Vortex unbinding transition in nonequilibrium photon condensates

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We present a theoretical study of a Berezinskii-Kosterlitz-Thouless-like phase transition in lattices of nonequilibrium photon condensates. Starting from linearized fluctuation theory and the properties of vortices, we propose an analytical formula for the critical point containing four fitting parameters, that captures well all our numerical simulations. We find that the ordered phase becomes more stable when driving and dissipation are increased.

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I. INTRODUCTION

Thermalization of cavity photons through repeated absorption and emission by dye molecules [1] has led to the creation of photonic Bose-Einstein condensates (BECs) [2–5] and presents an invitation to study photonic systems from a quantum fluid perspective [6,7]. However, the dimensional reduction implied by the microcavity structure that serves to confine the photons and to give them a nonzero rest mass, immediately raises the issue of the Hohenberg-Mermin-Wagner theorem that forbids BEC in two dimensions at a finite temperature [8]. Experimentally, this no-go theorem has been circumvented by adding a harmonic trapping potential that enables condensation in the ground state owing to the modification of the density of states [2,4,5]. In the presence of a harmonic trapping potential, however, the condensate is not spatially extended, limiting its appeal as a quantum fluid.

Even though BEC is absent in two-dimensional Bose gases, there is a Berezinskii-Kosterlitz-Thouless (BKT) transition [8–11] that separates a normal phase with free vortices from a superfluid phase where all vortex-antivortex pairs are bound. For this phase transition to occur, interactions are crucial: In their absence, the vortex core size tends to infinity and vortices cease to be well-defined excitations. The necessity of interactions seems to be fatal for the possibility of a thermal equilibrium BKT transition in photon condensate systems where interactions are negligible [12].

In experimental realizations of photon condensates, however, thermalization is never perfect, because photons can escape through the confining mirrors. These losses have to be compensated by the continuous pumping of the dye molecules, so that currently available photon condensates are actually driven-dissipative systems. We have shown recently that the nonlinear dynamics of driving and dissipation renders the vortex core size in an extended lattice of coupled photon condensates finite [13], raising the hope for the existence of a BKT-like transition in driven-dissipative photon condensates.

Motivated by experiments on exciton polaritons, it has already been numerically demonstrated that nonequilibrium interacting Bose gases feature a BKT-like transition [14–16]. At the same time it has been shown that the phase dynamics is actually in the Kardar-Parisi-Zhang (KPZ) universality class, which has been argued to destroy the superfluidlike phase [17–19]. In practice, however, the KPZ physics can be limited to very large system sizes, so that in experimental two-dimensional (2D) systems the BKT-like physics dominates [14–16,20]. Exciton polaritons are quasiparticles that arise from the strong coupling between a photon and an exciton [21]. Their hybrid light-matter nature gives them sizable interparticle interactions. Their degree of thermalization depends strongly on the polariton lifetime, that spans from a few ps to a few hundred ps, with close to thermal states only achieved in the samples with the longest lifetimes [15,22]. The maturity in manufacturing gives polariton systems the edge for what concerns the observation of physical phenomena in spatially extended condensates, such as the observation of quantized vortices, the polariton volcano effect, and the KPZ dynamics of the phase (see Ref. [7] for a recent review). Unfortunately, due to the complicated processes that govern their dynamics (scattering with excitons, scattering with photons, disorder), microscopic models of their dynamics are not as well rooted in microscopic physics as for photon condensates where the dye absorption and emission are thoroughly understood. This actually makes it easier to make quantitative theoretical predictions for photon condensates as for their polariton counterparts.

We will address here the BKT transition in a nonequilibrium photon condensate with vanishing interparticle interactions. We will show that numerical classical field simulations on a finite lattice of photon condensates do predict a BKT-like transition, stabilized by driving and dissipation even in the absence of interactions. To corroborate our numerical results, we construct an analytical expression containing a few fitting constants that explains the numerically obtained dependence of the critical point on the system parameters.

Our theoretical results are relevant for experiments on lattices of photon condensates, that can be realized by patterning the microcavity mirrors [23,24], analogous to lattices for exciton polaritons [25]. We opt for this system instead of a translationally invariant photon condensate, because of the possibility to reduce the density and phase fluctuations [26] and to have well-defined vortices [13]. Moreover, as long as

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the tunneling amplitude remains much smaller than the temperature, classical field theory is an excellent approximation to the exact quantum dynamics. This stands in contrast to translationally invariant systems where classical field theories suffer from an ultraviolet catastrophe.

The remainder of this paper is organized as follows. We recapitulate our model for a lattice of photon condensates in Sec. II. Our analytical estimate for the critical point is derived in Sec. III. The fitting parameters in this expression are fixed by the numerical simulations presented in Sec. IV. We present our conclusions and outlook in Sec. V.

II. MODEL

The simplest theoretical model to describe a lattice of coupled photonic cavities in the quantum degenerate regime is the generalized Gross-Pitaevskii equation (gGPE) [26],

$$i\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t} = \frac{i}{2}[B_{21}M_2(\mathbf{x},t)-B_{12}M_1(\mathbf{x},t)-\gamma]\psi(\mathbf{x},t) - (1-i\kappa)J\sum_{\mathbf{x}'\in\mathcal{N}_\mathbf{x}}\psi(\mathbf{x}',t)+\sqrt{2\mathcal{D}(\mathbf{x},t)}\,\xi(\mathbf{x},t). \tag{1}$$

Here, γ is the photon loss rate and J the coupling between the nearest-neighbor cavities [23,24]. The photons thermalize due to repeated absorption and emission by the dye with the respective rate coefficients B_{12} and B_{21}. The ground (excited) molecular state occupation is denoted by $M_{1(2)}$ satisfying at all times $M_1(\mathbf{x})+M_2(\mathbf{x})=M$, where M is the number of dye molecules at each lattice site. The Kennard-Stepanov relation [27–29] gives rise to energy relaxation with dimensionless strength $\kappa = B_{12}\bar{M}_1/(2T)$ (we set the Boltzmann constant $k_B = 1$) [26]. The last term describes the spontaneous emission noise [30,31]: $\mathcal{D}(\mathbf{x},t) = B_{21}M_2(\mathbf{x},t)$ and $\xi(\mathbf{x},t)$ is Gaussian white noise with the correlation function $\langle\xi(\mathbf{x},t)\xi(\mathbf{x}',t')\rangle = \delta_{\mathbf{x},\mathbf{x}'}\delta(t-t')$. The evolution of the number of excited molecules due to interactions with the photons is opposite to the change in the number of photons due to emission (both deterministic and stochastic), absorption, and energy relaxation. In order to compensate for the loss of energy in the system, external excitation with a pumping laser is needed. Under the condition $J \ll T$, which assures that the occupations of all momentum states are much larger than one, the generalized Gross-Pitaevskii classical field model (1) is valid for all the modes and there is no need to use a more refined quantum optical approach [32–34].

The noise in Eq. (1) provides a description of the density and phase fluctuations. For the simplest case of a single cavity, a crossover in the density fluctuations between a "grand canonical" regime with large fluctuations ($\delta n^2 \sim \bar{n}^2$), for $\bar{n}^2 \ll M_{\rm eff}$, and a "canonical" regime with small fluctuations ($\delta n^2 \ll \bar{n}^2$), for $\bar{n}^2 \ll M_{\rm eff}$, have been observed [35,36]. Here, the "effective" number of molecules is given by $M_{\rm eff} = (M+\gamma e^{-\Delta/T}/B_{21})/[2+2\cosh(\Delta/T)]$, where Δ is the detuning between the cavity and the dye zero-phonon transition frequency. For $e^{\Delta/T} \ll 1$, one has $M_{\rm eff} \approx \bar{M}_2 \approx \eta M e^{\Delta/T}$ with $\eta = 1+\gamma/(2\kappa T)$, while the energy relaxation parameter becomes $\kappa \approx B_{21}Me^{\Delta/T}/(2T)$.

III. BOGOLIUBOV ANALYSIS

While the linear Bogoliubov theory [8,26] breaks down in the vicinity of the BKT transition, that involves large phase differences between neighboring cavities, it nevertheless forms a good starting point to obtain insight into the analytical dependence of the transition temperature on the system parameters.

For the linear analysis, the stochastic density and phase variables are written as their average value plus a small deviation: $\psi(\mathbf{x}) = \sqrt{\bar{n}+\delta n(\mathbf{x})}e^{i\delta\theta(\mathbf{x})}$. The Fourier components of the phase fluctuations are defined by

$$\delta\theta(\mathbf{x}) = \frac{1}{\sqrt{L}}\sum_\mathbf{k}\delta\theta_\mathbf{k}\,e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{2}$$

where L is the number of lattice sites, and analogous for $\delta n(\mathbf{x})$. In linear approximation to Eq. (1), the phase fluctuations obey the equation of motion [26]

$$\frac{\partial}{\partial t}\delta\theta_\mathbf{k} = -\kappa\epsilon_\mathbf{k}\delta\theta_\mathbf{k} - \frac{\epsilon_\mathbf{k}}{2\bar{n}}\delta n_\mathbf{k} + \sqrt{2\mathcal{D}_\theta}\xi^{(\theta)}_\mathbf{k}. \tag{3}$$

For a tight-binding Hamiltonian with hopping amplitude J, the single-particle dispersion equals $\epsilon_\mathbf{k} = 2J[2-\cos(k_x)-\cos(k_y)]$. The white noise has zero average and variance $\langle\xi^{(\theta)}_\mathbf{k}(t)\xi^{(\theta)}_{\mathbf{k}'}(t')\rangle = \delta_{\mathbf{k},-\mathbf{k}'}\delta(t-t')$ where the phase noise strength equals

$$\mathcal{D}_\theta = \frac{B_{21}\bar{M}_2}{4\bar{n}} = \frac{\eta\kappa T}{2\bar{n}}. \tag{4}$$

In the steady state, one obtains from $d\langle|\theta_k|^2|\rangle = 0$ the relation

$$\kappa\langle|\delta\theta_\mathbf{k}|^2\rangle + \frac{1}{2\bar{n}}\langle\delta\theta_{-\mathbf{k}}\delta n_\mathbf{k}\rangle = \frac{\mathcal{D}_\theta}{\epsilon_\mathbf{k}}. \tag{5}$$

In equilibrium, invariance under time reversal ($\theta \to -\theta$ and $\delta n \to \delta n$) ensures that the second term in Eq. (5) vanishes. In nonequilibrium photon condensates, time-reversal symmetry breaks down and the density-phase correlator will play an important role in our discussion of the phase fluctuations that lead to the BKT transition.

At large momenta, the kinetic energy is much larger than the time-reversal breaking rates that involve the pumping and losses. The density-phase correlations therefore become negligible at large k, so that the phase fluctuations assume their thermal equilibrium value. At low momenta, on the other hand, the nonlinear dissipative dynamics kicks in and deviations from the thermal behavior appear. The lower bound of the momentum region, where the thermal equilibrium expression for the phase fluctuations is a good approximation, is given by [26,37]

$$k_c = \left[\frac{\gamma\kappa}{4J}\left(1+\frac{\bar{n}^2}{\bar{M}_2}\right)\frac{\bar{n}^2}{\bar{M}_2}\right]^{1/6}\left(\frac{\eta T}{J\bar{n}}\right)^{1/3}. \tag{6}$$

At low temperatures, where phase fluctuations are moderate, Eq. (5) is accurate for all momenta, but close to the BKT temperature the linear approximation breaks down and the system properties are determined by the full nonlinear equations. Even then, at momenta $k > k_c$, the linear relation (5) is expected to hold approximately.

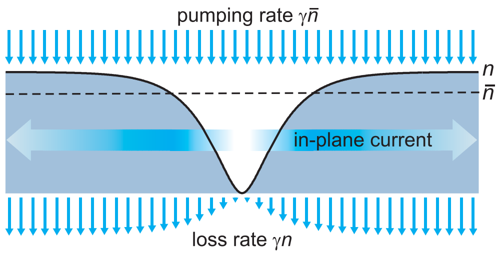

FIG. 1. Combination of a uniform pumping with losses proportional to the local density leads to outgoing particle flows from regions with reduced density.

In order to proceed further, we integrate (5) over all momenta [38] to obtain for the local fluctuations

$$\kappa\langle\delta\theta^2\rangle + \frac{1}{2\bar{n}}\langle\delta\theta\,\delta n\rangle = \frac{\mathcal{D}_\theta}{2\pi J}[c_1 + \ln(\pi/k_c)], \tag{7}$$

where the constant c_1 approximates the contribution from the momenta $k < k_c$, where (5) breaks down. It is clear from the logarithmic dependence of (7) on k_c that phase ordering is impossible in the absence of dissipative nonlinearity ($k_c \to 0$), reflecting the well-known fact that there is no phase transition for conservative noninteracting bosons in two dimensions.

Since phase fluctuations at the BKT transition are large, the parameter dependence of the transition point can be estimated with (7) by setting $\langle\delta\theta^2\rangle \sim 1$, provided that an estimate is available also for the the density-phase correlator. In order to obtain a first approximation, we restrict temporarily to one spatial dimension. Using partial integration to rewrite the density-phase correlator as $\langle\delta\theta\delta n\rangle = L^{-1}\int dx\,\delta\theta\delta n = -L^{-1}\int dx(\partial\theta/\partial x)\delta N$, where $\delta N = \int_0^x \delta n(x')dx'$, it can be related to the current by use of the identity $\partial j_x/\partial x = -\gamma\delta n$. This continuity relation shows that regions with density suppression, such as a vortex core, behave as a source of currents (see Fig. 1) [13,17,39–41]. With $j_x = 2J\bar{n}(\partial\theta/\partial x)$, this yields

$$\langle\delta\theta\,\delta n\rangle = \frac{1}{L}\frac{\gamma}{2J\bar{n}}\int dx\,\delta N^2(x) = \frac{\gamma}{2J\bar{n}}\langle\delta N^2\rangle. \tag{8}$$

In order to estimate the expectation value $\langle\delta N^2\rangle$ close to the transition, one can first consider a plane density wave of amplitude $a\bar{n}$, for which $\langle\delta N^2\rangle \propto \bar{n}^2a^2$. At the transition, vortices have to nucleate, which requires in a continuum model density fluctuations with amplitude $\bar{n}$ and hence $a = 1$. In a lattice geometry, however, the vortex core can be "in between" the lattice nodes and the density suppression smaller. In Ref. [13], the vortex core size was argued to roughly behave as $r_0 \sim \sqrt{J/\gamma}$. Assuming an exponential wave function in the vicinity of the vortex center, with density profile $n(r) = \bar{n}[1 - \exp(-r/r_0)]^2$, one can estimate the minimal density modulation depth sufficient to nucleate a vortex in the center of a plaquette as

$$a = 2e^{-c_3\sqrt{\gamma/J}} - e^{-2c_3\sqrt{\gamma/J}}, \tag{9}$$

where a constant $c_3 \sim 1$ was introduced. From the above arguments, we come to the following estimate for the dependence of the density-phase correlator on the system parameters close to the transition point, $\langle\delta\theta\delta n\rangle = 2c_2\bar{n}a^2\gamma/J$, with c_2 an additional fitting parameter.

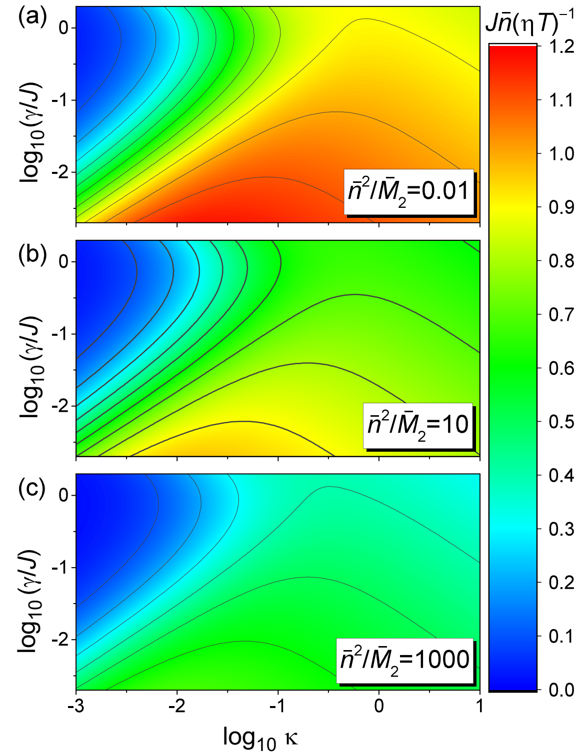

FIG. 2. Dimensionless coupling constant $J\bar{n}(\eta T)^{-1}$, given by Eq. (10), as a function of κ and γ/J for three different values of $\bar{n}^2/\bar{M}_2$.

Using $\langle\delta\theta^2\rangle = c_4 \sim 1$ together with the above estimate of $\langle\delta\theta\ \delta n\rangle$ allows us to rewrite Eq. (7) as a relation for the critical parameters,

$$\frac{J\bar{n}}{T} = \frac{\eta\kappa}{4\pi}\frac{c_1 + \ln(\pi/k_c)}{c_4\kappa + c_2a^2\gamma/J}, \tag{10}$$

where k_c and a are given by Eqs. (6) and (9). Because of the quite hand-waving arguments that have led us to relation (10), it cannot be expected to hold exactly. Nevertheless, we will show below that it offers a good description of the critical point, extracted from numerical simulations, for the following values of the fitting parameters: $c_1 = 3.82$, $c_2 = 0.139$, $c_3 = 1.23$, $c_4 = 0.510$. As implied by the results corresponding to moderate variations of the fitting parameters around the indicated values [42], fair agreement between the analytical and numerical results is mainly ensured by an adequate functional dependence on the relevant physical parameters in Eq. (10) rather than by an especially particular combination of the fitting constants c_1-c_4.

Figure 2 shows the variations of the dimensionless coupling constant $J\bar{n}/(\eta T)$ according to Eq. (10) as a function of the energy relaxation κ and the ratio of losses to hopping γ/J (note that both axes are logarithmic) for three values of the number of photons per cavity. We always restricted the dissipation strength to $\gamma/J < 2$ in order to keep a resolved photon dispersion.

Even though these parameters vary by orders of magnitude, the variations in the coupling constant are quite moderate. For large photon numbers (canonical regime, lower panel), the coupling parameter is close to 0.6 except for small κ, where nonequilibrium effects are strongest. For smaller numbers of photons (grand canonical regime), a larger coupling constant is needed in general and its variations are enhanced.

It is instructive to compare our relation (10) to the equilibrium BKT transition. The most elementary approximation is the reduction of the lattice Bose gas to the XY model, obtained by ignoring the density degree of freedom. The critical temperature has been determined to be $J\bar{n}/T = 0.56$ [43], which is close to the value that we obtain in a large part of parameter space in the deep canonical regime [see Fig. 2(c)].

In the limit of small γ, the second term in the denominator in Eq. (10), originating from the density-phase correlator, can be neglected and we obtain for the critical coupling parameter $J\bar{n}/T = \eta \ln(e^{c_1}\pi/k_c)/(4\pi c_4)$, whose form is reminiscent of the transition point of the weakly interacting Bose gas [11], that has been realized with dilute gases of ultracold atoms [44]. The main differences with the equilibrium case are that the crossover momentum k_c is now determined by losses instead of interactions and the appearance of the excess noise factor η. It is worth noting that in the limit of small γ, where $\eta \to 1$, the prefactor of the logarithm is in our fit equal to $1/(4\pi c_4) \approx 1/(2.04\,\pi)$, close to the equilibrium prefactor of $1/(2\pi)$ [11]. Not surprisingly, a reasonable agreement with the numerical data can be obtained also when fixing c_4 at its equilibrium value $1/2$ and using only three fitting parameters [42].

Formula (10) is also reminiscent of the heuristic expression $D_{\mathrm{BKT}}/n_{\mathrm{BKT}} \approx \kappa + 0.003c$, which has been shown to approximate fairly well the numerical results for the critical noise-to-density ratio as a function of κ and the "nonequilibrium parameter" $c \propto \gamma$ in interacting-polariton condensates [45].

IV. NUMERICAL RESULTS

Numerical simulations of the full gGPE (1) for an array of 100×100 cavities with periodic boundary conditions were done as explained in Ref. [26] and the location of the critical point was determined as in Ref. [45]: After a long-time evolution in the presence of noise, the system was evolved without noise for a short time ($\sim$10 ns) before checking for the presence of vortices. This noiseless evolution gives the advantage of cleaning up the photon phase while it is too short for the unbound vortex-antivortex pairs to recombine. The propensity for their recombination is reduced [16] with respect to the equilibrium case owing to outgoing radial currents that provide an effective repulsion between vortices and antivortices [17]. To determine the critical coupling J for the BKT transition, J_{BKT}, we use the following criterion. If for a coupling J vortex pairs are present after a noise exposure time t_{noise} (and hence $J < J_{\mathrm{BKT}}$), while for a certain coupling $J' > J$ no vortex pairs appear even at noise exposures a few times longer than t_{noise}, then J' lies either above J_{BKT} or below J_{BKT} and closer to J_{BKT} than to J. Therefore, the critical noise intensity can be estimated as $J_{\mathrm{BKT}} = J' \pm (J' - J)$.

Because the presence of vortices and antivortices is susceptible to statistical fluctuations, the numerical error on the transition point is not only due to our finite steps in parameter values, but also due to a statistical uncertainty. The stochastic contribution to the error bar is hard to quantify precisely, but

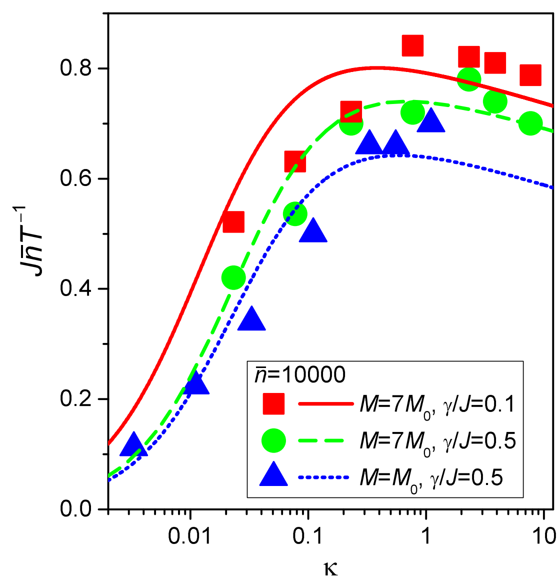

FIG. 3. Numerically determined dimensionless coupling strength $J\bar{n}T^{-1}$ at the BKT transition (symbols) as a function of κ for different values of M and γ/J. Here, $M_0 = 10^9$, $\Delta/T = -5.2$. The curves correspond to Eq. (10).

the analysis of many realizations of the dynamics allowed us to conclude that the statistical error bars are typically not larger than the symbol sizes in the figures.

As a first example of the parameter dependence of the critical coupling, we show in Fig. 3 $J\bar{n}/T$ as a function of κ, that was varied by changing both M and B_{21} around their values in current experiments [46]. The numerically obtained results are indicated with the symbols (symbols of the same type and color correspond to the same M but different B_{21}) and the fits with relation (10) are shown with solid lines. Good correspondence is observed over the whole range of κ, throughout which the critical coupling varies by one order of magnitude. The initial rise and subsequent saturation is clear from the explicit κ dependence in Eq. (10). As can be seen from the denominator in Eq. (10), in the regime of small κ the pumping and losses, proportional to γ, are dominant. The reduction of the critical coupling at small κ can therefore be interpreted as an increased robustness of the ordered phase due to driving and dissipation, in analogy with Ref. [45]. The decrease of $J\bar{n}/T$ at large values of κ originates from the k_c dependence on κ, while the increase with M is due to the dependence of k_c on $\bar{M}_2 \propto M$.

The dependence of the critical coupling on the number of photons per lattice site is illustrated in Fig. 4. Our relation (10) again captures most of the parameter dependence. According to Eq. (10), the decrease of the critical coupling parameter with the number of photons is due to the increase of the crossover momentum with increasing $\bar{n}$. This trend is reflected in the numerical results, but the numerical $\bar{n}$ dependence shows some features that are not entirely reproduced by our formula and require a more sophisticated theoretical approach. At first sight, it could be surprising that a phase transition still exists down to photon numbers as small as $\bar{n} = 1000$, well in the grand canonical regime with $\bar{n}^2/M_{\mathrm{eff}} = 0.18$ and 0.026 for $M = 10^9$ and $M = 7 \times 10^9$, respectively. Our

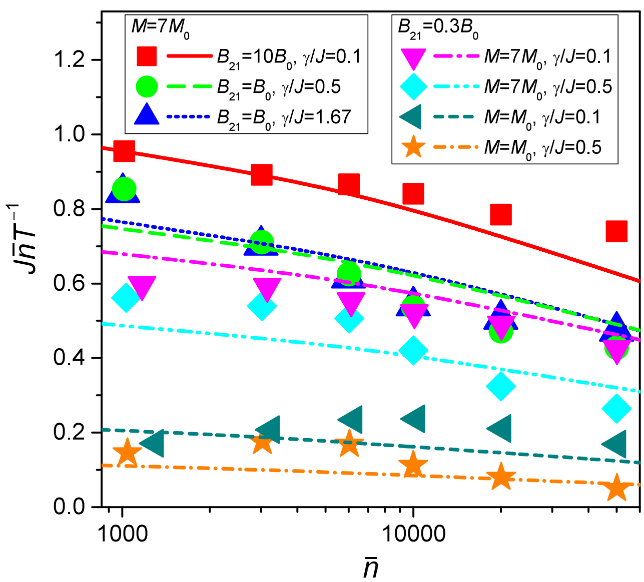

FIG. 4. Numerically determined dimensionless coupling strength $J\bar{n}T^{-1}$ at the BKT transition (symbols) as a function of $\bar{n}$ for different values of M, B_{21}, and γ/J. Here, $M_0 = 10^9$, $B_0 = 10^{-7}$ meV, $\Delta/T = -5.2$. The curves correspond to Eq. (10).

explanation is that for sufficiently strong coupling between the cavities, a subset of N cavities behaves collectively, thereby increasing the effective n^2/M_{eff} linearly with N.

At $\gamma/J < 1$ the critical coupling decreases with increasing γ/J (compare magenta to cyan or dark cyan to orange symbols and lines in Fig. 4; see also Fig. 2). For $\gamma/J \ll \kappa$ this decrease is determined by the behavior of $\ln(\pi/k_c)$ in Eq. (10), while for larger γ/J the effect of the term $c_2a^2\gamma/J$ dominates. In the case of $\gamma/J \sim 1$, where the vortex core size is comparable to the intercavity spacing and the density modulation depth a required for the BKT transition is significantly reduced, the aforementioned decrease of the critical coupling with increasing γ/J can be fully canceled or even reversed due to a strong decrease of a^2 in the term $c_2a^2\gamma/J$ (compare green to blue symbols and lines in Fig. 4; see also Fig. 2).

V. CONCLUSIONS AND OUTLOOK

Our numerical and analytical investigations of a lattice nonequilibrium Bose-Einstein condensate of noninteracting photons have shown that a BKT-like transition exists between states with and without unbound vortex-antivortex pairs. According to Eq. (10), the vortex-free phase is actually stabilized by driving and dissipation. Our findings are in line with previous numerical studies [14,15,45] of nonequilibrium polariton condensates, where interactions were included.

The experimental verification of our prediction for the spontaneous creation of vortices and antivortices should be possible by directly measuring the phase profile of a photon condensate by interferometry as used for the observation of phase jumps of localized photon condensates [47].

In our numerics, we have not found evidence for the destruction of the ordered phase as was predicted on the basis of the description of the phase dynamics by the nonlinear KPZ model [17–19]. This could be due to our finite simulation area, but the interplay of BKT and KPZ physics in nonequilibrium condensates [48–50] should be explored further. The stability of the vortex-free phase could be important for potential applications to analog optical computations [51–56] with photon condensates [24]. From the side of fundamental physics, it will also be interesting to study the dynamics of a photon condensate lattice after a density quench through the phase transition [20,57].

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