Nonequilibrium Dicke Quantum Phase Transition of an Ultracold Gas in an Optical Cavity

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We investigate the nonlinear light-matter interaction of a Bose-Einstein condensate in an optical cavity with transverse pump. This setup is described by a generalized Bose-Hubbard model which comprises the Dicke model of superradiance and reveals a nonequilibrium quantum phase transition from a superfluid condensate to a self-organized density-wave pattern. Due to the strong mutual dynamical backaction of the cavity light field and the interatomic correlations, we use a nonperturbative bosonic dynamical mean-field theory approach. For a narrow linewidth cavity as used in an experiment, we identify the Dicke quantum phase transition and the superradiant phase along the self-organization order parameter, density distributions and the cavity photon number. Moreover, we find a mixed phase in which the superfluid and the superradiant phases coexist.

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The interaction of an atomic ensemble with a photon field stays at the heart of quantum optics. The well-studied Jaynes-Cummings (JC) model describes the interaction of a single two-level atom and a single electromagnetic field mode \textsuperscript{[1]}. Since in free space a single photon mode is yet inaccessible, originally this model was introduced as an idealization of the light-matter interaction. However, nowadays optical cavities with an extremely high finesse can be fabricated routinely and are indispensable for a wide range of fundamental and applied research \textsuperscript{[2]}. Since a cavity intrinsically selects a single mode, the JC model turned into a precise description of the actual experimental situation \textsuperscript{[3]}. In fact, modern optical cavities provide a way to investigate collective matter-light interaction beyond a single-atom picture. This was first rigorously formulated by Dicke \textsuperscript{[4]}. He showed that when many atoms of an ensemble couple simultaneously to the same individual electromagnetic field mode, the ensemble radiation is strongly enhanced and occurs coherently and anisotropically within a much shorter time. This superradiance occurs because the atoms emit and absorb photons collectively and strong interatomic correlations build up. They act on the atom-field dynamics and lead to a highly nonlinear dynamical behavior \textsuperscript{[5]}. However, the realization of Dicke’s idea remained elusive because preparing a sufficiently dense ensemble of identical atoms in a resonator and then couple them to a single field mode is yet very challenging due to the optical field continuum.

For an experimental realization of the Dicke model, recently a hybrid setup of a Bose-Einstein condensate (BEC) inside a high-finesse optical cavity has been designed. A BEC per se is an ensemble of identical atoms and one can tailor a high-quality optical cavity to capture solely a single field mode to interact with the strongly correlated quantum many-body system.

An early insightful theoretical proposal \textsuperscript{[6]} showed that a quantum phase transition from the homogeneous superfluid BEC into a density modulated configuration, the so-called self-organized phase, emerges if one drives the BEC with a transverse laser pump sufficiently strongly. This scenario was shown to be directly connected to Dicke’s original concept of superradiance and was realized experimentally for the first time with thermal atoms \textsuperscript{[7]}, and, more recently, with a BEC \textsuperscript{[8–10]}. This latest progress has triggered a tremendous revisit of the Dicke model \textsuperscript{[11]}. To have a complete theoretical description of a BEC inside a cavity, one has to combine two paradigmatic models. The Bose-Hubbard (BH) model has to be joined with the JC model to derive a generalized BH model \textsuperscript{[12–14]} (hereafter, we follow Ref. \textsuperscript{[13]}). Due to the strong interaction of the atoms with the light field and among each other, the collective back action of the atoms on the photon field can readily be enhanced and the field dynamics becomes dependent on the collective interatomic interaction. In turn, the collective interatomic interaction is mediated by the photon-field and thus becomes itself strongly time-dependent. This gives rise to an inherently and strongly nonlinear dynamical collective behavior. An approach in terms of a static mean-field theory \textsuperscript{[15]}, which is very successful for the pure BH model \textsuperscript{[16]}, yields useful first insights by treating the interatomic interaction in terms of an effective static mean field. However, the collective interatomic interaction is an intrinsically time-dependent nonequilibrium quantity and a more refined treatment is necessary.

In this Letter, we use the bosonic dynamical mean field theory (BDMFT, see \textsuperscript{[17]} and references therein) in which the quantum many-body interaction dynamically evolves and eventually can be evaluated self-consistently. Due to its non-perturbative nature, it is applicable to the strongly correlated generalized BH model with its strong dynamical back action. Our realistic description of the
pumped optical cavity also includes the unavoidable cavity losses. For concreteness, we consider the setup of the high-finesse cavity realized as examples in Hamburg [9, 10] as well as the design realized in Zürich [8] with somewhat larger cavity losses. We quantify the self-organized phase by an order parameter \( \Phi \) which shows a clear quantum phase transition for increasing the transverse pump laser field. Moreover, we obtain atomic density distributions and effective lattice depths of the optical potential in the cavity and we compute the output photon number and the superfluid order parameter \( \varphi_{SF} \). This allows us to identify a mixed phase which is of particular interest in the experiments. Eventually, we address the individual role of the cavity decay rate and the pump-cavity detuning on the nonequilibrium quantum phase transition.

**Generalized Bose-Hubbard model** - The BEC consists of \( N \) identical atoms of mass \( m \), which are strongly interacting with a single standing wave cavity mode of frequency \( \omega_c \). Moreover, the BEC is pumped by a transverse laser field. Analogous to the experiments [9, 10], we consider a strong trapping potential in the \( y \)-direction (\( V_p = 25E_k \)) with the recoil energy \( E_k \). Then, the two-dimensional BH model in the cavity (\( x-z \)) plane results, with the Hamiltonian [13, 19]

\[
\mathcal{H} = - \sum_{\langle i,j \rangle} J_{\delta} b_i^\dagger b_j^0 + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + 2 \Re(\alpha) \eta^{\text{eff}} \int_0^\tau \sum_i (-1)^{i+1} \hat{n}_i + \sum_i (V_i^{\text{ext}} - \mu^{\text{eff}}) b_i^\dagger b_i.
\]

Here, \( b_i(b_i^\dagger) \) are bosonic annihilation (creation) operators that specify the local particle density \( n_i = b_i^\dagger b_i \) at site \( i \) and the total particle number \( N = \sum_i n_i \) where \( N_x = L^2 \) is the total number of sites in a \( L \times L \) square lattice with the linear lattice size \( L \). In addition to the standard BH-model, the key element of \( \mathcal{H} \) is the 3rd term. It crucially influences the cooperative effects via the cavity light field and the effective pump laser strength. It is responsible that two adjacent potential wells for the atoms are different in their depths. If this term is strong enough (i.e., for strong pumping), the self-ordered checkerboard phase becomes possible and a phase transition may occur. The effective pump laser strength is given by \( \eta^{\text{eff}} = -\sqrt{|U_0||V_p|} \) where \( U_0 \) is the refractive index due to a single atom and \( V_p \) is the pump laser strength. The cavity light field operator \( \hat{a} \) in the original form [13] enters via a coherent state complex number \( \alpha \) in \( \mathcal{H} \) [15] after eliminating the field. For this, the Heisenberg equation of motion for \( \hat{a} \) in presence of cavity losses characterized by the cavity decay rate \( \kappa \) is formulated and approximately solved. This effectively leads to the substitution \( \hat{a} \mapsto \alpha = \eta^{\text{eff}} \int_0^\tau \sum_i (-1)^{i+1} \hat{n}_i / (\Delta' + i\kappa) \) where \( \Delta' = \Delta_c - U_0 J_0 N \) with \( \Delta_c = \omega_k - \omega_c \) being the pump-cavity detuning. The site-independent on-site matrix element \( J_0 \) of the potential due to the cavity mode, the site-independent on-site potential \( J_0 \) due to the pump-cavity scattering, and the site-to-site hopping element \( J \) follow after an expansion in terms of Wannier states.

In passing, we note that the field elimination is strictly valid in the bad cavity limit for the setup of Ref. [8] when a large \( \kappa \) sets the fastest time scale [20]. In the good cavity limit with much smaller \( \kappa \) [9, 10], photons traverse much longer inside the cavity before they are lost and therefore the field elimination may not be strictly valid, but provides an improved approximation scheme. The explicit dynamical treatment of the light field is much more complicated and will be treated elsewhere.

Unlike for the standard BH model, the hopping amplitudes \( J_{x,z} \) and the on-site interaction \( U \) are not fixed a priori, but are given in terms of the momentum state of the photon field. In particular, we have that \( J_{x,z} = \frac{4}{\sqrt{\pi}} \left( \frac{V_{x,z}}{E_k} \right)^{3/4} \exp(-2\sqrt{V_{x,z}/E_k}) \) and \( U = 4\sqrt{2\pi}(\frac{1}{V_p}) \left( \frac{V_{x,z}V_p}{E_k} \right)^{1/4} \) with \( V_z = V_p \). Importantly, the effective potential \( V^{\text{eff}} = V_z = V_0 + U_0|\alpha|^2 \) along the cavity axis explicitly depends on the photon number which nicely illustrates that the lattice inside the cavity is dynamically

![Figure 1](image.png)

**FIG. 1.** Top: Order parameter \( \Phi \) of the self-organized phase and two exemplary density distributions. Middle: Effective potential \( V^{\text{eff}} = V_0 + U_0|\alpha|^2 \) along the cavity axis (left ordinate) and mean photon number \( |\alpha|^2 \) in the cavity (right ordinate). Bottom: Resulting hopping amplitude \( J_z \) along the cavity (\( x \)-axis) and calculated on-site interaction \( U \) (right ordinate). All panels are vs the transverse pump laser strength \( V_p \) (in units of \( E_k \)). The cavity decay rate, detuning and external classical potential are \( \kappa = 50E_k \), \( \Delta_c = -10E_k \) and \( V_0 = -5E_k \).
formed. For a realistic description, an extra lattice potential along the cavity axis with amplitude \( V_{\text{cl}} = -5E_R \) is added to ensure the validity of the tight-binding picture. We set the scattering length to \( a_s = 5.77 \text{nm} \) and the pump laser wavelength to \( \lambda_p = 803 \text{nm} \) according to the setup of Refs. [9] [15]. Also, the effective chemical potential depends on the state of the light-field and reads 
\[
\mu_{\text{eff}} = \mu_0 - U_0 |\alpha|^2 J_0.
\]
This directly expresses the interdependence between the state of the light field \( \alpha \) and the chemical potential (i.e., the particle number) which is the origin of the nonlinear behavior of this system [12]. In what follows, we focus on the homogenous system and set the external local potential to zero, i.e., \( V_{\text{ext}}^i = 0 \). Moreover, we consider a fixed temperature of \( T = 0.1 E_R \) and a given light shift of \( U_0 = -0.1 E_R \).

**Method** - To compute the resulting steady state of \( \mathcal{H} \), we use BDMFT which is analogous to the fermionic counterpart [21] and which is a nonperturbative approach to study a strongly correlated many-body bosonic system. The reliability of BDMFT depends on the behavior of the BH model in the limit of \( z \to \infty \) where \( z = 2d \) is the coordination number in a \( d \)-dimensional lattice [17]. In this limit, one can rigorously show that the BH model retains a local many-body self-energy. As a net result, the BH model is mapped onto an effective bosonic impurity model. Furthermore, a real-space extension of BDMFT has been developed recently which importantly incorporates any site-dependent behavior, either due to an external trapping potential [22] [23], or, solely by the underlying physics like the existence of a self-organized phase as in the current case. We eventually perform an exact diagonalization of the Anderson impurity model with fairly small numbers of orbitals (\( n_s = 4 - 6 \)) to obtain the local densities \( n_i \). Simultaneously, we monitor also the cavity photon number \( |\alpha|^2 \) until convergence for both parts is achieved. Throughout this work, we consider a \( 6 \times 6 \) lattice with a fixed total particle number \( N \approx 72 \). To quantify the self-organized quantum phase transition, we calculate the order parameter as \[ \Phi = \sum_i (-1)^i n_i / \sum_i n_i \]. In a normal and uniform BEC, \( \Phi = 0 \), while in an ideal self-organized phase with a perfect checkerboard pattern in which the density modulates between zero and one, we have \( \Phi = 1 \). However, in general, if the density modulation is between two non-zero values, then \( \Phi < 1 \).

**Results** - In the top panel of Fig. 1 we show the order parameter \( \Phi \) of the self-organized phase vs. the transverse pump laser strength \( V_p \). A clear quantum phase transition can be observed. A critical pump laser strength \( V_p^{\text{crit}} \) exists, below which the system is in a featureless superfluid BEC phase. The BEC is stable and the real-space density distribution is expectedly uniform with all \( n_i \approx 2 \) (see inset for an example).

For \( V_p < V_p^{\text{crit}} \), the scattering processes between the laser photon field and the BEC atoms are destructive and too weak for the cavity lattice to build up. In turn, this induces then a zero photon number \( |\alpha|^2 \) along the cavity axis that we show in the middle panel of Fig. 1 (right ordinate). The effective lattice depth \( V_{\text{eff}} \) along the cavity axis \( (x) \) is a sum of the external classical optical lattice with depth \( V_{\text{cl}} = -5E_R \) and the one from the photon field. For \( V_p < V_p^{\text{crit}} \), we have that \( V_{\text{eff}} = V_{\text{cl}} \) as shown in the middle panel, left ordinate. Moreover, we obtain finite values for the resulting hopping amplitude \( J_x \) along the cavity \( (x) \) axis (left ordinate). The interatomic on-site interaction \( U \) grows monotonously.

Upon increasing \( V_p \), a pronounced quantum phase transition occurs which stems from the constructive scattering between the atoms and the pump laser, see top panel of Fig. 1. The BEC atoms now redistribute themselves in a checkerboard density-wave pattern and the self-organization occurs. This phase transition from the superfluid BEC to the self-organized phase is associated to the Dicke phase transition [1] [24] and has been observed in recent experiments [8] [9]. The corresponding real-space density distribution for large \( V_p \) shows the density modulated checkerboard pattern. Therefore, the system faces a symmetry breaking when crossing \( V_p^{\text{crit}} \). A related result for \( \Phi \) vs \( V_p \) was obtained by a static mean-field approach [15], but we cannot quantitatively compare them with our results since in BDMFT the interactions are not fixed a priori, but are calculated dynamically and self-consistently. It is worth to note that the density modulation is between \( n_i = 1 \) and \( n_i = 3 \), such that we obtain \( \Phi < 1 \) even in deep self-organized phase.

We monitor also the photon number (right ordinate of the middle panel in Fig. 1). It shows a steady increase after crossing \( V_p^{\text{crit}} \) which originates from the constructive scattering. Regarding the behavior of \( V_{\text{eff}} \) in this regime (left ordinate of the middle panel), we note that similar to the experiments, both \( V_{\text{cl}} \) and \( U_0 \) have the same negative sign. Therefore, we observe a negative increase

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**FIG. 2.** Phase boundary between the super-fluid and the self-organized phase for varying cavity decay rates \( \kappa \) and critical pump laser strengths \( V_p^{\text{crit}} \) (both in units of \( E_R \)). The dashed line represents a square-root fit as suggested in [20].
of $V_{\text{eff}}$ beyond $V_p^{\text{crit}}$. The atom hopping along the cavity $J_c$, is clearly hindered because now the corresponding $V_{\text{eff}}$ is deeper. In turn, the onsite interaction $U$ changes smoothly.

The quality of the cavity is characterized by its decay (damping or photon loss) rate $\kappa$. Therefore, it is natural to examine the effect of $\kappa$ on the nonequilibrium Dicke quantum phase transition. In Fig. 2 we show the interdependence between $\kappa$ and $V_p^{\text{crit}}$ for several values of $\kappa$ and the associated phase boundary. We observe that for smaller values of $\kappa$ (i.e., higher $Q$ factors of the cavity), one needs a smaller $V_p^{\text{crit}}$ to drive the system over the quantum critical point. This is understandable because a smaller $\kappa$ implies a reduced photon leakage. Subsequently, a lower pump power is required to trigger the superradiance that appears upon crossing $V_p^{\text{crit}}$. Fig. 2 also shows a fit to a square-root behavior of the phase boundary as qualitatively suggested in Ref. [25].

The real-space BDMFT also allows us to calculate the superfluid order parameter $\varphi_{\text{SF}} = \langle b \rangle$. This is depicted in Fig. 3 together with $\Phi$. We observe that $\varphi_{\text{SF}}$ vanishes when $\Phi$ departs from zero, i.e., when the phase transition from the superfluid to the self-organized phase occurs. Interestingly, there is a sizable window in the vicinity of quantum critical point in which both the order parameters $\varphi_{\text{SF}}$ and $\Phi$ simultaneously coexist. This manifestation of both the long-range superfluid order and the spatially ordered density-wave is regarded as the supersolid phase. It is still a highly disputable phase of matter [20] due to its theoretical and experimental complexity. This phase has been discussed related to an experiment in Ref. [8] [27] and theoretically in Ref. [19].

A further decisive tunable parameter in the experiment is the pump-cavity detuning $\Delta_c$. In Fig. 4, we analyze its role for a fixed cavity decay rate $\kappa = 50E_h$. In accordance to the experiments [8][10], we observe two distinct features in the phase diagram with sharp phase boudries between super-fluid and self-organized phase. For small negative $\Delta_c$, i.e., $\Delta_c > -100$, the critical pump power scales inversely with $V_p$ while for large negative values of $\Delta_c$ it scales linearly. This phase diagram has been reported also in both experiments in the good cavity limit [9][10] and the bad cavity limit [8]. Theoretically the phase diagram resembles the one with large ensemble of particles obtained by semi-classical kinetic Vlasov equation which neglects all correlations [28]. Even though our particle number here is much smaller than Ref. [28], we still capture the same physics. This indicates also the robustness of BDMFT over a wide range of parameters and different phases.

In conclusion, we have solved the generalized Bose-Hubbard model for a correlated quantum gas which interacts collectively with an optical cavity mode. Since the photon field evolves dynamically over time, a strong back-action on the interatomic correlations occurs. Hence, a static mean-field approach is not realistic and has to be replaced by dynamical mean-field calculations. Similar to the current experiments, we find by means of the non-perturbative real-space BDMFT that this model shows a nonequilibrium quantum phase transition upon increasing the transverse pump laser field strength. We have quantified the order parameter of the self-organized phase which is the main characteristics of the Dicke quantum phase transition from a normal superfluid BEC to a density-modulated self-organized checkerboard pattern. We have elucidated how the crucial parameters in the experiment, namely the cavity decay rate, the pump-cavity detuning and temperature affect the critical point. Moreover, we have found a region of phase space where a supersolid can be identified which could be directly measurable.

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