Uniqueness of the Phase Transition in Many-Dipole Cavity Quantum Electrodynamical Systems

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The possibility of a superradiant phase transition in light-matter systems is the subject of much debate, due to numerous apparently conflicting no-go and counter no-go theorems. Using an arbitrary-gauge approach we show that a *unique* phase transition does occur in archetypal many-dipole cavity QED systems, and that it manifests unambiguously via a macroscopic gauge-invariant polarization. We find that the gauge choice controls the extent to which this polarization is included as part of the radiative quantum subsystem and thereby determines the degree to which the abnormal phase is classed as superradiant. This resolves the long-standing paradox of no-go and counter no-go theorems for superradiance, which are shown to refer to different definitions of radiation.

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Superradiance was originally described by Dicke [1], and since then it has received a great deal of attention (see, e.g., Ref. [2] for a recent introduction). A superradiant phase of a light-matter system is one in which a macroscopic number of photons arises due to the interaction between many dipoles. The possibility of such a phase transition within the Dicke model was first recognized some time ago [3,4]. Later, seminal contributions were made in the connection with quantum chaos [5–7]. The topic now includes extended Dicke models [8–12], driven and open systems, semiclassical descriptions [13–17], and artificial QED systems [18–29].

One of the most controversial aspects of theoretical studies has been the validity of so-called "no-go theorems," which prohibit a superradiant phase and are proved in the Coulomb gauge. The original no-go theorem [30] actually prohibits a phase transition of any kind, but neglects direct electrostatic interactions, whose presence are a defining feature of a correct Coulomb-gauge model. This theorem, and variants thereof, have been both refuted and confirmed in numerous subsequent works [11,12,18,21,25,31–41]. It has been suggested that where natural atomic systems admit a no-go theorem certain artificial atomic systems do not [21] (though see also Refs. [22,42]). However, in the multipolar-gauge the superradiant phase transition also appears to be automatically recovered for conventional cavity QED systems [37,38].

Further permutations of these results are available. For example, if explicit dipole-dipole interactions that are not naturally present are added into the multipolar-gauge description, then a no-go theorem reemerges [19,34,43,44]. A very recent contribution [41] argues without the two-level approximation that a superradiant phase is impossible, but this treatment considers only the radiative quantum subsystem and is again proved in the Coulomb gauge. If, rather than just the radiative subsystem, one also considers variations in the electrostatic interactions that are present within the Coulomb gauge, then an apparently different ferroelectric phase transition is predicted. This, however, does not lead to superradiance [36]. Thus, despite numerous contributions spanning several decades, the occurrence and nature of the phase transition in generic many-emitter light-matter systems, and how this relates to the choice of gauge, are fundamental questions whose answers remain unclear, yet still highly relevant [41,45–48].

Here we resolve these fundamental issues by proving that a *unique* physical phase transition does occur in generic many-dipole *cavity* QED systems and that the abnormal phase of the system is unambiguously signaled by a macroscopic average of the gauge-invariant transverse polarization field $\mathbf{P}_T$. This equals the longitudinal electric field $\mathbf{E}_L$ except at the point-dipole positions themselves. Crucial to the resolution provided is the recognition that QED subsystems are gauge relative, meaning that each gauge provides different *gauge-invariant* definitions of the light and matter subsystems. Whether the abnormal phase is characterized as ferroelectric or as superradiant depends on the extent to which $\mathbf{E}_L = \mathbf{P}_T$ is included within the radiative quantum subsystem and this is controlled by the gauge choice. We thereby show that the different viewpoints provided by different gauges are not contradictory, but in fact equivalent, as required. In particular, correct no-go statements such as in Ref. [41] are reconciled with correct counter no-go statements such as in Ref. [37]. Such results are found to be different ways of viewing the same phenomenon in terms of physically different quantum subsystems. By converting the apparent gauge non-invariance of the phase transition into a proof of gauge invariance, our results resolve the associated long-standing controversies.

A related but separate point is that level truncation of material dipoles causes a breakdown of gauge invariance [43,44,49,50]. Using numerical results for finite numbers of dipoles we show that accurate two-level model predictions can be identified. It is reasonable to conclude that the same two-level truncation will be accurate in the thermodynamic limit. Thus, arbitrary-gauge QED is also capable of eliminating any further quantitative ambiguity resulting from the use of material two-level truncation.

We begin by deriving an arbitrary gauge Dicke Hamiltonian. We adopt a general formulation of QED in which the gauge is selected by a real parameter α. We consider N identical electric dipoles each described by a classical center-of-mass position $\mathbf{R}_\mu$ and a dipole moment operator $\hat{\mathbf{d}}_\mu = -e\mathbf{r}_\mu$. The dipoles interact with a common electromagnetic field described by transverse-electric and magnetic fields $\mathbf{E}_T$ and $\mathbf{B}$, respectively. We obtain the Hamiltonian for the system from first principles [51], which can be written in the gauge-invariant form [49] $H = E_{\rm matter} + E_{\rm field}$, where $E_{\rm matter} \coloneqq \sum_{\mu=1}^N \frac{1}{2} m\dot{\mathbf{r}}_\mu^2 + V + V_{\rm dip}$ and $E_{\rm field} \coloneqq \frac{1}{2}\int d^3x[\mathbf{E}_T(\mathbf{x})^2 + \mathbf{B}(\mathbf{x})^2]$. Here V denotes the total intradipole potential, and $V_{\rm dip}$ denotes the interdipole electrostatic energy. The α-dependent canonical momenta are found to be

$$\mathbf{p}_{\mu\alpha} = m\dot{\mathbf{r}}_\mu - e(1-\alpha)\mathbf{A}(\mathbf{R}_\mu), \tag{1}$$

$$\mathbf{\Pi}_\alpha(\mathbf{x}) = -\mathbf{E}_T(\mathbf{x}) - \mathbf{P}_{T\alpha}(\mathbf{x}), \tag{2}$$

where $\mathbf{A}$ is the gauge-invariant transverse vector potential such that $\mathbf{E}_T = -\dot{\mathbf{A}}$ and $\mathbf{P}_{T\alpha}$ is the α-gauge transverse polarization given by $\mathbf{P}_{T\alpha}(\mathbf{x}) = \alpha\mathbf{P}_T(\mathbf{x})$, with $\mathbf{P}_T(\mathbf{x}) = \sum_{\mu=1}^N \hat{\mathbf{d}}_\mu \cdot \delta^T(\mathbf{x} - \mathbf{R}_\mu)$. The canonical commutation relations are $[r_{\mu,i}, p_{\nu,j}] = i\delta_{\mu\nu}\delta_{ij}$ and $[A_{T,i}(\mathbf{x}), \Pi_{T,j}(\mathbf{x}')] = \delta^T_{ij}(\mathbf{x} - \mathbf{x}')$. All other commutators between canonical operators vanish. The canonical momenta of different gauges are unitarily related via $\mathbf{X}_\alpha = R_{\alpha\alpha'}\mathbf{X}_{\alpha'}R_{\alpha'\alpha}$, where $\mathbf{X} = \mathbf{p}, \mathbf{\Pi}$ and $R_{\alpha\alpha'} = \exp[i(\alpha-\alpha')\sum_{\mu=1}^N \hat{\mathbf{d}}_\mu \cdot \mathbf{A}]$.

We now restrict our attention to a single cavity mode with volume v, frequency ω and unit polarization vector $\boldsymbol{\varepsilon}$, described by bosonic operators $a_\alpha, a_\alpha^\dagger$ with $[a_\alpha, a_\alpha^\dagger] = 1$. The restriction is imposed consistently on all fields including the transverse delta function δ^T. This eliminates the need to regularize $\mathbf{P}_T$ [54], and ensures that the transverse commutation relation for the canonical fields is preserved. The fundamental kinematic relations given by Eqs. (1) and (2) are therefore also preserved. In order to obtain a Dicke Hamiltonian we next take the limit of closely spaced dipoles around the origin; $\mathbf{R}_\mu \approx \mathbf{0}$ and we approximate the dipoles as two-level systems. Further details of all approximations used are given in Ref. [51]. We introduce the collective operators $J_\alpha^i = \sum_{\mu=1}^N \sigma_{\mu\alpha}^i$, with $i = \pm,\ z$, where $\sigma_{\mu\alpha}^\pm$ are the raising and lowering operators of the μth two-level dipole and $\sigma_{\mu\alpha}^z = [\sigma_{\mu\alpha}^+, \sigma_{\mu\alpha}^-]/2$. We also introduce cavity bosonic operators c_α and $c_\alpha^\dagger$, which incorporate both the bare cavity energy and the $\mathbf{A}^2$ term that results when Eq. (1) is substituted into the energy H [[51] Eqs. (72) and (73)]. The resulting arbitrary-gauge Dicke Hamiltonian is

$$\begin{aligned} H^{\alpha,2} = {} & \omega_m J_\alpha^z + \frac{N}{2}(\epsilon_0 + \epsilon_1) + \frac{1}{2}\rho d^2 + \omega_\alpha\left(c_\alpha^\dagger c_\alpha + \frac{1}{2}\right) \\ & - \frac{\mathcal{C}_\alpha}{N}(J_\alpha^+ + J_\alpha^-)^2 - i\frac{g'_\alpha}{\sqrt{N}}(J_\alpha^+ - J_\alpha^-)(c_\alpha^\dagger + c_\alpha) \\ & + i\frac{g_\alpha}{\sqrt{N}}(J_\alpha^+ + J_\alpha^-)(c_\alpha^\dagger - c_\alpha), \end{aligned} \tag{3}$$

where $\omega_m = \epsilon_1 - \epsilon_0$, $\omega_\alpha^2 = \omega^2 + e^2(1-\alpha)^2\rho/m$, $\mathcal{C}_\alpha \coloneqq \rho d^2(1-\alpha^2)/2$, $g'_\alpha \coloneqq (1-\alpha)\omega_m d\sqrt{\rho/(2\omega_\alpha)}$, and $g_\alpha \coloneqq \alpha d\sqrt{\rho\omega_\alpha/2}$, with $d \coloneqq \boldsymbol{\varepsilon}\cdot\mathbf{d}$. Here $\rho = N/v$ remains finite in the thermodynamic limit $N \to \infty$, $v \to \infty$. Although the nontruncated Hamiltonian H is unique, we now have a continuous infinity of Dicke Hamiltonians $H^{\alpha,2}$ such that $H^{\alpha,2}$ and $H^{\alpha',2}$ are not equal when $\alpha \neq \alpha'$ [43,44,49,50]. This breaking of gauge invariance will turn out not to be a barrier to eliminating all ambiguities regarding the occurrence and nature of a quantum phase transition.

To take the thermodynamic limit we use a Holstein-Primakoff map defined by $J_\alpha^z = b_\alpha^\dagger b_\alpha - N/2$, $J_\alpha^+ = b_\alpha^\dagger\sqrt{N - b_\alpha^\dagger b_\alpha}$, and $J_\alpha^- = (J_\alpha^+)^\dagger$, where $[b_\alpha, b_\alpha^\dagger] = 1$ [5–7]. The Hamiltonian obtained by substituting these expressions into Eq. (3) is denoted $H_{\rm th}^{\alpha,2}$. We first consider the material part of $H_{\rm th}^{\alpha,2}$, which can be written $H_{{\rm th},m}^{\alpha,2} = \tilde{\omega}_m^\alpha l_\alpha^\dagger l_\alpha + \frac{1}{2}(\tilde{\omega}_m^\alpha - \omega_m)$ where $[l_\alpha, l_\alpha^\dagger] = 1$ and

$$\tilde{\omega}_m^{\alpha\,2} = \omega_m(\omega_m - 4\mathcal{C}_\alpha). \tag{4}$$

The mode operators $l_\alpha, l_\alpha^\dagger$ are related to b_α and $b_\alpha^\dagger$ by a local Bogoliubov transformation that incorporates the contribution $V_{\rm dip}$ [see Eqs. (79) and (80) in Ref. [51]]. This results in the renormalized frequency $\tilde{\omega}_m^\alpha$ in Eq. (4). Reality of $\tilde{\omega}_m^\alpha$ requires that

$$\omega_m \geq 4\mathcal{C}_\alpha = 2\rho d^2(1-\alpha^2). \tag{5}$$

When the electrostatic interaction strength $\mathcal{C}_\alpha$ is large enough this inequality may be violated signaling a phase transition. We refer to this transition as ferroelectric, because it is completely independent of the radiative mode. Inequality (5) generalizes the result of Keeling obtained when $\alpha = 0$ (Coulomb gauge) [36]. Violation of inequality (5) cannot occur in the multipolar gauge $\alpha = 1$, which does not therefore admit a purely ferroelectric phase. In what follows this finding will be reconciled with our claim that a unique phase transition is predicted within all gauges. We show further that only in the Coulomb gauge does the phase transition appear purely ferroelectric.

We now consider the thermodynamic limit of the total Hamiltonian, which is [51]

$$H_{\rm th}^{\alpha,2,i} = E^i_{\alpha+} f^{i\,\dagger}_\alpha f^i_\alpha + E^i_{\alpha-} c^{i\,\dagger}_\alpha c^i_\alpha + \frac{1}{2}(E^i_{\alpha+} + E^i_{\alpha-}) + C^i \quad (6)$$

where the superscript i is either $i = n$ for normal phase, or $i = a$ for abnormal phase. The polariton operators f^i_α, c^i_α are bosonic satisfying $[f^i_\alpha, f^{i\,\dagger}_\alpha] = 1 = [c^i_\alpha, c^{i\,\dagger}_\alpha]$ with all other commutators vanishing. In the normal phase, $i = n$, the zero-point constant in Eq. (6) is $C^n = N\epsilon_0 + (\rho d^2 - \omega_m)/2$ and the polariton energies are

$$2E^n_{\alpha\pm}{}^2 = 8\tilde{g}_\alpha \tilde{g}'_\alpha + \tilde{\omega}^{\alpha\,2}_m + \omega^2_\alpha \pm \sqrt{([\tilde{\omega}^{\alpha\,2}_m - \omega^2_\alpha]^2 + 16[\tilde{\omega}^\alpha_m \tilde{g}'_\alpha + \omega_\alpha \tilde{g}_\alpha][\tilde{\omega}^\alpha_m \tilde{g}_\alpha + \omega_\alpha \tilde{g}'_\alpha])}, \quad (7)$$

where $\tilde{g}_\alpha = g_\alpha\sqrt{\omega_m/\tilde{\omega}^\alpha_m}$ and $\tilde{g}'_\alpha = g'_\alpha\sqrt{\tilde{\omega}^\alpha_m/\omega_m}$. The coupling strength at which the lower polariton energy $E^n_{\alpha-}$ is no longer real signals the onset of the abnormal phase and the breakdown of $H_{\rm th}^{\alpha,2,n}$. Reality of $E^n_{\alpha-}$ requires that

$$\omega_m(\omega_m - 2\rho d^2)[\omega^2_\alpha - 2\omega_m \rho d^2(1-\alpha)^2] \geq 0. \quad (8)$$

From the Thomas-Reiche-Kuhn (TRK) inequality $e^2/m \geq 2\omega_m d^2$ it follows that $\omega^2_\alpha \geq 2\omega_m \rho d^2(1-\alpha)^2$. Therefore, by inequality (8) $E_{\alpha-}$ is real if and only if

$$\omega_m \geq 2\rho d^2. \quad (9)$$

This simple gauge-invariant result defines the normal phase. Inequality (9) is stronger than inequality (5), so $\tilde{\omega}^\alpha_m$ in Eq. (4) is also real when inequality (9) is satisfied.

The Hamiltonian $H_{\rm th}^{\alpha,2,a}$ for the abnormal phase takes over from $H_{\rm th}^{\alpha,2,n}$ when inequality (9) is violated. It is obtained as the thermodynamic limit of $H^{\alpha,2}$ written, via the Holstein-Primakoff map, in terms of displaced modes f_α and c'_α such that $b_\alpha = f_\alpha - \sqrt{\beta_\alpha}$ and $c_\alpha = c'_\alpha + i\sqrt{\gamma_\alpha}$, where $\beta_\alpha = \beta \coloneqq N(1-\tau)/2$ and $\gamma_\alpha = N g^2_\alpha(1-\tau^2)/\omega^2_\alpha$ are of order N, with $\tau = \omega_m/(2\rho d^2)$. Note that $\beta_\alpha = \beta$ is α independent indicating that the "material" mode is always displaced by the same macroscopic quantity. On the other hand, γ_α is α dependent, so the extent to which the "radiative" mode is displaced depends on the chosen definition of radiation. In particular, $\gamma_0 = 0$, so in the Coulomb gauge *only* the material mode is displaced. In the abnormal phase, $i = a$, the zero-point constant in Eq. (6) is $C^a = N[\epsilon_0 - \omega_m(1-\tau)^2]/(4\tau) - \rho d^2/2$ and the polariton energies are

$$2E^a_{\alpha\pm}{}^2 = 8\underset{\sim}{g}_\alpha \underset{\sim}{g}'_\alpha + \underset{\sim}{\omega}^{\alpha\,2}_m + \omega^2_\alpha \pm \sqrt{([\underset{\sim}{\omega}^{\alpha\,2}_m - \omega^2_\alpha]^2 + 16[\underset{\sim}{\omega}^\alpha_m \underset{\sim}{g}'_\alpha + \omega_\alpha \underset{\sim}{g}_\alpha][\underset{\sim}{\omega}^\alpha_m \underset{\sim}{g}_\alpha + \omega_\alpha \underset{\sim}{g}'_\alpha])}, \quad (10)$$

where $\underset{\sim}{\omega}^{\alpha\,2}_m = \omega_m{}^2[1-(1-\alpha^2)\tau^2]/\tau^2$, while $\underset{\sim}{g}'_\alpha = g'_\alpha\sqrt{\tau\underset{\sim}{\omega}^\alpha_m/\omega_m}$, and $\underset{\sim}{g}_\alpha = g_\alpha\sqrt{\tau\omega_m/\underset{\sim}{\omega}^\alpha_m}$. The material frequency $\underset{\sim}{\omega}^\alpha_m$ is real provided $(2\rho d^2)^2 \geq \omega_m{}^2(1-\alpha^2)$ and the lower polariton energy $E^a_{\alpha-}$ is real provided

$$([2\rho d^2]^2 - \omega_m{}^2)[\omega^2_\alpha - \omega_m{}^2(1-\alpha)^2] \geq 0. \quad (11)$$

In the abnormal phase we have $2\rho d^2 \geq \omega_m$ implying that $\omega^2_\alpha - \omega_m{}^2(1-\alpha)^2 \geq 0$ and therefore that $E^a_{\alpha-}$ is real. At the critical coupling point where $2\rho d^2 = \omega_m$ the Hamiltonians $H_{\rm th}^{\alpha,2,n}$ and $H_{\rm th}^{\alpha,2,a}$ coincide. We have therefore obtained a description of the thermodynamic limit for all coupling strengths. The polariton energies constitute different two-level approximated results in each different gauge α. This is shown in [51], Fig. 1. However, every gauge's approximate (Dicke) model predicts exactly one ground state phase transition occurring when $\omega_m = 2\rho d^2$ and the ground state is unique within the nontruncated theory. Therefore, inequality (9) should be interpreted as predicting a unique phase transition. However, the nature of the phase transition appears to be different depending on the value of α. In the Coulomb gauge for example, it is necessarily purely ferroelectric, whereas this is impossible in the multipolar gauge.

The radiative classification of a unique phase transition will naturally depend on the definition of radiation and the latter is controlled by the gauge. Evidently, the *subsystem*

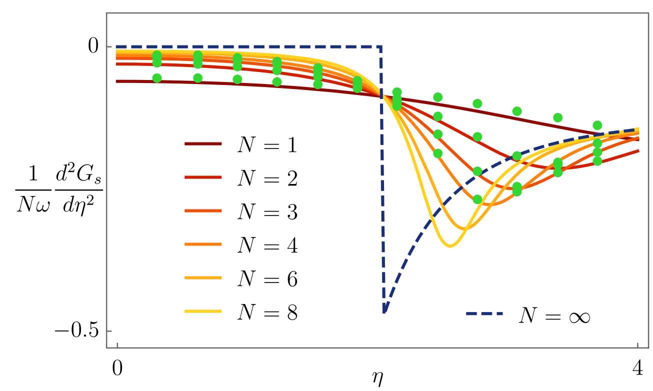

FIG. 1. Second derivative of the normalized ground energy $(N\omega)^{-1}d^2G_s/d\eta^2$ plotted for various values of N as a function of η found using the multipolar-gauge two-level model (solid curves). A precursor to the discontinuity that locates the phase transition in the limit $N = \infty$ can clearly be seen. The green dotted curves provide exact (gauge-invariant) predictions found without two-level truncation. Agreement already occurs at $N = 4$. $\beta = 3.3$ and $\mathcal{E}$ is chosen such that $\omega_m = \omega$.

gauge-relativity of QED [55], is strongly exemplified by the phase transition phenomenon. To understand the physical meaning of "matter" and "radiation" in the gauge α we note that the *total* multipolar polarization of N dipoles is $\mathbf{P}(\mathbf{x}) = \sum_{\mu=1}^{N} \mathbf{d}_\mu \delta(\mathbf{x} - \mathbf{R}_\mu)$. Since $\nabla \cdot \mathbf{E} = \rho = -\nabla \cdot \mathbf{P}$ it follows that for $\mathbf{x} \neq \mathbf{R}_\mu$ we have $\mathbf{P}_T = \mathbf{E}_L$ and therefore $\mathbf{\Pi}_\alpha = -\mathbf{E}_T - \alpha \mathbf{E}_L$ [cf. Eq. (2)]. Similarly, the material momentum $\mathbf{p}_\alpha$ of a dipole is given by Eq. (1) in which $q\mathbf{A}(\mathbf{0})$ is the electric dipole approximation of $q\mathbf{A}(\mathbf{r}) = \mathbf{P}_{\rm long} = \int d^3x \mathbf{E}_{L\mathbf{r}}(\mathbf{x}) \times \mathbf{B}(\mathbf{x})$, which is the momentum of the longitudinal field generated by q at $\mathbf{r}$ with $\nabla \cdot \mathbf{E}_{L\mathbf{r}}(\mathbf{x}) = q\delta(\mathbf{x} - \mathbf{r})$.

As an example, one may consider the Coulomb gauge in which "matter" is fully dressed by $\mathbf{E}_L$, i.e., $\mathbf{p}_0 = m\dot{\mathbf{r}} + \mathbf{P}_{\rm long}$, so matter as defined by $\mathbf{p}_0$ is not fully localized. Correspondingly, radiation is defined using the field $\mathbf{\Pi}_0 = -\mathbf{E}_T$ alone. In the multipolar-gauge (within the electric dipole approximation) matter is completely bare, i.e., $\mathbf{p}_1 = m\dot{\mathbf{r}}$, and therefore fully localized. Radiation is correspondingly defined for $\mathbf{x} \neq \mathbf{0}$ by the local (causal) total field $\mathbf{\Pi}_1 = -\mathbf{D}_T = -\mathbf{E}_T - \mathbf{E}_L = -\mathbf{E}$. More generally, α controls how the longitudinal electric degrees of freedom are shared out, thereby controlling the balance between localization and electrostatic dressing in defining the quantum subsystem called "matter." Radiation is then defined using the canonical degrees of freedom left over.

There are noteworthy gauges in between $\alpha = 0$ and $\alpha = 1$, such as gauges relative to which ground state "virtual photons" are highly suppressed and for which the corresponding two-level model can sometimes offer a more accurate representation of the ground state than conventional quantum Rabi models [49] (see also Ref. [51]). What differs between gauges is the spacetime localization properties of "material sources" and their dressing by virtual photons. In general the most operationally relevant definitions of the subsystems may depend on the available measurements, including their time and length scales. As a result, general statements about *measurable* photon condensation (superradiance), that are independent of experimental context, cannot be made. What can be demonstrated and is demonstrated below, is that there are no internal theoretical inconsistencies and no fundamental paradoxes. Previous no-go and counter no-go theorems refer to different definitions of radiation and so are not contradictory. They are in fact equivalent.

We now calculate the ground-state momentum $\mathbf{\Pi}_\alpha$ of radiation defined relative to gauge α. This directly demonstrates strict equivalence of all gauges and reveals an unambiguous macroscopic manifestation of the abnormal phase. We allow the two-level truncation to be performed in an arbitrary gauge α'. The α'-gauge two-level approximation of an operator $o_\alpha = o_\alpha(\mathbf{p}_\alpha, \mathbf{\Pi}_\alpha)$, denoted $o_\alpha^{\alpha',2}$, is found by expressing o_α in terms of α'-gauge canonical operators followed by two-level truncation. For $\Pi_\alpha = \boldsymbol{\varepsilon} \cdot \mathbf{\Pi}_\alpha$ we have $\Pi_\alpha^{\alpha',2} = \Pi_{\alpha'} - d(\alpha - \alpha')(J_{\alpha'}^+ + J_{\alpha'}^-)/v$. We will see that in the thermodynamic limit the ground state value of $\Pi_\alpha^{\alpha',2}$ is actually independent of α', i.e., the prediction is gauge invariant, so we return to the simpler notation $\Pi_{\alpha,\rm th}$. Using the Holstein-Primakoff representation, we find that $\Pi_{\alpha,\rm th}$ vanishes in the normal phase and in the abnormal phase is proportional to the identity. The calculation in Ref. [51] yields the simple result

$$\Pi_{\alpha,\rm th}^a = \alpha\rho d\sqrt{1-\tau^2} = \frac{\alpha}{2d}\sqrt{(2\rho d^2)^2 - \omega_m{}^2}. \quad (12)$$

The factor of α in Eq. (12) is highly significant. It demonstrates that the degree of superradiance in the abnormal phase is proportional to α, with the minimum value of zero occurring only in the Coulomb gauge.

To demonstrate equivalence between all gauges we calculate the α-gauge transverse polarization $P_{T\alpha} = \alpha\boldsymbol{\varepsilon} \cdot \mathbf{P}_T = \alpha(\Pi_0 - \Pi_1)$, which is such that $P_{T\alpha}^{\alpha',2} = \alpha(d/v)(J_{\alpha'}^+ + J_{\alpha'}^-)$. This quantity is also α' independent in the thermodynamic limit. In the normal phase $P_{T\alpha,\rm th}$ vanishes, whereas in the abnormal phase it is found by the same method that leads to Eq. (12) to be $P_{T\alpha,\rm th}^a = -\alpha\rho d\sqrt{1-\tau^2}$. Equation (12) then yields $\Pi_{\alpha,\rm th}^a = -P_{T\alpha,\rm th}^a$, which since $-E_{T,\rm th}^a = \Pi_{0,\rm th}^a = 0$, is seen to be nothing but the fundamental kinematic relation, Eq. (2). This establishes consistency between all gauges. The quantity $|P_{T,\rm th}^{\alpha',2,a}| = |P_{T\alpha,\rm th}^{\alpha',2,a}/\alpha|$ provides a gauge-invariant monotonic measure of the coupling distance past the phase transition point. Thus, independent of the gauge the onset of the abnormal phase manifests in the form of a macroscopic value of the gauge-invariant field $\mathbf{P}_T$;

$$P_{T,\rm th}^a = -\rho d\sqrt{1-\tau^2} \quad (13)$$

which is plotted in [51], Fig. 2. Within the present simplified Dicke-type treatment the field $\mathbf{P}_T$ is independent of spatial position $\mathbf{x}$, but at a more fundamental level $\mathbf{P}_T$ coincides with the longitudinal electric field $\mathbf{E}_L$ away from the dipole positions, i.e., for $\mathbf{x} \neq \mathbf{R}_\mu$. Whether one considers $\mathbf{E}_L = \mathbf{P}_T$ to be "material" or "radiative" determines whether one calls the phase transition "purely ferroelectric" or "superradiant," and this in turn is determined by the gauge choice as discussed earlier.

We finally consider a concrete example. We assume that each dipole has canonical operators pointing along $\boldsymbol{\varepsilon}$ and a double-well potential $V(\theta, \phi) = -\theta r^2/2 + \phi r^4/4$ where θ and ϕ control the shape of the double well. The Hamiltonian of each dipole is therefore $H_m^\alpha = (\mathcal{E}/2)[-\partial_\zeta^2 - \beta\zeta^2 + (\zeta^4/2)]$ [43] where we have defined $\zeta = r/r_0$ with $r_0 = (1/[m\phi])^{1/6}$, along with $\mathcal{E} = 1/(mr_0^2)$ and $\beta = \theta m r_0^4$. We also define the gauge-invariant dimensionless coupling parameter $\eta = (e/\omega)\sqrt{\rho/m}$. The parameters e, m, and ρ can now be eliminated in favor of $\mathcal{E}$, β, and η. To demonstrate that it is possible to obtain accurate two-level model predictions and to show a clear precursor to the phase transition, in Fig. 1 we consider the normalized second derivative of the (shifted) ground energy [7]. In the abnormal phase of the thermodynamic limit this is given by

$$\frac{1}{N\omega}\frac{d^2G_s^{\alpha,2}}{d\eta^2}\bigg|_{\mathrm{th},a} = -\frac{\omega_m}{\omega}\frac{d^2}{d\eta^2}\frac{(1-\tau)^2}{4\tau} \tag{14}$$

where $G_s = G - \rho d^2/2$ is the ground energy G shifted by the coupling-dependent term $\rho d^2/2$ in Eq. (3). We choose $\beta = 3.3$, which provides a highly anharmonic single-dipole spectrum such that $(\epsilon_2 - \epsilon_0)/\omega_m \approx 36$. The two-level truncation within the multipolar gauge $\alpha = 1$ is subsequently found to be accurate in predicting low energy properties. This was first confirmed in the case of the Rabi model $N = 1$ in Ref. [43]. The accuracy actually increases with N and convergence of exact (gauge-invariant, no two-level truncation) and approximate predictions already occurs at $N = 4$. The situation may change if the double well is parameterized differently such that the multipolar truncation is not optimal [49], see also additional analysis in Ref. [51].

The situation may also change if additional cavity modes are taken into account [50,56]. In particular, the multipolar-gauge coupling scales as $\sqrt{\omega}$ such that the single-mode approximation appears least favorable in this gauge, and has been shown to breakdown in the ultrastrong-coupling regime [56]. To incorporate some of the effects of non-resonant modes within a Dicke-type model a formal procedure of adiabatic elimination can be used and this also has the advantage of enabling an exploration of more diverse dipolar geometries [29]. Nevertheless, for our purpose of determining whether a physical phase transition can be supported by systems describable using a Dicke model and on understanding its relationship to the choice of gauge, the single-mode restriction is sufficient, because the qualitative behavior of the thermodynamic limit of the single-mode Dicke model is known to carry over to the multimode case [10,57]. The extension to general dipolar arrangements, and to more sophisticated cavity models warrants further study.

We have shown that a unique physical phase transition can occur in simple many-dipole cavity QED systems. We have resolved all ambiguities pertaining to the choice of gauge by determining both the origin and properties of the phase transition in terms of any gauge's definitions of the quantum subsystems, and by demonstrating equivalence between all gauge choices. We have shown that the original "no-go theorem" [30] does not apply, and also that one need not look beyond ordinary cavity QED in order to find systems supporting a superradiant phase transition. A no-go *theorem* for ground state superradiance occurs for, and only for, the Coulomb-gauge definition of radiation. We have shown that although the two-level approximation ruins the gauge invariance of the theory, unambiguous predictions can still be obtained. The framework developed here should be straightforwardly extendable to artificial solid-state and superconducting systems, as well as to driven and dissipative systems. This will elucidate both qualitatively and quantitatively the underlying causes and physical natures of thermodynamic phase transitions therein, and in each case, determine optimal approximate descriptions.

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