum variance (QV), $\mathrm{Var}_Q(O) = \mathrm{Var}(O) - k_B T\chi^{(0)}_O > 0$ [24]. Our central result is that, at thermal criticality, the QV of the order parameter (along with a whole family of coherence measures to which it belongs) acquires a singular part scaling as

$$[\mathrm{Var}_Q(O)]_s \approx A_1|T - T_c|^{2\nu z-\gamma} + A_2|T - T_c|^{4\nu z-\gamma} + \cdots. \qquad (3)$$

Given that $2\nu z - \gamma \geq 0$ for all the universality classes reported in the literature [1,5] this result has the immediate implication that the QV of the order parameter does *not* diverge at the critical point, despite being the difference between two divergent quantities. This is consistent with the intuition that quantum fluctuations do not alter the long wavelength behavior of the system at thermal criticality—in fact, their characteristic length scale, the quantum coherence length, remains finite even at T_c [34]. At the same time, the weak singularity of the QV fully exposes the dynamical critical exponent, despite depending only on equilibrium fluctuations and the static response of the system.

Proof of the main result.—Equation (3) follows directly from the dynamical scaling hypothesis [Eq. (2)]. It is indeed a basic result of linear response theory that both $\mathrm{Var}(O)$ and $\chi^{(0)}_O$ can be expressed in terms of the imaginary part of the dynamical susceptibility [1,33]:

$$\mathrm{Var}(O) = \hbar \int_0^\infty \frac{d\omega}{\pi} \coth(\beta\hbar\omega/2)\chi''_O(\omega),$$
$$\chi_O^{(0)} = 2\int_0^\infty \frac{d\omega}{\pi}\frac{\chi''_O(\omega)}{\omega}. \quad (4)$$

The first line is a consequence of the fluctuation-dissipation theorem [35], and the second of causality [1,33]. Consequently, the QV admits the following expression

$$\mathrm{Var}_Q(O) = \hbar \int_0^\infty \frac{d\omega}{\pi} h_{\mathrm{QV}}(\beta\hbar\omega)\chi''_O(\omega), \quad (5)$$

where $h_{\mathrm{QV}}(x) = \coth(x/2) - 2/x$ filters out the low frequency modes in the integral (namely, the modes such that $\hbar\omega \ll k_B T$). In contrast, the functions of which is it composed [$\coth(x/2)$ and $2/x$] both diverge at zero frequency. The dynamical scaling hypothesis, Eq. (2), suggests that the characteristic frequency singled out by $\chi''_O(\omega)$ (corresponding, e.g., to its maximum), moves to zero as $T \to T_c$, and therefore the critical singularity of both $\mathrm{Var}(O)$ and $\chi_O^{(0)}$ stems from the critical enhancement of the zero frequency contribution to the integrals Eq. (4). Similarly, the singular part of the quantum variance must also stem from the low-frequency part of the integral Eq. (5). Assuming on other hand that $\chi''_O(\omega)$ vanishes as $\omega \to \infty$ faster than any power [36] we may then Taylor expand $h_{\mathrm{QV}}(x)$ at low frequency as $h_{\mathrm{QV}}(x) = x/6 - x^3/360 + \ldots$, to obtain

$$[\mathrm{Var}_Q(O)]_s \approx [\chi_O^{(0)}]_s \left[\frac{(\hbar\omega_c)^2}{k_B T}\mathcal{I}_1 + \frac{(\hbar\omega_c)^4}{(k_B T)^3}\mathcal{I}_2 + \cdots\right], \quad (6)$$

where $\mathcal{I}_1 = (6\pi)^{-1}\int_0^\infty dx\, x g(x)$, $\mathcal{I}_2 = -(360\pi)^{-1} \times \int_0^\infty dx\, x^3 g(x)$, etc. Given the critical behavior of $[\chi_O^{(0)}]_s$ and ω_c, we obtain Eq. (3).

Extension to asymmetry measures.—Equation (5) is very similar to an expression derived for the quantum Fisher information (QFI) [26] [with $h_{\mathrm{QFI}}(x) = \tanh(x/2)$], and in fact, both the QV and the QFI belong to a larger family of so-called quantum coherence (or "asymmetry") estimators [25], all admitting an analogous expression in term of χ'' (see the Supplemental Material [37] for further details). Most importantly, for all the coherence measures of this family the "quantum filter" $h(x)$ appearing in the frequency integrals of the dynamical susceptibility has an odd parity, and therefore is linear at low frequency [26,37]. The latter property, together with the dynamical scaling hypothesis [Eq. (2)], are the only requirements leading to Eq. (3); hence our result immediately applies to all of them. In the specific case of the QFI, our result rectifies a statement of Ref. [26] on the absence of thermal singularities [37].

Two exactly solvable models.—We first illustrate our findings with two quadratic models which belong to the same static universality class, yet have different z exponents (we also treat the case of a quantum Ising model with infinite range interaction in Supplemental Material [37]). The first one is the so-called quantum spherical model (QSM) on a d-dimensional lattice [44–46], defined by the Hamiltonian $\mathcal{H}_{\mathrm{QSM}} = (g/2)\sum_i P_i^2 + (1/2g)\sum_{i,j} U(i,j) X_i X_j + \lambda[\sum_i X_i^2 - (N/4)]$, where $[X_i, P_i] = i\hbar\delta_{ij}$, and $U(i,j)$ defines the interaction. The second model describes a Bose-Einstein condensation (BEC) transition [47–49], and is defined by $\mathcal{H}_{\mathrm{BEC}} = -\mu N_B + \sum_{\mathbf{k}}(\epsilon_k + \mu)a^\dagger_{\mathbf{k}} a_{\mathbf{k}}$, $[a_{\mathbf{k}}, a^\dagger_{\mathbf{l}}] = \delta_{kl}$. The Lagrange parameter λ (μ) imposes the constraint $\sum_i \langle X_i^2\rangle = N/4$ ($\sum_{\mathbf{k}}\langle a^\dagger_{\mathbf{k}} a_{\mathbf{k}}\rangle = N_B$), with N the number of sites (N_B the number of bosons). In both models, we assume that at small momenta $\epsilon_k \sim U_k \sim k^x$, with $d < x < 2d$ ($x = 2$ corresponds to short-range interactions in the QSM). Both models have a phase transition at a critical temperature T_c, and belong to the universality class of the spherical model [50,51], with exponents $\nu = [1/(d-x)]$ and $\gamma = [x/(d-x)]$ [46,49,51], so that $\lambda, \mu \propto |T - T_c|^{[x/(d-x)]}$. In the Supplemental Material [37], we show that for the QSM, the dynamical exponent is $z_{\mathrm{QSM}} = x/2$, and that the QV of the order parameter ($O_{\mathrm{QSM}} = N^{-1/2}\sum_i X_i$) is $\mathrm{Var}_Q(O_{\mathrm{QSM}}) = (\hbar g/2\omega_0) h_{\mathrm{QV}}(\beta\hbar\omega_0)$, with critical frequency $\omega_0 = \sqrt{2g\lambda}$. For the bosons ($O_{\mathrm{BEC}} = a_{\mathbf{0}} + a^\dagger_{\mathbf{0}}$), we find $z_{\mathrm{BEC}} = x$ and $\mathrm{Var}_Q(O_{\mathrm{BEC}}) = h_{\mathrm{QV}}(\beta\mu)$. Close to criticality, we therefore obtain

$$\mathrm{Var}_Q(O_{\mathrm{QSM}}) = \frac{\hbar^2 g}{12 k_B T} - \frac{\hbar^4 g^2 \lambda}{720(k_B T)^3} + \ldots,$$
$$\mathrm{Var}_Q(O_{\mathrm{BEC}}) = \frac{\mu}{6 k_B T} - \frac{\mu^3}{360(k_B T)^3} + \ldots. \quad (7)$$

The singular part of the QV in the QSM model stems from the (negative) $\mathcal{I}_2$ contribution to Eq. (6), scaling as $|T - T_c|^{4\nu z - \gamma}$, which is consistent with $z_{\mathrm{QSM}} = x/2$. Remarkably, the QV vanishes at the BEC transition, as well as in the whole BEC phase [52]. The singular contribution scales as $|T - T_c|^{2\nu z - \gamma}$ [Eq. (3)], which is consistent with $z_{\mathrm{BEC}} = x$.

Extraction of the dynamical exponent using QMC.— The QV can be calculated for *any* quantum model whose thermodynamics can be calculated efficiently [24], opening the route for a systematic calculation of the z exponent in a large class of quantum many-body systems. We illustrate this possibility by focusing on four paradigmatic models exhibiting a finite-temperature transition, defined on d-dimensional (hyper-)cubic lattices of size L^d: (i) the $2d$ ferromagnetic transverse-field Ising model (TFIM) $\mathcal{H}_{\mathrm{TFIM}} = -J\sum_{\langle ij\rangle} S_i^z S_j^z - \Gamma\sum_i S_i^x$ with $\Gamma/J = 1.3$; and the XXZ model $\mathcal{H}_{\mathrm{XXZ}} = -J\sum_{\langle ij\rangle}(S_i^x S_j^x + S_i^y S_j^y - \Delta S_i^z S_j^z)$ (with $J < 0$) in the three following cases: (ii) $2d$ easy-axis model ($\Delta = 1.2$); (iii) $3d$ XX model ($\Delta = 0$); and (iv) $3d$ Heisenberg model $\Delta = 1$) [53]. For all models $\langle ij\rangle$ are nearest-neighbor pairs on a d-dimensional lattice. All four models possess a finite-temperature transition. For models (i) and (ii), the transition belongs to the $2d$ Ising universality class. However in model (ii) the magnetization along z is conserved: it represents a diffusive mode which could potentially couple to the order parameter and alter the z exponent with respect to model (i) [1]. Model (iii) is representative of the $3d$ XY universality class, and model (iv) of the $3d$ Heisenberg class. We investigate all models using quantum Monte Carlo based on stochastic series expansion [54] which allows us to reconstruct the QV (as already shown in Refs. [24,27,28]). The system sizes we analyze ($L = 64$ in $d = 2$; $L = 28$ in $d = 3$) are not the largest ones we can simulate, but the QV exhibits very little scaling beyond these sizes [37], while its precision degrades significantly in the ordered phase, as the QV (per spin) is the nondiverging difference between two divergent quantities. For all the models, T_c is estimated by a scaling analysis of the full variance of the order parameter (scaling as $L^{\gamma/\nu}$ at the transition point).

The QV per spin of the order parameter (uniform magnetization $O = J^z$ for the $2d$ TFIM, $O = J^x$ for the $3d$ XX model, and staggered magnetization $O = J^z_{\rm st}$ for the $2d$ XXZ model and the $3d$ Heisenberg model) shows a clear anomaly at the phase transition (Fig. 1). It is then fitted as

$$\mathrm{Var}_Q(O)(T) = a_0 + a_1 T + a_2 T^2 + [A_+\theta(\delta) + A_-\theta(-\delta)]|\delta|^{2\nu z-\gamma}, \quad (8)$$

where $\delta = T - T_c$, and θ is the Heaviside step function. The first line is a parabolic fit to the regular part, while the second line is a fit to the dominant term of the singular part (the critical exponents ν and γ are known for each universality class [55]). In principle we have six fitting parameters $(a_0, a_1, a_2, A_+, A_-, z)$, which are nonetheless further reduced: (a) for the $d = 2$ models [(i) and (ii)], we set $A_- = 0$, as suggested by the smallness of A_- when treated as a free parameter; (b) for the $d = 3$ models, we set $A_+ = 0$ (for the same reason as above) as well as $a_2 = 0$. A subtle aspect of the fits is the discrimination of the singular part from the regular one, since both are nondivergent. This is particularly true for the models (i) and (ii), for which an alternative fitting analysis is presented in the Supplemental Material [37].

We perform our fits to Eq. (8) over windows of variable width $[T_c - w, T_c + w]$ around the critical point. Figure 1 shows the results: the fit quality is always very good for all four models, with $(\chi^2)_{\rm red}$ (χ^2 per degree of freedom) systematically reaching values around 1 upon shrinking the fitting window down to the relevant critical region. As for our final estimates of z, we retain the values at which $(\chi^2)_{\rm red} \approx 1$ and for which the fitted value has converged upon reducing w (within the error bar): (i) $z = 1.95(15)$; (ii) $z = 1.95(10)$; (iii) $z = 1.61(15)$; and (iv) $z = 1.36(10)$. Models (i) and (ii) ($2d$ Ising universality class) could potentially be captured by Model C ($z = 2$) [1,5]. The alternative fitting strategy presented in the Supplemental Material [37] gives $z = 1.88(10)$ for model (ii), compatible with $z = 1.95(10)$ obtained above, while it gives $z \simeq 1.65(5)$ for model (i), closer to experimental results on quasi-$2d$ magnets ($z \approx 1.6$–1.8) [8,9,56–58]. For model (iii), our estimate is compatible with that obtained by Ref. [13] ($z = 1.62$) via a dynamical simulation of the classical 3D XY model. As for model (iv), our estimate is slightly lower but compatible with $z = 1.49(3)$ obtained via dynamical simulations of classical Heisenberg antiferromagnets [12,14,59], and with the experimental estimate from neutron scattering studies of quantum Heisenberg antiferromagnets [60,61].

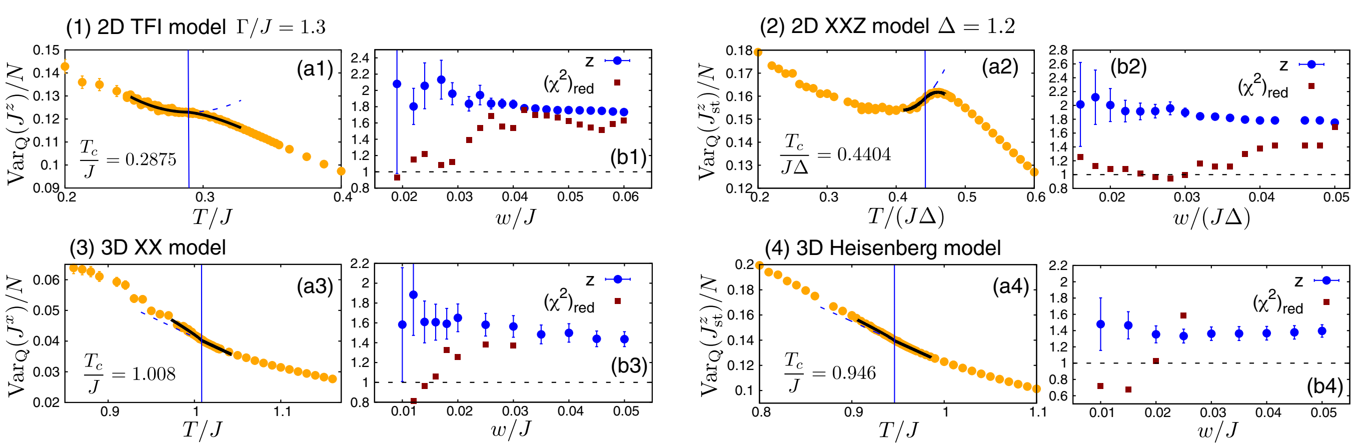

FIG. 1. Thermal singularity of the quantum variance from QMC results, and fitted z exponents. The (a1)–(a4) panels show the quantum variance of the order parameter close to the transition, together with a representative fit (black line) and the fitted regular part (blue dashed line); the vertical line marks the transition point. The (b1)–(b4) panels show the resulting fitted z exponent as a function of the fitting window width w around T_c, along with the reduced χ^2 (the dashed line marks the unity threshold). (a1)–(b1): $2d$ TFIM ($\Gamma/J = 1.3$—lattice size $L = 64$); (a2)–(b2) $2d$ antiferromagnetic XXZ model ($\Delta = 1.2$, $L = 64$); (a3)–(b3) 3D XX model ($L = 28$); (a4)–(b4) 3D Heisenberg model ($L = 28$).

Conclusions.—We have shown that the dynamical exponent z, governing the critical slowing down of the dynamics close to a second-order thermal phase transition of a quantum system, manifests itself in a weak singularity of the quantum fluctuations of the order parameter. This general result was illustrated by two exactly solvable models with the same thermodynamic criticality but different critical dynamics; by a quantum spin model with infinite-range interactions amenable to exact diagonalization for large system sizes (as discussed in the Supplemental Material [37]); and exploited to extract the exponent z in four quantum spin models in $d = 2$ and $d = 3$ from unbiased QMC data. Our scheme gives access to the z exponent associated with the *intrinsic* Hamiltonian dynamics (in the absence of any external bath) without the need to simulate the real-time quantum dynamics itself (which is a prohibitive numerical task); and the z exponent can be extracted from numerical (e.g., QMC) data without the need for analytic continuation (which is also a very demanding task). Here we have focused on the singularity of quantum fluctuations of the order parameter, but other quantities are expected to display similar singularities exposing the z exponent, offering alternative strategies for its numerical evaluation. Therefore our approach opens a way to the calculation of dynamical critical exponents for the Hamiltonian dynamics of a large class of quantum many-body models—something which is of extreme importance in the light of the recent generation of experiments addressing the dynamics of closed quantum systems close to critical points [4,10,62,63]. Moreover, the ability of inelastic neutron scattering experiments to reconstruct quantum coherence estimators [64–67] along with dynamical critical scaling [6] could lead to a direct test of our predictions within the same experimental platform. Finally, at a fundamental level, the precise connection between microscopic quantum models (as studied in this Letter) and effective classical theories [1,5,13–15] is a fascinating topic for future investigations.

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[37] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.128.130601, which contains Refs. [38–43], for (i) a discussion of the singularity of quantum coherence estimators; the calculation of the z exponent and the quantum variance for (ii) the quantum spherical model and (iii) the Bose-Einstein condensation model with mean-field interactions; (iv) the discussion of the singularity of the quantum variance and quantum Fisher information for the transverse-field Ising model with all-to-all interactions; and (v) a detailed discussion of the quantum Monte Carlo results and their fits.

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