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Emergent crystallinity and frustration with BECs in multimode cavities

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In this document, we elaborate on the derivation of the atom-only action, i.e., Eq. (4) of the main text, and on the reduction of Eq. (4) to the order-parameter-based actions Eqs. (7) and (11). We begin with the second-quantized Hamiltonian of the theory, written out in detail:

$$\begin{aligned}\mathcal{H} \;=\; & \int d^dx \left\{ \Psi_g^\dagger(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu \right) \Psi_g(\mathbf{x}) + \Psi_e(\mathbf{x}) \left(-\frac{\hbar^2\nabla^2}{2M} - \mu + \hbar\omega_A \right) \Psi_e(\mathbf{x}) \right. \\ & \left. + U\,|\Psi_g(\mathbf{x},\tau)|^2 (|\Psi_g(\mathbf{x},\tau)|^2 + |\Psi_e(\mathbf{x},\tau)|^2) \right\} \\ & + i\hbar \int d^dx \left\{ \Psi_g^\dagger(\mathbf{x}) \Psi_e(\mathbf{x}) \left(\sum\nolimits_\alpha g_\alpha(\mathbf{x})\, a_\alpha^\dagger + \Omega \right) - \text{h.c.} \right\} + \hbar\omega_C \sum\nolimits_\alpha a_\alpha^\dagger\, a_\alpha + \mathcal{H}' \end{aligned} \tag{1}$$

where the terms describing the environmental modes and their coupling to the system are given by

$$\mathcal{H}' = \sum\nolimits_\varepsilon \hbar\,\omega_\varepsilon A_\varepsilon^\dagger A_\varepsilon + \sum\nolimits_{\alpha,\varepsilon} (\hbar\,\widetilde{\kappa}_{\alpha,\varepsilon} A_\varepsilon^\dagger\, a_\alpha + \text{h.c.}) + i\hbar \int d^dx \sum\nolimits_\varepsilon \left\{ \widetilde{\gamma}_\varepsilon(\mathbf{x})\, A_\varepsilon^\dagger\, \Psi_g^\dagger(\mathbf{x}) \Psi_e(\mathbf{x}) - \text{h.c.} \right\} \tag{2}$$

contains the terms describing, respectively, the environmental photon modes, their coupling to the cavity modes (with coupling constants $\widetilde{\kappa}$), and their coupling to the intracavity atoms (with coupling constants $\widetilde{\gamma}$). These terms, when the environmental modes are integrated out, generate the dissipative effects due to cavity photon loss and spontaneous emission.

Quasi-adiabatic switching

We now justify the limit of approximately adiabatic switching (discussed in the Effective Action section of the main text), which underpins our functional-integral formalism. The extent to which the assumption of adiabatic switching fails is given by the flux of energy through the system, which is the sum of the irreversible contributions due to (i) spontaneous emission and (ii) cavity-photon loss, viz., $N\gamma(\Omega^2/4\Delta_A^2) + 2\kappa \sum_\alpha \langle n_\alpha \rangle$ [1]. Below the threshold for self-organization, $\langle n_\alpha \rangle \propto N\Omega^2$; slightly above threshold, $\langle n_\alpha \rangle \propto \Omega^2 \rho_\alpha^2$, where $\rho_\alpha (\propto N)$ is the order parameter for self-organization. Our model, whose focus is to describe the threshold regime, is concerned only with the flux near threshold. We shall see that Ω_{th} (i.e., the laser's Rabi frequency at threshold) scales as $N^{-1/2}$; therefore, below thresohld, the energy flux is independent of particle number, and contributes negligibly, per particle, as $N \to \infty$.

Above but near threshold, $\rho_\alpha/N \ll 1$, because the transition is weakly first-order; together with the assumption that $\kappa/\Delta_C \ll 1$ (see the section on Experimental Considerations in the main text), this implies that the dissipative dynamics due to cavity loss is dominated by the Hamiltonian dynamics of the atom-cavity coupling, and for sufficiently large particle number it is therefore valid to neglect the departure from equilibrium near the transition.

Effective atomic action

In the approximately adiabatic limit, the dynamics described by $\mathcal{H}$ can be encapsulated in a coherent-state functional integral by the procedure described in, e.g., Ref. [2]. We transform the fields into a frame rotating with the laser as follows: $\Psi_e \to \Psi_e e^{-i\omega_L t}, a_\alpha \to a_\alpha e^{-i\omega_L t}$. After doing this, we Wick-rotate all the fields into imaginary time, as described in Ref. [2]. The central object in the functional-integral formalism is the quantum partition function,

$$Z = \int [d(\Psi_g, \Psi_g^*, \Psi_e, \Psi_e^*, \{a_\alpha, a_\alpha^*\}, \{A_\varepsilon, A_\varepsilon^*\})] \exp(-S), \tag{3}$$

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from which densities and correlation functions—which are the objects of primary physical interest—can be obtained by means of functional differentiation with respect to suitable source terms. The action is given by Eqs. (3) of the main text, which we reproduce here:

$$\begin{aligned}
S &= S_{\rm at} + S_{\rm em} + S_{\rm int} + S_{\rm dis}, \\
S_{\rm at} &= \int d^d x\, d\tau \left[\Psi_g^*(\mathbf{x},\tau) \left(\partial_\tau - \frac{\hbar\nabla^2}{2M} - \frac{\mu}{\hbar} \right) \Psi_g(\mathbf{x},\tau) \right. \\
&\quad + \Psi_e^*(\mathbf{x},\tau) \left(\partial_\tau - \frac{\hbar\nabla^2}{2M} + \omega_A - \frac{\mu}{\hbar} \right) \Psi_e(\mathbf{x},\tau) \\
&\quad \left. + \frac{U}{\hbar} |\Psi_g(\mathbf{x},\tau)|^2 (|\Psi_g(\mathbf{x},\tau)|^2 + |\Psi_e(\mathbf{x},\tau)|^2) \right], \\
S_{\rm em} &= \int d\tau \sum\nolimits_\alpha a_\alpha^*(\tau) \left(\partial_\alpha + \omega_C \right) a_\alpha(\tau), \\
S_{\rm int} &= \int d\tau\, d^d x \left[\sum\nolimits_\alpha i g_\alpha(\mathbf{x}) \Psi_e^*(\mathbf{x},\tau)\, \Psi_g(\mathbf{x},\tau)\, a_\alpha(\tau) + i\Omega\, \Psi_e^*(\mathbf{x},\tau) \Psi_g(\mathbf{x},\tau) + \text{h.c.} \right], \\
S_{\rm dis} &= \int d\tau \sum\nolimits_\varepsilon A_\varepsilon^* \left(\partial_\tau + \omega_\varepsilon \right) A_\varepsilon + \sum\nolimits_{\alpha,\varepsilon} [\widetilde{\kappa}_{\alpha,\varepsilon}\, a_\alpha^\dagger A_\varepsilon + \text{h.c}].
\end{aligned}$$

To proceed, we first note that the action is entirely linear or quadratic in (Ψ_e, Ψ_e^*). These fields can therefore be integrated over by completing the square; if we assume that $\hbar\Delta_A \gg U \int d^d x |\Psi_g(\mathbf{x})|^2$, as is true for weak repulsive contact interactions, this yields

$$\begin{aligned}
Z = \int [d(\Psi_g, \Psi_g^*, \Psi_e, \Psi_e^*, \{a_\alpha, a_\alpha^*\}, \{A_\varepsilon, A_\varepsilon^*\})] \exp(-\widetilde{S}) \qquad (4) \\
\times \exp\left\{ -\frac{k_B T}{\hbar} \int d\tau\, d\tau' d^d x \sum_{\omega_\nu,\alpha,\beta} \frac{e^{-\omega_\nu|\tau-\tau'|}}{i\omega_\nu - \Delta_A} \left[\Psi_g^*(\mathbf{x},\tau)\, g_\alpha(\mathbf{x})\, a_\alpha^*(\tau)\, \Psi_g(\mathbf{x},\tau')\, \Omega + \text{h.c.} \right] \right\}
\end{aligned}$$

where $\widetilde{S}$ comprises all terms in S that do not depend on (Ψ_e, Ψ_e^*), and we have omitted terms that involve exchange of photons between cavity modes, which are similar in form to the one written out above. The neglected terms are subleading near threshold, as the cavity photon populations are small relative to that of the laser mode. For Δ_A larger than the other relevant energy scales, the atom-cavity interaction is local in time as well as space (intuitively, because the virtual "excited particle" is formed locally and decays almost instantaneously), and the exponent then reduces to the following simpler form:

$$\frac{g\Omega}{\Delta_A} \int d\tau\, d^d x \left(|\Psi_g(\mathbf{x},\tau)|^2\, \Xi_\alpha(\mathbf{x})\, a_\alpha^* + \text{h.c.} \right). \qquad (5)$$

(Recall that Ξ_α is the normalized mode function.) Our next step is to integrate out the environmental fields A_ε; each such integration adds a term to the effective action, and their overall contribution is as follows [3]:

$$\int [d(A_\varepsilon, A_\varepsilon^*)] \exp(-S_{\rm dis}) \equiv \exp(-S_{CL}), \qquad (6)$$

where

$$S_{CL} = \widetilde{\kappa} \int d\tau d\tau' \sum_\varepsilon \frac{e^{-\omega_\varepsilon|\tau-\tau'|}}{4\omega_\varepsilon} \sum\nolimits_\alpha a_\alpha^*(\tau)\, a_\alpha(\tau'). \qquad (7)$$

The expression above can generically be rewritten, at low temperature, as follows:

$$S_{CL} = \widetilde{\kappa} \sum_{\nu,\alpha} |a_\alpha(\omega_\nu)|^2 f(\omega_\nu), \qquad (8)$$

where $f(\omega_\nu)$ is some non-analytic function of ω_ν that depends on the details of the mode-environment coupling, and is most commonly of the form $|\omega_\nu|^\beta$. In the regime where dissipative effects dominate dispersive ones, this term might modify the physics in interesting ways; in the present case, however, this term is dominated by the energy of the photons ($\sim \hbar\Delta_C$) and the important point to note is that the integrating out of the environment leaves the action quadratic in the cavity photon modes; these modes can therefore be integrated out along the same lines as the previous integrations, leaving the effective action given in Eq. (4) of the main text:

$$\begin{aligned} S_{\rm eff} &= \sum_\nu \int d^dx\, \Psi^*(\omega_\nu,\mathbf{x}) \left[i\omega_\nu - \frac{\hbar\nabla^2}{2M} - \frac{\mu}{\hbar} \right] \Psi(\omega_\nu,\mathbf{x}) + \frac{U}{\hbar}\int d\tau\, d^dx\, |\Psi(\tau,\mathbf{x})|^4 \\ &- \widetilde{\zeta}\frac{k_BT}{\hbar}\sum_\alpha \int d\tau\, d\tau'\, d^dx\, d^dx' \sum_\nu \frac{e^{-\omega_C|\tau-\tau'|}}{i\omega_\nu - \omega_C}\, \Xi_\alpha(\mathbf{x})\, |\Psi(\tau,\mathbf{x})|^2\, \Xi^*_\alpha(\mathbf{x}')\, |\Psi(\tau',\mathbf{x}')|^2 + \cdots \quad (9) \end{aligned}$$

where $\widetilde{\zeta} \equiv \Delta_C\zeta$, and $\zeta \equiv \Omega^2 g^2 \Delta_C/[\Delta_A^2(\Delta_C^2+\kappa^2)]$. In the case at hand, $\hbar\Delta_C$ being larger than the typical atomic kinetic energy, the second line of $S_{\rm eff}$ simplifies to Eq. (4) of the main text.

Order-parameter theory at nonzero temperatures

The next step is to re-express the effective action in terms of the order parameter ρ_{mn} defined in the main text. We proceed as follows: we note that the cavity mediated interaction term can be written as $\int d\tau \sum_{mn} \zeta_{mn}\rho_{mn}(\tau)\,\rho_{-mn}(\tau)$, where ζ_{mn} is the cavity-mediated interaction for modulation at wavenumber $m+n$. The coupling ζ_{mn} is to be considered as being sharply peaked about modes obeying $m+n = K_0R/2\pi$. It is helpful to rewrite the partition function as follows, introducing a Dirac delta functional:

$$Z = \int [d(\Psi,\Psi^*)][d\widehat{\rho}_{mn}]\, \delta\left(\widehat{\rho}_{mn}(\tau) - \int d^dx\, \Psi^*(\mathbf{x},\tau)\Psi(\mathbf{x},\tau)\, \Xi_\alpha(\mathbf{x}) \right) e^{-S_{\rm eff}}. \quad (10)$$

We now use the path-integral identity[1]:

$$\delta[x(\tau)] = \int [dy] \exp\left(2i \int d\tau\, x(\tau)\, y(\tau) \right)$$

to introduce an additional functional integral over a field ρ, so that the partition function takes the form:

$$Z = \int [d(\Psi,\Psi^*)][d\widehat{\rho}_{mn}][d\rho_{mn}]\, e^{-S_{\rm eff} - 2i\sum_{mn}(k_BT/\hbar)\int d\tau \rho_{mn}\left[\widehat{\rho}_{mn}(\mathbf{x},\tau) - \int d^dx \Psi^*(\mathbf{x},\tau)\Psi(\mathbf{x},\tau) g_\alpha(\mathbf{x})\right]}, \quad (11)$$

which is a path integral over Ψ, Ψ^* and $\rho, \widehat{\rho}$ with the action

$$\begin{aligned} S' &= \int d\tau \int d^dx\, \Psi^*(\mathbf{x},\tau) \left(\partial_\tau - \frac{\hbar\nabla^2}{2M} - \frac{\mu}{\hbar} + 2i\sum_{mn} \frac{k_BT}{\hbar}\rho_{mn}(\tau)\Xi_{mn}(\mathbf{x}) \right) \Psi(\mathbf{x},\tau) \\ &- \int d\tau \sum_{mn} \left(\zeta_{mn}\, \widehat{\rho}_{mn}(\tau)\, \widehat{\rho}_{-mn}(\tau) + 2i\frac{k_BT}{\hbar}\widehat{\rho}_{mn}(\tau)\, \rho_{-mn}(\tau) \right). \quad (12) \end{aligned}$$

(The above action S' does not explicitly contain an interatomic contact repulsion term, but such a term could, in principle, be included via a redefinition of ζ_{mn}.) For a Bose-condensed gas below the self-organization threshold, the field operators $\Psi(\mathbf{x},\tau)$ can be written in terms of condensate and non-condensate parts as $\Psi(\mathbf{x},\tau) = \sqrt{N_0/V} + \Phi(\mathbf{x},\tau)$, where $N_0(T)$ is the equilibrium condensate fraction at temperature T. Expanding the Bose fields in the basis of m,n mode functions, in which

[1] Factors of 2π are absorbed into the functional-integral measure.

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they are diagonal, one finds that $\Psi_{mn}(\omega_\nu) = \sqrt{N_0}\,\delta_{m,0}\,\delta_{n,0}\,\delta_{\nu,0} + \Phi_{mn}(\omega_\nu)$. Integrating out $\widehat{\rho}$ and (Φ^*, Φ), which appear quadratically in the action and are not coupled to each other, one arrives at the action

$$S = \frac{1}{2}\mathrm{Tr}\ln(\mathbf{M}) + \frac{k_B T}{\hbar}\sum_{mn\nu}\left[\frac{1}{\zeta_{mn}}\rho_{mn\nu}\,\rho_{-mn-\nu} - N_0\,\rho_{mn\nu}\,(\mathbf{M}^{-1})_{mn\nu,m'n'\nu'}\,\rho_{m'n'\nu'}\right], \tag{13}$$

where the (infinite-dimensional) matrix $\mathbf{M}$ is defined by

$$\mathbf{M}_{mn\nu,m'n'\nu'} \equiv \left[i\omega_\nu - \frac{\hbar(m+n)^2}{2MR^2}\delta_{mn,m'n'}\right]\delta_{\nu\nu'} + \frac{k_B T}{\hbar}\sum_{pq\nu''}\rho_{pq\nu''}\,\delta_{mm'+p}\,\delta_{nn'+q}\,\delta_{\nu+\nu'',\nu}. \tag{14}$$

Below threshold, one can expand the matrix $\mathbf{M}$ in powers of the order parameter ρ; the quadratic term in the action is then given by[2]

$$\sum_{mn}\rho_{mn}\,\rho_{-mn}\left[\frac{k_B T}{\hbar\zeta_{mn}} - \frac{N_0 k_B T}{\frac{\hbar^2(m+n)^2}{2MR^2}} - \frac{(k_B T)^2}{2\hbar^2}\sum_{pq\nu}\frac{1}{i\omega_\nu - \frac{\hbar(p+q)^2}{2MR^2} - \mu}\,\frac{1}{-i\omega_\nu - \frac{\hbar(m+n-(p+q))^2}{2MR^2} - \mu}\right]. \tag{15}$$

The last expression can be rearranged, if one recalls that $\sum_{mn\nu}(i\omega_\nu - (m+n)^2 - \mu)^{-1} = N - N_0$ for a Bose-Einstein condensate [2]. (This statement also holds for a non-Bose-condensed gas, if one sets $N_0 = 0$.) We now use the fact that the particles in a Bose-Einstein condensate typically have energies that are low compared with the recoil energy to evaluate the last term approximately, and find that at low temperatures the quadratic term in the action is then given by

$$\frac{k_B T}{\hbar}\sum_{mn}\rho_{mn}\,\rho_{-mn}\left[\frac{1}{\zeta_{mn}} - \frac{N}{\hbar(m+n)^2/2MR^2}\right], \tag{16}$$

which is the mean-field expression for threshold. Note that this result holds only for sub-recoil temperatures at which quantum effects are the primary reason for delocalization. We choose $\zeta_{mn} \equiv \zeta(1 - \chi(m+n-\Lambda_0)^2)$, where χ is the broadening term discussed in the main text. Likewise, we arrive at the term quartic in ρ by adding up the appropriate terms in the power-series expansions of $\log(\mathbf{M})$ and $\mathbf{M}^{-1}$ and keeping the leading term in a gradient expansion:

$$\frac{(k_B T)^2 N}{\hbar^4 K_0^4/4M^2}\sum_{m_i n_i}\rho_{m_1 n_1}\,\rho_{m_2 n_2}\,\rho_{m_3 n_3}\,\rho_{m_4 n_4}\,\delta_{\sum m_i,0}\,\delta_{n_1+n_2,n_3+n_4}. \tag{17}$$

To express the action in Brazovskii's form, we make the rescaling $\rho \to \rho\sqrt{\hbar\zeta/k_B T\chi}$. In terms of the rescaled fields, the full action is given by the following expression, which is of precisely the same form as Brazovskii's free energy [4]:

$$S_{\mathrm{LW}} = \sum_{mn}\left[\frac{1}{\chi}\left(1 - \frac{N\zeta}{\hbar K_0^2/2M}\right) + (m+n-(K_0 R/2\pi))^2\right]\rho_{mn}\,\rho_{-mn} \tag{18}$$

$$+ \frac{\zeta^2 N}{\chi^2\hbar^2 K_0^4/4M^2}\sum_{m_i n_i}\rho_{m_1 n_1}\,\rho_{m_2 n_2}\,\rho_{m_3 n_3}\,\rho_{m_4 n_4}\,\delta_{\sum m_i,0}\,\delta_{n_1+n_2,n_3+n_4}. \tag{19}$$

Having reduced the action to Brazovskii's form [4], we can apply his analysis of the critical behavior to our model, and in particular the two-dimensional result [5] that the threshold including fluctuations, ζ_{th} is related to the mean-field threshold $\zeta_{\mathrm{th}}^{\mathrm{mf}}$ by the relation

[2] We specialize to the $\nu = 0$ sector of the order-parameter theory, as this is the only sector of the theory that plays an important role for thermal phase transitions.

$$\zeta_{\rm th} - \zeta_{\rm th}^{\rm mf} \approx \frac{\chi}{N}\frac{\hbar K_0^2}{2M}\left(\frac{K_0 R}{2\pi}\,\frac{\zeta^2 N}{\chi^2\hbar^2 K_0^4/4M^2}\right)^{\frac{2}{3}}, \tag{20}$$

which, upon substituting the definition of ζ in terms of physical parameters, yields the result given in the main text.

Features of Brazovskii's model

The free energy functional that Brazovskii originally introduced on phenomenological grounds [4] has the form

$$F = \sum\nolimits_{\mathbf{k}} \left(r + (|k| - k_0)^2\right) \psi_{\mathbf{k}}\, \psi_{-\mathbf{k}} + \frac{\lambda}{12} \sum\nolimits_{\mathbf{k}_i} \psi_{\mathbf{k}_1}\psi_{\mathbf{k}_2}\psi_{\mathbf{k}_3}\psi_{\mathbf{k}_4}\delta_{\sum \mathbf{k}_i,\mathbf{0}}. \tag{21}$$

As discussed in the main text, this action appears, according to mean-field theory, to have a continuous phase transition at $r = 0$. Brazovskii's transition differs from many commonly studied phase transitions in an important respect: near most phase transitions, the active low-energy fluctuations are clustered about a point, or isolated set of points, in momentum space (frequently the origin). By contrast, for the Brazovskii case, as long as the spatial dimension d of the system is two or greater, the low-energy fluctuations are clustered about a circular shell of nonzero radius given by the stripe wavevector. (In our realization, we have a ribbon $m+n = K_0 R$ rather than a shell, but the essential physics depends only on the dimensionality of the phase space of fluctuations, which is the same in both cases.) This has the important consequence that the low-energy density of states is effectively one-dimensional, regardless of d. Fluctuation effects therefore play a strong role, as they commonly do in 1D systems: in the present case, they control not only the details of critical behavior at the phase transition but even the order of the transition itself.

Order-parameter theory at zero temperature

In principle, we could follow the procedure we followed above to construct the order-parameter theory at $T = 0$, the key difference being that the sum over Matsubara frequencies would become an integral. At $T = 0$, however, there is a more straightforward way to arrive at the effective action. Let us assume that the quantum depletion of the condensate in the absence of the cavity is relatively small: then $\rho_{mn} \approx \sqrt{N_0}(\Phi_{mn} + \Phi^*_{mn})/2$. Inserting this value of ρ into $S_{\rm eff}$ gives the result:

$$\begin{aligned} S_{\rm eff} \;=\; & \sum_{mn}\int d\omega\, \Phi^*_{mn}\left(i\omega - \frac{\hbar(m+n)^2}{2MR^2} - \frac{\mu}{\hbar}\right)\Phi_{mn} + N\frac{\zeta_{mn}}{2}\left(\Phi_{mn}\Phi_{-mn} + \Phi^*_{mn}\Phi^*_{-mn} + 2\Phi^*_{mn}\Phi_{mn}\right) \\ & + \frac{U}{\hbar}\int d\tau\, d^d x\, |\Phi(\tau,\mathbf{x})|^4. \end{aligned} \tag{22}$$

(Note that we have dropped the quadratic contributions coming from U but kept the quartic ones; this is because $U \ll \zeta$ near threshold, but couplings mediated by ζ do not contribute to the quartic term.) By analyzing this action in the manner of Ref. [6], one finds that in the region near threshold, the quadratic part of the action simplifies to

$$S = \frac{1}{\zeta}\int d\omega \sum_{mn}\left[\omega^2 + \frac{\hbar(m+n)^2}{2MR^2}\left(\frac{\hbar(m+n)^2}{2MR^2} - \zeta_{mn}\right)\right]\left(\Phi^*_{mn} + \Phi_{-mn}\right)^2. \tag{23}$$

For an appropriate choice of ζ_{mn}, this gives us back the result given in the main text.

Correlation functions of emitted light

The formalism described in the main text and supplementary material can be used to compute the spatio-temporal correlations of the light emitted from the cavity as well as those of the atoms. One proceeds as follows: one adds a source term $\sum_\alpha (h^*_\alpha a_\alpha + \text{h.c.})$ to the action before integrating out the

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intracavity photons. Functional derivatives of the partition function with respect to h then generate photon correlators: e.g.,[3]

$$\left.\frac{\delta Z}{\delta h_\alpha^* \delta h_\beta}\right|_{h=0} = \langle a_\alpha^* a_\beta \rangle. \tag{24}$$

If one then integrates out the cavity photons prior to setting $h = 0$, the functional derivatives of the effective atomic action with respect to h still generate the cavity-photon correlators. In the weak single-atom-cavity coupling regime we have considered in this paper, one finds that

$$\langle a_\alpha^\dagger(\omega)\, a_\beta(\omega)\rangle - \frac{1}{\Delta_C}\delta_{\alpha\beta} \propto \langle \rho_\alpha(\omega)\, \rho_\beta(\omega)\rangle, \tag{25}$$

i.e., that the photon correlators are directly proportional to the order-parameter correlations. This is a particularly simple relationship, which arises because the order parameter couples linearly to the cavity mode. The utility of the functional-differentiation approach is that it extends to cases in which the mode-mode scattering term,

$$\int \sum_{\alpha\beta} d\tau\, d^d x\, d^d x'\, g_\alpha^*(\mathbf{x})\, a_\alpha g_\beta(\mathbf{x}')\, a_\beta^* |\Psi(\mathbf{x})|^2\, |\Psi(\mathbf{x}')|^2, \tag{26}$$

is retained. (This would be the case, for instance, at strong single-atom-cavity coupling.) In this case, the photonic and atomic correlators at equal times are related to one another by the expression

$$\langle a_\alpha^\dagger a_\beta \rangle \propto \int d^d x\, d^d x'\, g_\epsilon(\mathbf{x})\, g_\phi(\mathbf{x}')\, \left\langle |\Psi(\mathbf{x})|^2\, |\Psi(\mathbf{x}')|^2\, (\Delta^{-1})_{\epsilon\alpha} (\Delta^{-1})_{\phi\beta} \right\rangle, \tag{27}$$

where Δ is a matrix in mode space given by

$$\Delta_{ij} = \Delta_C\, \delta_{ij} - \int d^d x\, |\Psi(\mathbf{x})|^2\, g_\alpha(\mathbf{x})\, g_\beta(\mathbf{x}). \tag{28}$$

Note that, in the regime of strong single-atom-cavity coupling, the two-photon correlation function depends on arbitrarily high-order atomic correlations. Once the intracavity correlations are obtained, they can be straightforwardly translated into extracavity correlations using the input-output formalism [7].

Defects and frustration

We now elaborate on the situation depicted in Fig. 3 of the main text, which is reproduced at the end of this document, first focusing on the non-equatorial sheet marked (i). Near the center of the sheet, crystallization into $l = 1$ modes is suppressed because such modes have low intensity, whereas crystallization into $l = 2$ modes is favored because they have maximal intensity; away from the center, the opposite is true. The change in l forces a change in m or n, owing to the degeneracy condition $2\pi(l+m+n) = K_0 R$, so the mode functions in the sheet must change across an interfacial zone between the $l = 1$ and $l = 2$ regions. Therefore, either a dislocation, associated with a change in m, or an abrupt change in lattice periodicity (i.e., a discommensuration), associated with a change in n, is expected. (This picture assumes that, as is always the case near threshold, the self-organized lattice is not strong enough to trap the entire atomic distribution at the center or the edge of the sheet. The kinetic energy cost of localization, as well as the cost in repulsive energy, act to spread out the atomic cloud.)

Now consider a situation in which two symmetrically disposed sheets on opposite sides of the equator are populated with atoms, e.g., sheets (i) and (ii) of Fig. 1b. Atoms in sheet (i) and those in sheet (ii) are coupled via the cavity modes. Because the $l = 2$ ($l = 1$) mode functions are symmetric (antisymmetric) about the equatorial plane, atoms in the $l = 2$ ($l = 1$) arrangement in sheet (ii) occupy the same (opposite) checkerboard as those in sheet (i). If there are no dislocations,

[3]Strictly speaking, these are the temperature Green's functions, which yield temporal correlations upon analytic continuation [2].

atoms in the interfacial zone remain disordered, because it is impossible for the atoms to satisfy both desiderata (or, equivalently, because the corresponding cavity modes interfere destructively in sheet (i) and constructively in sheet (ii)). The introduction of dislocations enables the system to order in part of the interfacial zone, as shown in the right hand side of Fig. 1b, and is therefore favored as it decreases the energy of the system.

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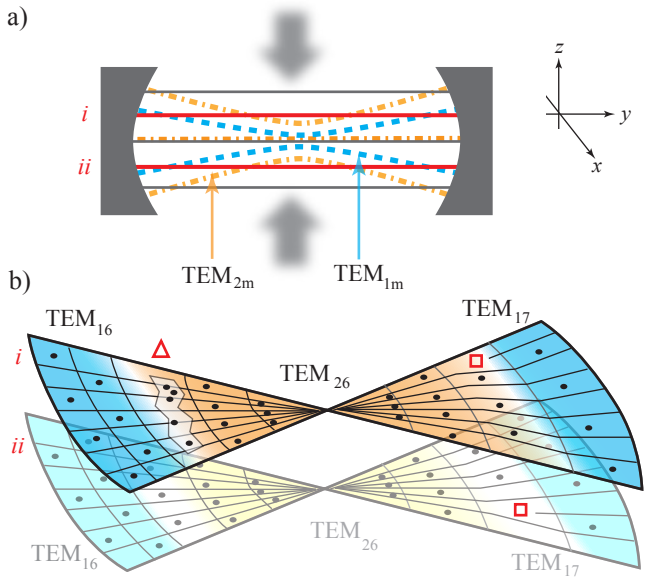

Figure 1: **Effects due to frustration.** Atoms are loaded into sheets (i) and (ii), marked in thick red lines in panel (a), which are an integer number of pump wavelengths apart. The blue (dashed) and orange (dash-dot) curves are, respectively, antinodal regions of the modes TEM_{1m}, which have low intensity near the centers of sheets (i) and (ii), and modes TEM_{2m}, which have low intensity away from the centers of sheets (i) and (ii). Near the center of each sheet, atoms crystallize into mode TEM_{2m}; away from the center, they crystallize into $\mathrm{TEM}_{1m'}$. Within a sheet, regions may be separated by a discommensuration, e.g., in the left side of panel (b), or a dislocation, e.g., in the right-hand side of panel (b). Between sheets, the opposite parity of adjacent modes leads to frustration, which precludes ordering, as in the regions indicated by a △ and a □. Dislocations (□), being more localized, are less energetically costly than discommensurations (△).