Universality class and exact phase boundary in the superradiant phase transition

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The Dicke model and the Rabi model can undergo phase transitions from the normal phase to the superradiant phase at the same boundary, which can be accurately determined using some approximated approaches. The underlying mechanism for this coincidence is still unclear, and the universality class of these two models is elusive. Here we prove this phase transition exactly using the path-integral approach based on the faithful Schwinger fermion representation, and give a unified phase boundary condition for these models. We demonstrate that at the phase boundary, the fluctuation of the bosonic field is vanished, thus, it can be treated as a classical field, based on which a much simplified method to determine the phase boundary is developed. This explains why the approximated theories by treating the operators as classical variables can yield the exact boundary. We use this method to study several similar spin and boson models, showing its much wider applicability than the previously used approaches. Our results demonstrate that these phase transitions belong to the same universality by the classical Landau theory of phase transition from a more general way, which can be confirmed using the platforms in the recent experiments.

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I. INTRODUCTION

The Dicke model has been studied for more than half a century [1–4]. This model considers the coupling between N identical atoms (or two-level systems) with a bosonic field, which can be written as

$$\mathcal{H} = \omega b^\dagger b + \sum_{i=1}^{N} \frac{\Omega}{2}\sigma_i^z + \frac{g}{\sqrt{N}}\sigma_i^x(b + b^\dagger). \tag{1}$$

Here b is the annihilation operator for the bosonic field, σ_i^x, σ_i^z are the Pauli operators for the ith atom, and N is the total number of atoms. This model undergoes a phase transition from a normal phase to a superradiant phase at $g_c^2 = \frac{\Omega\omega}{4}\coth\frac{\beta\Omega}{2}$ [5–7], where $\beta = 1/k_B T$ with k_B as the Boltzmann constant and T is the temperature. The phase transition can be obtained from the Holstein-Primakoff (HP) method [8,9] and semiclassical method [10,11] in which negative or complex eigenvalues mark the ground-state instability. It is challenging to be realized with atoms in radiation-plus-matter field due to not only the required large density, but also the no-go theorem [12–15]. However, it can be realized with ultracold atoms [16–22], driven-dissipative quantum simulators [23,24], spin-orbit coupled condensates in a trap [25], and electron gases in a cavity [26].

Recently, the phase transition with only one atom has attracted widespread attention [27–32]. When $N = 1$, Eq. (1) is reduced to the exact solvable quantum Rabi model [33–35]. A great effort has been devoted in experiments trying to push the light-matter interaction strength g from the strong-coupling regime (with g larger than the dissipation rate) [36–38] to the ultrastrong coupling ($g \sim 0.1\Omega$) [39–42] and even the deep strong-coupling regimes [43]. This model has broad application in cold atoms [44], trapped ions [45–49], quantum dots [50], cavity QED [51,52], and superconducting circuits [41,53]. It plays as a testing ground for strong-coupling physics. Meanwhile, the calculation of its full spectra with the help of integrability is also of general interest [54]. It was shown [27,29] that the phase transition is realized when $\frac{\omega}{\Omega} \to 0$ at g_c. In Ref. [29], the critical exponent $\nu = 1/2$ is the same as that from the Landau theory of phase transition. The universal dynamics is also formulated using the Kibble-Zurek mechanism, which was established based on second-order phase transitions [55,56].

The phase transition in the Rabi model can be obtained using the simplest perturbation theory and the effective Hamiltonian approach by some truncation at $T = 0$ [27,29]. However, it is surprising that whereas approximations are involved in various approaches, the predicted critical boundary is shown to be exact. This should not be regarded as some kind of coincidence [57,58], which is an unsolved puzzle in theory. We unveil the underlying origin based on the path-integral approach with Schwinger fermion representation. We demonstrate that the phase transitions in the above two models belong to the same universality class by the Landau theory of phase transitions from which the previous conclusions,

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such as the critical exponent and Kibble-Zurek dynamics in consistency with the mean-field theory will become straightforward. The unified boundary condition we want to prove is given by

$$\omega_c = \frac{(\eta g)^2}{\Omega}\tanh\frac{\beta\Omega}{2}, \quad \frac{\omega}{N\Omega} \to 0. \tag{2}$$

Physically, it means a classical phase transition since the quantization of the bosonic field is vanishing. The parameter η in both models accounts for the effect of the rotating-wave approximation in which $\eta = 1$ for the presence of it and $\eta = 2$ for its absence. At this point, the fluctuation of the bosonic field is negligible, based on which we derive a much simpler method to study the phase transition in some similar models with interaction between boson fields and atoms, showing that the same phase transition can happen in models with non-identical atoms, Hubbard interaction, and nonlinearity, all of which belong to the Landau paradigm of phase transition. This method is demonstrated to have much broader applicability than the previous approximated approaches.

II. THEORETICAL METHOD

We implement Eq. (1) using the path-integral approach developed by Popov [59–62] in which the spins are represented by the Schwinger fermions [63,64],

$$\sigma_i^+ = \frac{\sigma_i^x + i\sigma_i^y}{2} = \alpha_i^\dagger\beta_i, \quad \sigma_i^z = \alpha_i^\dagger\alpha_i - \beta_i^\dagger\beta_i. \tag{3}$$

Here α_i and β_i are fermion operators, and the number of fermions $\sum_i \alpha_i^\dagger\alpha_i + \beta_i^\dagger\beta_i = N_F$ is constrained by the number of spins $N_F = N$. This is a faithful representation since the Hilbert spaces in these two theories are the same. In the few-spin models, we can directly verify that the partition function of the Hamiltonian in these two representations is exactly the same. This is different from the approximated HP method in which the spin and boson have different Hilbert spaces. The partition function reads as

$$Z = \text{Tr}\,\exp(-\beta\mathcal{H}) = i^N \text{Tr}\,\exp\left(-\beta\mathcal{H}_F - \frac{i\pi}{2}N_F\right), \tag{4}$$

where N_F is the constraint defined above. In this new representation, we can take the constraint into account and write the partition function in terms of these fermions as following:

$$Z = i^N \int \mathcal{D}\bar{\alpha}\,\mathcal{D}\alpha\,\mathcal{D}\bar{\beta}\,\mathcal{D}\beta\,\mathcal{D}\bar{b}\,\mathcal{D}b\,e^{-S}, \tag{5}$$

where $S = \int(\bar{b}\frac{\partial}{\partial\tau}b + \sum_{i=1}^N \bar{\alpha}_i\frac{\partial}{\partial\tau}\alpha_i + \bar{\beta}_i\frac{\partial}{\partial\tau}\beta_i + \mathcal{H})d\tau$. We first make a rotating-wave approximation to Eq. (1), which corresponds to the Jaynes-Cummings model. Via the fermion coherent representation we have

$$\mathcal{H} = \omega\bar{b}b + \sum_i \frac{\Omega}{2}(\bar{\alpha}_i\alpha_i - \bar{\beta}_i\beta_i) + \frac{g}{\sqrt{N}}(\bar{\alpha}_i\beta_i b + \bar{\beta}_i\alpha_i\bar{b}) + \frac{i\pi}{2\beta}N_F. \tag{6}$$

The trace in Eq. (4) is carried out over different N_F spaces of $\mathcal{H}$ in which only the state with $N_F = N$ is physical, whereas all the other modes are canceled exactly [60,61]. We solve the above model based on Fourier transformation $b(\tau) = \sum_n b_n e^{i\omega_n\tau}$ and $\psi_i(\tau) = \sum_q \psi_i(q)e^{i\omega_q\tau}$, with ψ_i for fields α_i and β_i, where $\omega_n = 2n\pi/\beta$, $\omega_q = (2q+1)\pi/\beta$ $(n, q \in \mathbb{Z})$ are Matsubara frequencies for bosons and fermions. The total action is decoupled into two parts $S = S_0 + S_{\text{int}}$, where $S_0 = \sum_{k,q}\bar{\psi}_k(q)G_0^{-1}(q)\psi_k(q)$ with $\psi_k(q) = [\alpha_k(q), \beta_k(q)]^T$, and

$$G_0(q) = \begin{pmatrix} \mathcal{G}_q^+ & 0 \\ 0 & \mathcal{G}_q^- \end{pmatrix}, \quad \mathcal{G}_q^\pm = \frac{1}{\beta\left(i\omega_q + i\frac{\pi}{2\beta} \pm \frac{\Omega}{2}\right)}. \tag{7}$$

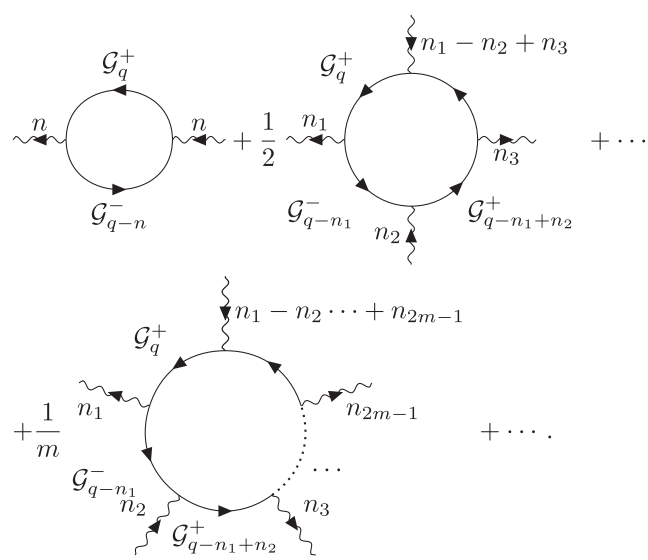
The interaction term can be written as $S_{\text{int}} = \sum_k \sum_{q,q'} \bar{\psi}_k(q)\Sigma(q-q')\psi_k(q')$, where

$$\Sigma(q-q') = \frac{g\beta}{\sqrt{N}}\begin{pmatrix} 0 & b_{q-q'} \\ \bar{b}_{q'-q} & 0 \end{pmatrix}. \tag{8}$$

We see that for the fermion fields, the interacting term is in a quadratic form; whereas for the bosonic field by treating the fermion field as a Grassmannian constant, the interacting term is just a linear displacement of the bosonic field. We take advantage of this feature and integrate out of the fermion fields ψ_i, leaving only the bosonic field in the following form $Z = \int \mathcal{D}\bar{b}\,\mathcal{D}b\,e^{-S_{\text{eff}}[\bar{b},b]}$, where

$$S_{\text{eff}}[\bar{b}, b] = \sum_n \beta(i\omega_n + \omega)\bar{b}_n b_n - N\,\text{tr}\,\ln\,G^{-1}, \tag{9}$$

with $G^{-1} = G_0^{-1} + \Sigma$. The previous literature tries to solve the above model from the saddle-point solution of S_{eff} [59–62] and its fluctuation around this point. We choose a different strategy by expanding the solution to infinite orders via Taylor expansion of the bosonic field. In the second term of S_{eff}, we utilize $-\text{tr}\,\ln\,G^{-1} = -\text{tr}\,\ln\,G_0^{-1} + \text{tr}\sum_{m\geqslant 1}\frac{1}{2m}(G_0\Sigma)^{2m}$, which can be represented by the following Feynman diagrams:



(10)

In these diagrams, the bosonic field can be written as

$$\mathcal{V}_{\{n_i\}}^{(2m)} = \sum_{\{n_i\}} \chi_{\{n_i\}}^{(2m)} b_{n_1}\bar{b}_{n_2}b_{n_3}\bar{b}_{n_4}\cdots b_{n_{2m-1}}\bar{b}_{k_{2m}} \tag{11}$$

for $k_{2m} = \sum_{i=1}^{2m-1}(-1)^{i+1}n_i$ in which the Matsubara summation of ω_q is performed. The leading term yields

$$S_{\rm eff}^{(2)} = \sum_n \left(i\omega_n + \omega - \frac{g^2}{i\omega_n + \Omega}\tanh\frac{\beta\Omega}{2}\right)|b_n|^2. \tag{12}$$

The real part of $S_{\rm eff}^{(2)}$, which should be positive for all modes for the normal phase, has been used to determine the superradiant phase transition in the Dicke model [59–62]. It is given by the mode b_0 by Eq. (2) with $\eta = 1$. However, whether the phase transition occurs or not also depends critically on the higher-order terms [65]. For example, the next leading term in $S_{\rm eff}$ is $\chi_0^{(4)}|b_0|^4$, where

$$\chi_0^{(4)} = \frac{g^4\beta}{2N\Omega^3}\left(2\tanh\frac{\beta\Omega}{2} - \beta\Omega\,{\rm sech}^2\frac{\beta\Omega}{2}\right) \leqslant \frac{g\beta}{N}\left(\frac{g}{\Omega}\right)^3. \tag{13}$$

We see that $\chi_0^{(4)}$ is always a positive number (for the stability of the ground state), which is bounded from above by some universal scaling law as a function of g/Ω. We expect the same feature for all the other higher terms, although they will be complex valued for nonzero $\{n_i\}$ after performance of the Matsubara summation of frequencies ω_q. This action obviously can not yield exact phase transition.

To this end, we need to calculate the upper bound of

$$\left|\chi_{\{n_i\}}^{(2m)}\right| = \left|\sum_q \frac{(g\beta)^{2m}}{mN^{m-1}}\mathcal{G}_q^+\mathcal{G}_{q-n_1}^-\mathcal{G}_{q-n_1+n_2}^+\cdots\mathcal{G}_{k_{2m}}^-\right|$$
$$\leqslant \sum_q \frac{(g\beta)^{2m}}{mN^{m-1}}|\mathcal{G}_q^+||\mathcal{G}_{q-n_1}^-||\mathcal{G}_{q-n_1+n_2}^+|\cdots|\mathcal{G}_{k_{2m}}^-|. \tag{14}$$

We noted that the non-negative-valued elements $|\mathcal{G}_{q-n}^\pm|$ are elements of the sets $\Lambda^\pm = \{|\mathcal{G}_q^\pm||q \in \mathbb{Z}\}$, and the above some is nothing but just the product of all these elements from this set upon some kind of permutation. From the two theorems in Appendix B which are based on the rearrange inequality (see the last chapter of Ref. [66] by Hardy *et al.*), we have an estimation of the upper bound for $\beta\Omega \gg 1$ as

$$\left|\chi_{\{n_i\}}^{(2m)}\right| \leqslant \frac{\beta g}{2mN^{m-1}\sqrt{\pi}}\left(\frac{2g}{\Omega}\right)^{2m-1}\frac{\Gamma(m-1/2)}{\Gamma(m)}. \tag{15}$$

The right-hand side is just $\chi_0^{(2m)}$. This inequality is the major basis of this paper. When $m = 2$, it reduces to Eq. (12). We have confirmed this upper bound numerically in Appendix A in which the different $\{n_i\}$'s will approach the same upper bound. We see that the phase transition can happen only when all these terms are vanished, which can be reached by either $N \to \infty$ as discussed in the Dicke model; and $g/\Omega \to 0$ as discussed in the Rabi model. We can also combine these two limits into a unified one using $g^2/(\Omega^2 N) \to 0$. By the critical boundary at $g^2 \simeq \omega\Omega$, we naturally have $\omega/(\Omega N) \to 0$, yielding the second condition of Eq. (2).

This estimation can also be applied to the full Dicke model. In this case, the self-energy Σ should be changed accordingly by setting its off-diagonal component $b_{q-q'}$ to $(b_{q-q'} + \bar{b}_{q'-q})$ in Eq. (8). However, the propagators $\mathcal{G}_q^\pm$ are unchanged. Thus, the estimation is still applicable. We have

$$S_{\rm eff}^{(2)} = \sum_n (i\omega_n + \omega)\bar{b}_n b_n - \frac{g^2\tanh\frac{\beta\Omega}{2}}{i\omega_n + \Omega}(b_n + \bar{b}_{-n})^2, \tag{16}$$

which has the same symmetry— U(1) in the Jaynes-Cummings model with $\eta = 1$ and $\mathbb{Z}_2$ in the Dicke and Rabi models with $\eta = 2$—as the original Hamiltonian. The above action with vanished higher-order terms yields the boundary in Eq. (2).

The second requirement of Eq. (2) means that only the leading term of $S_{\rm eff}^{(2)}$ to be important. Thus, the phase transition is exact by even mean-field theory. This feature will not be changed by other types of interactions. This conclusion has some immediate consequences. By considering only the mean-field term with relevant field b_0, we only need to treat the field as a classical variable. Let us assume $b \to b_0$ and $b^\dagger \to b_0^*$, then

$$\mathcal{H} = \omega|b_0|^2 + \frac{\Omega}{2}\sum_i \sigma_i^z + \frac{g}{\sqrt{N}}\sum_i^N(\sigma_i^\dagger b_0 + b_0^*\sigma_i^-). \tag{17}$$

The N two-level atoms are now independent. We can calculate the free energy of the above model at finite temperature from $Z = e^{-\beta F} = {\rm Tr}(e^{-\beta\mathcal{H}})$, which yields $F = \omega|b_0|^2 - \frac{N}{\beta}\ln[2\cosh(\beta E)]$ with $E = \sqrt{\Omega^2/4 + g^2|b_0|^2/N}$. Around $b_0 \sim 0$, we have

$$F = F_0 + |b_0|^2\left(\omega - \frac{g^2\tanh\frac{\beta\Omega}{2}}{\Omega}\right) + \sum_{n\geqslant 2}F_{2n}|b_0|^{2n}, \tag{18}$$

where $F_0 = -\frac{N}{\beta}\ln(2\cosh\frac{\beta\Omega}{2})$. This result naturally yields Eq. (2). Here b_0 is a classical variable, thus, it forbids the superposition of two different states for spontaneous symmetry breaking. The higher-order terms F_{2n} are ignored in the previous literature for phase transition [27–30], which may not be correct. When $\beta\Omega \gg 1$, we have

$$F_4 \to \frac{g^4}{N\Omega^3}, \quad F_6 \to -\frac{2g^6}{N^2\Omega^5}, \quad F_8 \to \frac{5g^8}{N^3\Omega^7}. \tag{19}$$

One may even find analytically for any $\beta\Omega$ that $F_{2m} = (-1)^m\tanh(\frac{\beta\Omega}{2})\frac{g^{2m}}{N^{m-1}\Omega^{2m-1}}\frac{2^{2m-1}\Gamma(m-1/2)}{2m\sqrt{\pi}\Gamma(m)}$, which is the same as Eq. (14). The negative signs of the higher-order terms may lead to failure of the Landau theory of second-order phase transitions (e.g., see the first-order phase transitions by Landau theory in Ref. [65]). This result confirms our previous conclusion that the exact phase transition happens only when $F_{2n} \to 0$ for all $n \geqslant 2$, leaving only the leading term $S_{\rm eff}^{(2)}$ for instability. In this sense, at the critical point, the fluctuation of the bosonic field is negligible. This justifies why even the simplest approximations in the previous literature can yield the accurate phase boundary. It also means that the phase transition is exactly described by the Landau theory with the number of photon as $\langle b^\dagger b\rangle \sim |g - g_c|^{-\nu}$, where $\nu = 1/2$ is the same as the mean-field theory [27,29,67–69].

III. APPLICATIONS

Our result is useful to understand the phase transitions in the other models with spin and boson interactions for

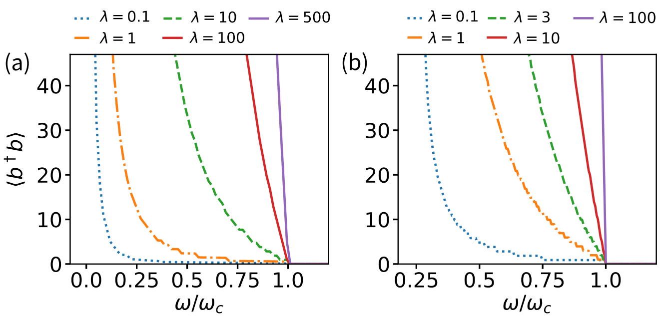


FIG. 1. Phase transitions for model (I) in (a) and model (III) in (b) based on the exact diagonalization method at $T = 0$. In (a), $N = 3$, $(\tilde{g}_1, \tilde{g}_2, \tilde{g}_3) = (12, 1, 100)$, and $(\tilde{\Omega}_1, \tilde{\Omega}_2, \tilde{\Omega}_3) = (9, 50, 110)$. Different lines are plotted with $g_i = \sqrt{\lambda}\tilde{g}_i$ and $\Omega_i = \lambda\tilde{\Omega}_i$, which yield $\omega_c = 35.6$ from Eq. (20). In (b), $N = 1$, $\kappa = 0.5$, $\tilde{g} = 12$, and $\tilde{\Omega} = 100$ with $\omega_c = 1.94$ from Eq. (22) using λ defined in the same way as (a).

second-order phase transition in which the HP method and the effective Hamiltonian approaches are failed. We discuss several models (I)–(III), which have been justified by the exact numerical method with high accuracy (Fig. 1). This approach applies to physics even at finite temperatures.

(I) *Inhomogeneous interaction*. This model reads as

$$\mathcal{H} = \omega b^\dagger b + \sum_i \Omega_i \sigma_i^z + \sum_i \left(\frac{g_i}{\sqrt{N}} \sigma_i^\dagger b + \text{H.c.} \right) \tag{20}$$

for nonidentical atoms interacting with a common field. The dynamics in this model has been studied in Refs. [70–72]. The phase transition happens at

$$\omega_c = \frac{1}{N} \sum_{i=1}^{N} \frac{g_i^2}{\Omega_i} \tanh \frac{\beta \Omega_i}{2}, \quad \frac{1}{N} \sum_i \frac{\omega}{\Omega_i} \to 0. \tag{21}$$

This expression is inconsistent with the result in Ref. [73] with inhomogeneous interaction. We confirm this phase transition in Fig. 1(a) in which a divergence of $\langle b^\dagger b \rangle$ is expected from $S_{\text{eff}}^{(2)}$ across the phase boundary due to the vanished higher-order terms [67].

(II) *Antirotating term and Hubbard interaction*. In this case, we consider the anisotropic interaction of the form of $(g_1\sigma_i^+ + g_2\sigma_i)b/\sqrt{N} + \text{H.c.}$ and Hubbard interaction of $Un(n-1)$ with $n = b^\dagger b$. It is frequently termed as the anisotropic Rabi model when $g_1 \neq g_2$ [74]. In this case we find the energy-level spacing mediated by this term is $\sqrt{\Omega^2/4 + |g_1 b_0 + g_2 b_0^*|^2/N}$, which preserves the $\mathbb{Z}_2$ symmetry. The Hubbard term U is unimportant for the phase transition. We have the phase transition at

$$\omega_c = \frac{(g_1+g_2)^2}{\Omega} \tanh \frac{\beta\Omega}{2}, \quad \frac{\omega}{N\Omega} \to 0. \tag{22}$$

This condition has been shown in literature [27,29], and it can be obtained much more straightforward in this paper. Thus, we have $\eta = 2$ in Eq. (2) when all $g_i = g$.

(III) *Nonlinearity effect*. It is inevitable that the higher-order correction by the bosonic field can slightly modify the energy-level spacing of the atoms [24]. We mimic this effect using the model $\mathcal{H} = \omega b^\dagger b + \sum_i (\Omega/2 + \kappa b^\dagger b)\sigma_i^z + g/\sqrt{N}\sum_i (b^\dagger \sigma_i + \text{H.c.})$ where the term κ maybe introduced via the higher-order perturbation theory. This model cannot be solved by the HP method for the reason of nonlinear interaction. We find the phase transition happens at

$$\omega_c = \frac{g^2 + \kappa N \Omega}{\Omega} \tanh \frac{\beta\Omega}{2}, \quad \frac{\omega}{N\Omega} \to 0. \tag{23}$$

We confirm this phase transition in Fig. 1(b). This result will have some interesting predictions. When κ is independent of N, it is relevant, and the phase transition is forbidden in the thermodynamic limit. When $\kappa = \kappa_0/N$, which is most likely to happen since the bosonic field is proportional to $1/\sqrt{N}$, we find that this phase transition is still presented. However, when $\kappa \propto \kappa_0/N^\gamma$, where $\gamma > 1$, this nonlinear effect is irrelevant in the thermodynamic limit, which will not influence the phase boundary. Thus, $\gamma = 1$ is marginal. This result means that the Dicke phase transition can still happen even taking the nonlinear correction into account.

IV. CONCLUSION

To conclude, this paper is stimulated by the coincident phase boundary in the Dicke and quantum Rabi models, which is exact although derived by some approximated approaches. We explore the underlying origin using the path-integral approach and give a unified boundary condition for these two models at which the fluctuation of the bosonic field is vanished. In this limit, we can treat the bosonic field as a classical variable, which has much broader applicability than all the above approximated approaches in the determination of phase boundaries in some of the spin and boson interacting models. All these phase transitions belong to the classical Landau theory of phase transition, thus, the critical exponent and the associated universal dynamics should be the same as that from the mean-field theory, which can be confirmed using cold atoms, trapped ions, and superconducting circuits.

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APPENDIX A: ESTIMATION OF THE UPPER BOUND

The effective action of the Dicke model can be written as

$$S_{\text{eff}} = \sum_n (i\omega_n + \omega)|b_n|^2 - \ln \det G. \tag{A1}$$

Taylor series expansion of the second term is

$$-\ln \det G = N\Bigg\{ -\text{tr} \ln G_0^{-1} + \frac{1}{2}\text{tr}(G_0\Sigma G_0 \Sigma) + \frac{1}{4}\text{tr}(G_0\Sigma G_0\Sigma G_0\Sigma G_0\Sigma) + \cdots \Bigg\}, \tag{A2}$$

where $G^{-1} = G_0^{-1} + \Sigma$ with Σ being the self-energy. According to the Feynman rules given in the main text and for the leading term we have

$$\begin{aligned}&\frac{N}{2}\mathrm{tr}(G_0\Sigma G_0\Sigma)\\&=\sum_{n,q}(g\beta)^2 g_q^+ g_{q-n}^-|b_n|^2\\&=g^2\beta^2\sum_{n,q}\frac{|b_n|^2}{\beta^2\left(i\omega_q+i\frac{\pi}{2\beta}+\frac{\Omega}{2}\right)\left(i\omega_{q-n}+i\frac{\pi}{2\beta}-\frac{\Omega}{2}\right)}\\&=-\sum_n\frac{g^2\beta}{i\omega_n+\Omega}\tanh\frac{\beta\Omega}{2}\bar{b}_n b_n,\end{aligned} \tag{A3}$$

where $\omega_q=(2q+1)\pi/\beta$, $\omega_n=2n\pi/\beta$ are fermionic and bosonic Matsubara frequencies, respectively. This term contributes to the quadratic energy to the free energy, which is exactly the same as that from the mean-field theory. The superradiant phase happens when the coefficient of the $\bar{b}_0 b_0$ term becomes negative, yielding a phase transition described by the Landau theory of phase transition. Following this route, the next leading term is given by the fourth order,

$$\begin{aligned}&\frac{1}{2}N\left(\frac{g}{\sqrt{N}}\right)^4\sum_{q,n_1,n_2,n_3}\left\{\frac{b(n_1)\bar{b}(n_2)b(n_3)\bar{b}(n_1-n_2+n_3)}{\left(i\omega_q+i\frac{\pi}{2\beta}+\frac{\Omega}{2}\right)\left(i\omega_{q-n_1}+i\frac{\pi}{2\beta}-\frac{\Omega}{2}\right)\left(i\omega_{q-n_1+n_2}+i\frac{\pi}{2\beta}+\frac{\Omega}{2}\right)\left(i\omega_{q-n_1+n_2-n_3}+i\frac{\pi}{2\beta}-\frac{\Omega}{2}\right)}\right\}\\&\quad=\sum_{n_1,n_2,n_3,}\chi^4_{\{n_i\}}b_{n_1}\bar{b}_{n_2}b_{n_3}\bar{b}_{n_1-n_2+n_3},\end{aligned} \tag{A4}$$

where n_1, n_2, and n_3 are arbitrary integers. By performing the Matsubara frequency summation of $\omega_q=\pi(2n+1)/\beta$ for the fermion fields via the residue theorem (it may also be calculated directly with the aid of *Mathematica* for their excellent convergence), we find

$$\begin{aligned}\chi^{(4)}_{\{n_i\}}&=\frac{\beta g^4\cot\left(\frac{1}{4}(\pi-i\beta\Omega)\right)}{4N(\omega_{n_2-n_3})(i\omega_{n_1}+\Omega)(i\omega_{n_2}+\Omega)}+\frac{\beta^4 g^4\cot\left(\frac{1}{4}(\pi+i\beta\Omega)\right)}{4N(\omega_{n_1-n_2})(i\omega_{n_2}+\Omega)(i\omega_{n_3}+\Omega)}\\&\quad+\frac{\beta g^4\cot\left(\frac{1}{4}(\pi-i\beta\Omega)\right)}{4N(\omega_{n_2-n_3})(i\omega_{n_2-n_1-n_3}-\Omega)(i\omega_{n_3}+\Omega)}+\frac{\beta g^4\cot\left(\frac{1}{4}(\pi+i\beta\Omega)\right)}{4N(\omega_{n_1-n_3-n_2})(i\omega_{n_1}+\Omega)(\omega_{n_1-n_2+n_3}+\Omega)}\\&=\frac{\beta g^4\tanh\left(\frac{\beta\Omega}{2}\right)(2\Omega+i\omega_{n_1+n_3})}{2N\left(\Omega+i\omega_{n_1-n_2+n_3}\right)\prod_{j=1}^3\left(\Omega+i\omega_{n_j}\right)}.\end{aligned} \tag{A5}$$

This expression has salient features that it is a complicated expression with complex values. One can image that the expression can become much more complicated in the higher-order terms, making the Matsubara frequency summation too complex to be unrealistic. However, we observe that

$$|\chi^{(4)}_{\{n_i\}}|\leqslant\frac{\beta g}{N}\left(\frac{g}{\Omega}\right)^3\tanh\left(\frac{\beta\Omega}{2}\right)\leqslant\frac{\beta g}{N}\left(\frac{g}{\Omega}\right)^3. \tag{A6}$$

Especially, in the special case of $n_1=n_2=n_3=0$, the coefficient can be calculated analytically,

$$\chi^{(4)}_0=\frac{g\beta}{2N}\left(\frac{g}{\Omega}\right)^3\left(2\tanh\frac{\beta\Omega}{2}-\beta\Omega\,\mathrm{sech}^2\frac{\beta\Omega}{2}\right), \tag{A7}$$

which obviously satisfies the upper bound set in Eq. (A6). This result is stimulating because what we need to do is actually try to estimate the upper bounds of these coefficients instead of their analytical forms. Following the Feynman diagram in the main text, the coefficient of the $2m$th order of the effective action is as follows:

$$\chi^{(2m)}_{\{n_i\}}=\sum_q\frac{(g\beta)^{2m}}{mN^{m-1}}\mathcal{G}_q^+\mathcal{G}_{q-n_1}^-\mathcal{G}_{q-n_1+n_2}^+\cdots\mathcal{G}_{k_{2m}}^-, \tag{A8}$$

where $k_{2m}=q-n_1+n_2-n_3+n_4\cdots-n_{2m-1}$. We find

$$\begin{aligned}\left|\chi^{(2m)}_{\{n_i\}}\right|&\leqslant\sum_q\frac{g^{2m}}{mN^{m-1}}\frac{1}{\sqrt{\left(\omega_q+\frac{\pi}{2\beta}\right)^2+\left(\frac{\Omega}{2}\right)^2}}\frac{1}{\sqrt{\left(\omega_{q-n_1}+\frac{\pi}{2\beta}\right)^2+\left(\frac{\Omega}{2}\right)^2}}\cdots\frac{1}{\sqrt{\left(\omega_{q-n_1+n_2\cdots-n_{2m-1}}+\frac{\pi}{2\beta}\right)^2+\left(\frac{\Omega}{2}\right)^2}}\\&\leqslant\frac{g^{2m}}{mN^{m-1}}\sum_q\frac{1}{\left[\left(\omega_q+\frac{\pi}{2\beta}\right)^2+\left(\frac{\Omega}{2}\right)^2\right]^m}=\left|\chi^{(2m)}_0\right|.\end{aligned} \tag{A9}$$

This is the major inequality used in the main text. The reasoning of the above inequality using the rearrangement theorem which will be discussed shortly in Appendix B. Let us define

$$\mathcal{A}^{(2m)}=\sum_q\frac{1}{\left[\omega_q'^2+\left(\frac{\Omega}{2}\right)^2\right]^m}, \tag{A10}$$

where

$$\omega'_q = \omega_q + \frac{\pi}{2\beta} = \left(2q + \frac{3}{2}\right)\frac{\pi}{\beta}. \tag{A11}$$

This expression exhibits an upper bound with a specific scaling law in the limit when $\beta\Omega \to \infty$ as that discussed in the main text. By performing of binomial theorem expansion to $\mathcal{A}^{(2m)}$, we find

$$\mathcal{A}^{(2m)} = \sum_q \frac{1}{\left(\frac{\Omega}{2}\right)^{2m} + C_m^1\left(\frac{\Omega}{2}\right)^{2(m-1)}\omega_q'^2 + C_m^2\left(\frac{\Omega}{2}\right)^{2(m-2)}\omega_q'^4 + C_m^3\left(\frac{\Omega}{2}\right)^{2(m-3)}\omega_q'^6 + C_m^4\left(\frac{\Omega}{2}\right)^{2(m-4)}\omega_q'^8 + \cdots} < \sum_q \frac{1}{\left(\frac{\Omega}{2}\right)^{2m} + m\left(\frac{\Omega}{2}\right)^{2(m-1)}\omega_q'^2}$$
$$= \frac{4^{m-1}\beta \tanh\left(\frac{\beta\Omega}{2\sqrt{m}}\right)}{\Omega^{2m-1}\sqrt{m}}, \tag{A12}$$

where $\{C_m^k\}$'s are the expansion coefficients. In the limit of $\beta\Omega \to \infty$, only the leading term of ω'_q is dominated, yielding

$$\lim_{\beta\Omega\to\infty} \mathcal{A}^{(2m)} < \frac{\beta}{\Omega^{2m-1}} \frac{4^{m-1}}{\sqrt{m}}. \tag{A13}$$

By comparing Eqs. (A13) and (A9) we can obtain

$$\lim_{\beta\Omega\gg 1} \left|\chi^{(2m)}_{\{n_i\}}\right| < \frac{g\beta}{2m^{3/2}N^{m-1}}\left(\frac{2g}{\Omega}\right)^{2m-1}. \tag{A14}$$

This bound naturally yields the same scaling as Eq. (A6) when $m = 2$. However, it cannot be numerically correct due to the neglecting the higher-order terms during the binomial theorem expansion. To obtain a much better estimation of the upper bound, we use the following identity:

$$\begin{aligned} Q(b,a) &= (a)^{2m} \sum_q \frac{1}{b + a^2\omega_q'^2} \\ &= \frac{a^{2m-1}\beta \tanh\left(\frac{\sqrt{b}\beta}{a}\right)}{2\sqrt{b}} \\ &\to \frac{\beta a^{2m-1}}{2\sqrt{b}}, \end{aligned} \tag{A15}$$

where $a = 2/\Omega$. Based on this identity, we find

$$\begin{aligned} \mathcal{A}^{(2m)} &= \sum_q \frac{a^{2m}}{(a^2\omega_q'^2 + 1)^m} \\ &= \frac{1}{(-1)^{m-1}(m-1)!} \frac{\partial^{m-1} Q}{\partial b^{m-1}}\bigg|_{b=1} \\ &\to \frac{\beta a^{2m-1}}{2(m-1)!}\frac{F(m)}{2^{m-1}} \\ &= \frac{\beta a^{2m-1}}{(m-1)!}\frac{F(m)}{2^m}, \end{aligned} \tag{A16}$$

where $F(1) = 1$ and $F(m > 1) = 1 \cdot 3 \cdot 5 \cdots (2m-3)$. So we have the supremum,

$$\mathrm{Sup}\left[\left|\chi^{(2m)}_{\{n_i\}}\right|\left(\frac{\Omega}{g}\right)^{2m-1}\right] = \frac{2^{m-1} g\beta}{m! N^{m-1}} F(m) \tag{A17}$$

$$= \frac{4^{m-1}\beta g}{mN^{m-1}\sqrt{\pi}} \frac{\Gamma(m-1/2)}{\Gamma(m)}. \tag{A18}$$

The right-hand side is nothing, but just the integration of q in the whole $\mathbb{R}$ axis by replacing the summation to integration in Eq. (A15) when $1/\beta\Omega \ll 1$. Based on this result, we can obtain the analytical expression of $\chi^{2m}_{\{n_i\}}$ at $\beta\Omega \to \infty$ as

$$\lim_{\beta\Omega\to\infty} |\chi^{(2m)}_{\{n_i\}}| = \frac{\beta g}{2mN^{m-1}\sqrt{\pi}}\left(\frac{2g}{\Omega}\right)^{2m-1} \frac{\Gamma(m-1/2)}{\Gamma(m)}. \tag{A19}$$

One can see that the above upper bound has the same scaling law as Eq. (A14). Moreover, this new upper bound naturally yields Eq. (A6) by setting to $m = 2$. We can even show that the ratio between these two expressions is $\sqrt{\pi}$ when $m \to \infty$, thus, Eq. (A14) overestimates the summation by a factor of $\sqrt{\pi}$ due to the truncation to the quadratic term. The upper bound in Eq. (A19) is used in the main text. We have also verified its correctness numerically by setting different $\{n_i\}$'s in Fig. 2, which agrees well with our calculation.

APPENDIX B: REARRANGEMENT INEQUALITIES

The estimation of the upper bound in Eq. (A9) is the most essential mathematical trick used in this paper. We need to following rearrangement inequality.

Theorem 1. (Rearrangement theorem). For two sequences $\{a_i\}_{i=1}^n$ and $\{b_i\}_i^n$ in nondecreasing order, that is, $a_i \leqslant a_{i+1}$ and $b_i \leqslant b_{i+1}$ have the following inequalities:

$$\sum_{i=1}^n a_{n+1-i} b_i \leqslant \sum_{i=1}^n a_{\sigma_i} b_i \leqslant \sum_{i=1}^n a_i b_i, \tag{B1}$$

where σ_i is any permutation of $\{1, 2, 3, \ldots, n\}$.

The proof of the above theorem can be found in most of the textbooks about inequality using only elementary techniques in mathematics. The above theorem is also true for three sequences and even arbitrary number of sequences with the following generalized rearrangement theorem for *non-negative valued* sequences:

Theorem 2. (Generalized rearrangement theorem). For non-negative valued sequences $\{a_{l,i}\}_{i=1}^n$ for $l = 1, 2, \ldots, k$ $(k \geqslant 2)$ in nondecreasing order, that $0 \leqslant a_{l,i} \leqslant a_{l,i+1}$ for all l's and i's, we have

$$\sum_{i=1}^n \prod_{l=1}^k a_{\sigma_i^{(l)}} \leqslant \sum_{i=1}^n \prod_{l=1}^k a_{l,i}, \tag{B2}$$

where $\sigma^{(l)}$ are permutations of $\{1\text{–}3, \ldots, n\}$.

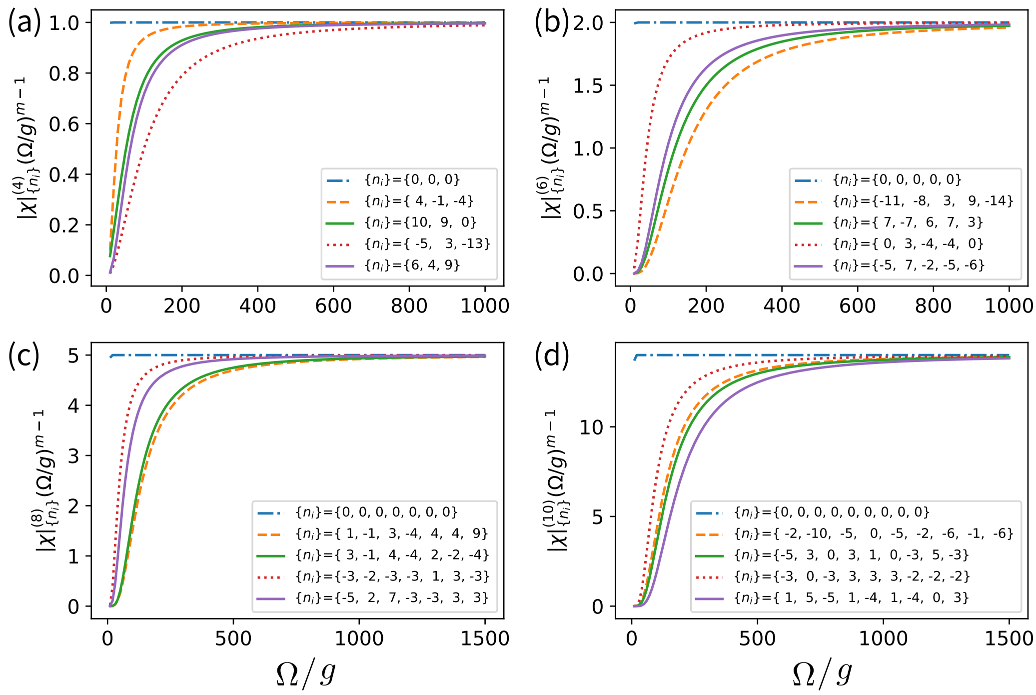

FIG. 2. $|\chi^{(2m)}_{n_i}|(\Omega/g)^{m-1}$ for $2m = 4,\ 6,\ 8$, and 10 for various $\{n_i\}$'s. The horizon lines are the upper bound estimated by Eq. (A18). For $\beta = 1,\ g = 1$, we have the upper bounds of $|\chi^{(2m)}_{n_i}|(\Omega/g)^{m-1}$ to be 1, 2, 5, and 14 for $2m = 4,\ 6,\ 8,$ and 10, respectively.

The systematic study of rearrangement inequalities has been systematically studied in the final chapter of "*Inequalities*" by Hardy *et al.* [66], which is correct both for the discrete sequences and for the continuous sequences.

In the following, we only explain the above-generalized theorem for $k = 3$ intuitively based on the concept of combined sequence; whereas its generalization to arbitrary k follows the same procedure. We only need to explain the case with three short sequences as $0 \leqslant a_1 \leqslant a_2,\ 0 \leqslant b_1 \leqslant b_2$, and $0 \leqslant c_1 \leqslant c_2$. We denote these three sequences as $a,\ b$, and c, respectively. We assume $a'_i,\ b'_i$ being the possible permutation of these sequences. We need to prove

$$a'_1 b'_1 c_1 + a'_2 b'_2 c_2 \leqslant a_1 b_1 c_1 + a_2 b_2 c_2. \tag{B3}$$

We may have four different cases. (1) $a'_1 = a_1,\ a'_2 = a_2$ and $b'_1 = b_1,\ b'_2 = b_2$; (2) $a'_1 = a_1,\ a'_2 = a_2$ and $b'_1 = b_2,\ b'_2 = b_1$; (3) $a'_1 = a_2,\ a'_2 = a_1$ and $b'_1 = b_1,\ b'_2 = b_2$; (4) $a'_1 = a_2,\ a'_2 = a_1$ and $b'_1 = b_2,\ b'_2 = b_1$. In the case of (1), the equal sign of Eq. (B3) is achieved. In the case of (3), we can combine the sequences of b and c into a new sequence bc, satisfying $0 \leqslant b_1c_1 \leqslant b_2c_2$, based on which Theorem 1 can be used to prove Eq. (B3) for the two new sequences a and bc. For the case of (2), we can treat ac as a new combined sequence for Eq. (B3). For the case of (4), we can combine ab as a new sequence for the proof of Eq. (B3). We see that the requirement of non-negative sequences naturally keep the basic features of the combined sequences. The above reasoning can be applied to much longer sequences for $k = 3$ and to the condition of arbitrary number $k > 3$.

With these two theorems, we next explain the trick used in Eq. (A9). It is realized using two steps,

$$|\mathcal{G}_q| = 1/[\beta\sqrt{(\omega_q + \pi/2\beta)^2 + (\Omega/2)^2}], \quad q \in \mathbb{Z}. \tag{B4}$$

We denote the set by non-negative valued $|\mathcal{G}_q|$ as Λ, via $\Lambda = \{|\mathcal{G}_q|, q \in \mathbb{Z}\}$. Obviously, Λ is independent of n_i. We find that the Matsubara summation used in Eq. (A9) is nothing but the product of all elements from the $2m$ sets of Λ upon some kind of permutation (shifted by n_i). The inequality naturally holds using Theorem 2 for $k = 2m$. The numerical results in Fig. 2 confirm this result. Phase transition with only one atom has attracted widespread attention [27–32].

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