Self-organization of atoms in a cavity field: threshold, bistability and scaling laws

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(Dated: August 10, 2005)

We present a detailed study of the spatial self-organization of laser-driven atoms in an optical cavity, an effect predicted on the basis of numerical simulations [P. Domokos and H. Ritsch, Phys. Rev. Lett. 89, 253003 (2002)] and observed experimentally [A. T. Black et al. in Phys. Rev. Lett. 91, 203001 (2003)]. Above a threshold in the driving laser intensity, from a uniform distribution the atoms evolve into one of two stable patterns that produce superradiant scattering into the cavity. We derive analytic formulas for the threshold and critical exponent of this phase transition from a mean-field approach. Numerical simulations of the microscopic dynamics reveal that, on laboratory timescale, a hysteresis masks the mean-field behaviour. Simple physical arguments explain this phenomenon and provide analytical expressions for the observable threshold. Above a certain density of the atoms a limited number of “defects” appear in the organized phase, and influence the statistical properties of the system. The scaling of the cavity cooling mechanism and the phase space density with the atom number is also studied.

I. INTRODUCTION

The manipulation of cold atoms and molecules by laser light is a rapidly growing field and has become a suitable ground for studying fundamental phenomena of physics both experimentally and theoretically \cite{1}. In the last decade, the emphasis has partly been shifted towards many-body effects in the dynamics of weakly interacting atoms \cite{2, 3}. The mechanical action of the electromagnetic radiation field on free atoms rarely manifests these effects. The refractive index of a cloud of atoms is simply composed of the product of the single atom polarizability and the optical density. Standard laser cooling methods were also conceived on the basis of single-atom processes. Only at densities as high as the ones achievable in a high-

The dynamics of atoms in a resonator is inherently a many-body problem even at a small density of the ensemble \cite{13, 14}. As all atoms are coupled to the same cavity mode, the modification of the field by one atom is experienced by a remote atom as well as by itself. The cavity cooling mechanism may become inefficient since the delicate dynamical correlation between one atom and the field mode could be perturbed by the motion of another atom \cite{17, 18}. Indeed, one of the cavity cooling schemes was found to slow down linearly with increasing number of atoms \cite{19}.

In a recent Letter we have predicted a cooperative behavior of the atoms driven by a laser in a direction perpendicular to the axis of a standing wave cavity \cite{20}. At high pump laser intensities (above a threshold) the homogeneous atomic cloud self-organizes into one of two regular checkerboard patterns that maximize scattering into the cavity. The constructive interference of fields radiated by the individual atoms produces an intensity which depends quadratically on the number of atoms (superradiance). Corresponding to the two patterns, there are two possible phases of the output field with 180 de-
degrees difference, which have been observed in an experi-
ment by Black, Chan, and Vuletic [21].

The onset of self-organization is relatively fast, on the
microsecond time scale. A basic property of the present
system is that the field created by the atoms traps and
simultaneously cools them so that the organized pattern
remains stable on a long time scale (10’s of ms). The cav-
ity cooling mechanism now acts on many atoms without
losing efficiency. There is no external finite-temperature
heat bath to define the temperature which, instead, is
set by the dynamical equilibrium of the dipole force fluc-
tuations and the cavity cooling effect. This is a distinct-
ive feature with respect to the recently demonstrated
collective atomic recoil laser in a ring cavity (CARL)
[22, 23, 24, 25], where a magneto-optical trap is nec-
essary to stabilize the organized phase and the otherwise
transient gain [20], and also to inject noise for obtaining
the phase transition-like behavior [27, 28, 29].

In the present paper we discuss in detail the self-
analysis process, from the viewpoint of phase tran-
sitions. A mean-field approach leads to a well-defined
threshold in the pumping strength. Comparison to nu-
merical simulations reveals effects scaling unusually with
the atom density, a characteristic feature of this cavity-
coupled many-atom system.

The paper is organized as follows. In Sect. II the equa-
tions of a semiclassical model are recapitulated, where
the atoms are represented as simple linearly polarizable
particles. Thereby the theory applies to a much wider
class of particles than alkali atoms. The main features of
the self-organization process, such as time scales, sup-
erradiance, collective cooling, are surveyed using a numeri-
cal example in Sect. III. Then, in Sect. IV we introduce
a one-dimensional mean-field model and determine the
threshold and critical exponent. In Sect. V we present
the results of detailed numerical simulations, which show
effects beyond mean-field. The atom number enters the
physics of the system in a form other than the density.
Above a certain atom number, stable defects appear in
the self-organized pattern and modify the system prop-
erties, which is accounted for in Sect. VI. In Sect. VII
the cooperative atomic behavior is discussed in detail by
demonstrating the superradiance, and the ensuing im-
provement of localization by collectivity. We conclude in
Sect. VIII.

II. SEMICLASSICAL MODEL

We consider \( N \) atoms in an open optical resonator
(Fig. 1). The atoms are illuminated from the side by
a “transverse” standing-wave laser pump with frequency
\( \omega \). This geometry corresponds to various experimen-
tal setups realizing the controlled transport of atoms from
the side into a cavity [14, 30] where the standing-wave
down is magnified. In an experiment in Sect. III. Then, in Sect. IV, we introduce
"transverse" standing-wave laser pump with frequency
\( \omega \). The atoms are illuminated from the side by
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tal setups realizing the controlled transport of atoms from
the side into a cavity [14, 30] where the standing-wave
pump coupling described by the single-photon Rabi fre-
quency \( g = \omega_C/2|2\gamma_0 n V|^{-1/2}d_{eg} \), for a mode volume \( V \)
and atomic transition dipole moment \( d_{eg} \) along the cav-
ity mode polarization. Large detuning of the laser from
the atomic transition \( |\omega - \omega_A| \gg \gamma \), where \( 2\gamma \) is the full
atomic linewidth at half maximum, ensures that the up-
ner level of the atoms can be adiabatically eliminated.
This model then describes a very general class of lin-
erly polarizable particles—in the following, we continue to use “atoms” for convenience. For the sake of sim-
plicity, we restrict the atomic motion to two dimensions,
along the pump laser and the cavity axis, coordinates \( x \)
and \( z \), respectively, without losing any relevant physical
effect. Motion in the third dimension could be taken into
account in the same way as along \( x \).

The quantum master equation for the density matrix
reads

\[
\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + \mathcal{L}\rho .
\]

Here the Hamiltonian is

\[
H = \sum_{j=1}^{N} \frac{\mathbf{p}_j^2}{2M} - h\Delta_C a^\dagger a + hU_0 \sum_{j=1}^{N} E^\dagger(\mathbf{r}_j)E(\mathbf{r}_j) ,
\]

where \( a, a^\dagger \) are the boson operators of the cavity mode,
\( \mathbf{r}_j = (x_j, z_j) \) and \( \mathbf{p}_j = (p_{x_j}, p_{z_j}) \) are the position and
momentum vectors of the \( j \)th atom. The Liouville op-
erator describing the cavity photon losses with rate \( 2\kappa \),
and the spontaneous emission reads

\[
\mathcal{L}\rho = 2\kappa \left( a\rho a^\dagger - \frac{1}{2}a^\dagger a\rho - \frac{1}{2}\rho a^\dagger a \right) - \Gamma_0 \sum_{j=1}^{N} \left( E^\dagger(\mathbf{r}_j)E(\mathbf{r}_j)\rho + \rho E^\dagger(\mathbf{r}_j)E(\mathbf{r}_j) \right) - 2 \int d^2\mathbf{u} N(\mathbf{u})E(\mathbf{r}_j)e^{-ik_A\mathbf{u}\cdot \mathbf{r}_j}\rho e^{ik_A\mathbf{u}\cdot \mathbf{r}_j}E^\dagger(\mathbf{r}_j) .
\]

In the above formulas, \( E(\mathbf{r}) \) is the dimensionless electric
field,

\[ E(r) = f(r)a + \eta(r)/g \approx \cos(kz)a + \cos(kx)\eta/g . \quad (2c) \]

The Rabi frequency of the driving laser is \( \eta(r) \), whose position dependence is given by a \( \cos(kz) \) mode function for a standing-wave field. In the following, we are going to refer to the maximum value of the Rabi frequency \( \eta \) as “pumping strength”. The variation of the pump field along the cavity axis and that of the cavity mode function \( f(r) \) along the transverse direction (Gaussian envelope) are neglected. The detunings are defined as \( \Delta_C = \omega - \omega_C \) and \( \Delta_A = \omega - \omega_A \). The parameters

\[ U_0 = \frac{g^2\Delta_A}{\Delta_A^2 + \gamma^2}, \quad \Gamma_0 = \frac{g^2\gamma}{\Delta_A^2 + \gamma^2}, \quad (3) \]

describe the dispersive and absorptive effects of the atoms, respectively, as they shift and broaden the resonance line of the cavity. In the last term of Eq. (2d), the integral represents the averaging over the angular distribution \( N(\alpha) \) of the random recoil due to spontaneous emission into the free-space modes.

Instead of directly using the density matrix, we consider the evolution of the corresponding joint atom-field Wigner function \[33]. This can be systematically approximated by semiclassical equations for a set of classical stochastic variables, \( \alpha, p_j, r_j \), the index \( j = 1, \ldots, N \) labeling the atoms,

\begin{align*}
\dot{\alpha} &= i\left[\Delta_C - U_0 \sum_j \cos^2(kz_j)\right] \alpha - \left[\kappa + \Gamma_0 \sum_j \cos^2(kz_j)\right] \alpha \\
& \quad - \eta_{\text{eff}} \sum_j \cos(kz_j) \cos(kx_j) + \xi_\alpha , \quad (4a) \\
\dot{p}_{xj} &= -\hbar U_0 (\eta/g)^2 \frac{\partial}{\partial x_j} \cos^2(kx_j) \\
& \quad - i\hbar (\eta_{\text{eff}}^* \alpha - \eta_{\text{eff}} \alpha^*) \frac{\partial}{\partial x_j} \cos(kx_j) \cos(kz_j) + \xi_{xj} , \quad (4b) \\
\dot{z_j} &= -\hbar U_0 |\alpha|^2 \frac{\partial}{\partial z_j} \cos^2(kz_j) \\
& \quad - i\hbar (\eta_{\text{eff}}^* \alpha - \eta_{\text{eff}} \alpha^*) \frac{\partial}{\partial z_j} \cos(kx_j) \cos(kz_j) + \xi_{zj} , \quad (4c)
\end{align*}

where the effective pumping strength for the cavity mode is

\[ \eta_{\text{eff}} = \frac{\eta g}{i \Delta_A + \gamma} . \quad (5) \]

These equations include Langevin noise terms \( \xi_\alpha, \xi_{xj}, \) and \( \xi_{zj} \), defined by the non-vanishing second-order correlations,

\begin{align*}
\langle \xi^*_\alpha \xi_\alpha \rangle &= \kappa + \sum_{j=1}^{N} \Gamma_0 \cos^2(kz_j) , \quad (6a) \\
\langle \xi_\alpha \xi_m \rangle &= i\hbar \Gamma_0 \partial_\alpha \mathcal{E}(r_j) \cos(kz_j) , \quad (6b) \\
\langle \xi_n \xi_m \rangle &= 2\hbar^2 k^2 \Gamma_0 |\mathcal{E}(r_j)|^2 \delta_{nm} \delta_{nm} + \hbar^2 \Gamma_0 \\
& \quad \left[ \partial_n \mathcal{E}^*(r_j) \partial_m \mathcal{E}^*(r_j) + \partial_n \mathcal{E}(r_j) \partial_m \mathcal{E}^*(r_j) \right] , \quad (6c)
\end{align*}

where the indices \( n, m = x, z \). The noise terms associated with different atoms are not correlated. The complex dimensionless electric field \( \mathcal{E}(r) \) is derived from Eq. (2a), replacing the field operator \( a \) by the complex variable \( \alpha \). We iterate the coupled, stochastic Itô-style differential equations \[1\] by a Monte Carlo-type algorithm.

There are two types of force terms in the equations of the momentum components. The terms in the first lines derive from the usual one-dimensional “optical lattice” potentials, the laser pump keeps the atoms inside the resonator via this term. In the second lines, the force terms originate from the coherent redistribution of photons between the pump and the field mode. The potentials depending on the amplitude \( \alpha \), which itself is a variable, are not conservative (all but the optical lattice created by the transverse pump). The time-delayed correlations in the dynamics of the atomic motion and the field mode can result in a friction force on the atoms, known as cavity cooling \[11, 33, 34, 35, 36, 37, 38, 39\].

### III. SELF-ORGANIZATION

We study the motion of the atoms in the cavity by numerically integrating the set of stochastic ordinary differential equations \[1\]. To be specific, \(^{85}\text{Rb} \) were considered, with the \( 5S_{1/2} \rightarrow 5P_{3/2}, F = 4 \) transition. Starting from a gas of thermal atoms (random positions from a uniform, and velocities from a thermal distribution) and no light in the cavity mode (\( \alpha = 0 \)), with the right choice of parameters we observe a buildup of the cavity field accompanied by the appearance of an organized pattern in the spatial distribution of the atoms. This is illustrated in Fig. 2, where the trajectories of 40 atoms during the initial 50 \( \mu \)s of a run are shown. The grid lines denote points of maximum coupling to the standing-wave cavity or pump field. Trapped atoms are oscillating about intersections of grid lines, where a single atom can scatter pump photons into the cavity mode most efficiently. For many atoms, however, destructive interference can inhibit the scattering process: the source term in Eq. (1a) contains the factor \( \sum_j \cos(kx_j) \cos(kz_j) \), which can be small even if all the atoms are maximally coupled due to the alternating signs of the summands. In contrast to this, in Fig. 2 only every second “maximally coupled” site—the black or the white fields of a checkerboard—is occupied, leading to an efficient Bragg scattering of pump photons into the cavity.
...tistical fluctuations either the in-phase or opposite-phase axis but some meander along the cavity axis. Due to stau-

FIG. 2: Two-dimensional trajectories of 40 rubidium atoms in a cavity, during the initial 50 μsec. A checkerboard pattern of trapped atoms emerges, untrapped atoms move mainly along the cavity axis. Parameters: $\gamma = 20/\mu$sec, $(g, \kappa) = (2.5, 0.5)\gamma$, atomic detuning $\Delta_A = -500\gamma$, cavity detuning $\Delta_C = -\kappa + NU_0$, and the pumping strength $\eta = 50\gamma$.

The emergence of a checkerboard pattern of atoms with every second point of maximum coupling empty happens only due to the good choice of the parameters ensuring positive feedback, as explained in the following. Initially, in the random position distribution some atoms scatter into the cavity in a given phase and some with an opposite phase, and thus most of the scattered field is canceled. The dipole force (first term of Eq. (115)) attracts atoms towards antinodes of the pump (for red detuning, $\Delta_A < 0$), but almost no field in the cavity means no substantial modification of the uniform position distribution along the cavity axis. This can be seen in Fig. 4 where most atoms are well trapped along the transverse axis but some meander along the cavity axis. Due to statistica fluctuations either the in-phase or opposite-phase scatterers will be in tiny majority, and a small cavity field...
transverse pump is too weak to induce any noticeable spatial modulation at temperatures $k_B T \approx \hbar \kappa$. Thus $\langle \Delta z \Delta p_z \rangle = \text{const.}$ and $\langle \Delta x \Delta p_x \rangle = \text{const.}$ reveal that the temperature itself does not change in either direction. At the cavity cooling limit $k_B T = \hbar \kappa$, the numerical value for the phase space volume from the last paragraph is $13.4\hbar$, in accordance with the value along the transverse $x$ direction. Along the cavity axis $z$, however, the phase space volume is greater than the estimate, indicating a higher temperature. Above threshold, the phase space volume transiently jumps to high values for both directions, and then it is gradually decreased. Compression is apparently more efficient along the cavity axis, here the phase space goes considerably below the value corresponding to the uniform distribution. In both plots the two curves corresponding to $N = 40$ and $N = 160$ are very similar, which manifests that the cooling rate of the ensemble is independent of the atom number. This is a very important observation, being at variance with the expectation that the efficiency of cavity cooling mechanism is reduced for increasing number of atoms. This prediction was made for a setup where the external pump field is injected directly into the cavity. Apparently it does not apply to the transverse pumping case studied here.

With the help of these few examples, we surveyed three important properties appearing in the dynamics of a laser-driven atomic ensemble coupled to a cavity mode: (i) the system rapidly self-organizes into a checkerboard pattern in a trapping field, (ii) which is generated by a collective, superradiant scattering into the cavity, and finally, (iii) the energy of the atoms is dissipated at a rate independent of the number of atoms. This behaviour requires a sufficiently strong pumping strength, indicating the possibility of a well-defined threshold separating two different stability regions. This threshold is discussed in the next section within the framework of a mean field approximation.

**IV. MEAN-FIELD APPROXIMATION**

The essence of the self-organization process can be understood on the ground of conservative mean-field forces acting on the atoms. This amounts to treating the cavity field as if it responded immediately to the positions of the atoms. Cavity cooling, which is directly related to the time lag of the cavity field, is absent in this model. Moreover, the mean-field approach corresponds to the thermodynamic limit of the system: $N \to \infty$, $g \to 0$, $\kappa = \text{const.}$ with $Ng^2 = \text{const.}$ Physically, the limit can be thought of as taking larger cavities (cavity length $l_{\text{cav}} \to \infty$) filled with a gas of atoms of constant density (atom number $N \propto l_{\text{cav}}^{-1}$). Due to the $V^{-1/2}$ dependence of the coupling constant $g$ on the mode volume $V$, one then has $Ng^2 = \text{const.}$, neglecting the variation of the waist of the mode. Moreover, due to larger photon travel time between the mirrors, the reflectivity has to scale like $\propto l_{\text{cav}}^{-1}$ to keep $\kappa = \text{const.}$ For the sake of simplicity, we analyze one-dimensional motion along the cavity.

**A. Potentials**

Taking $x_j = 0$, $j = 1, \ldots, N$, according to Equation 4g each atom moves in a potential

$$V(z) = U_2 \cos^2(kz) + U_1 \cos(kz)$$

composed of the sum of a $\lambda/2$ periodic potential stemming from the cavity field and a $\lambda$ periodic one arising from the interference between cavity and pump fields. The potential depths are given by

$$U_2 = N^2 \langle \cos(kz) \rangle^2 \hbar I_0 U_0$$

$$U_1 = 2N \langle \cos(kz) \rangle \hbar I_0 \left( \Delta C - NU_0 \langle \cos^2(kz) \rangle \right).$$

These, in the mean-field approximation, depend on the position of the individual atoms only via the mean value

$$\Theta = \langle \cos(kz) \rangle = \frac{1}{N} \sum_{i=1}^{N} \cos(kz_i)$$.

**FIG. 4:** Evolution of the phase space volume, along the cavity axis (up) and along the transverse pump (bottom), on a long time scale for various settings, same parameters as in Fig. 3. The number of atoms is $N=40$ and $N=160$ (black line), and $N=40$ but pumped below threshold, $\eta = 10\gamma$, for the dashed line.
which can be considered a spatial order parameter, and via the bunching parameter

\[ B = \langle \cos^2(kz) \rangle = \frac{1}{N} \sum_{i=1}^{N} \cos^2(kz_i). \]  

(10)

The order parameter \( \Theta \) has characteristic values: (i) \( \Theta \approx 0 \) describes the uniform distribution, (ii) \( \Theta \to \pm 1 \) corresponds to a self-organized phase with atoms in the even or odd antinodes, respectively. Finally, \( I_0 \) represents the maximum number of photons each atom can scatter into the cavity:

\[ I_0 = \frac{|\eta| \eta^*|}{|\kappa + N|B^2| + |\Delta_c - NU|B^2|}. \]  

(11)

In equilibrium the spatial distribution of the atoms and the above averages are time-independent, which makes it possible to attribute a physical meaning to the potential \( \Theta \). Since the potential depends on the position distribution, however, the system is highly nonlinear.

For \( U_0 < 0 \), obviously \( U_2 < 0 \) and the cavity field gives a potential with “even” wells at \( kz = 2n\pi \) and “odd” ones at \( kz = (2n + 1)\pi \). The interference term \( \alpha \cos(kz) \) discriminates between the even and odd sites, raising the energy of one of them and lowering that of the other. If \( 2 |U_2| < |U_1| \) this effect is so strong that \( V(z) \) yields a potential with wells at the even and hills at the odd sites — or the other way around, depending on the sign of \( U_1 \).

The sign of \( U_1 \) is crucial. To simplify the dependence, let us require a cavity detuning \( \Delta_c < -N|U_0| \) so that the second factor in \( U_1 \) is always negative regardless the momentary configuration of the atoms. To be specific, in the following we are going to use

\[ \Delta_c = NU_0 - \kappa. \]  

(12)

If the atoms accumulate around the even (odd) antinodes, then \( \Theta \approx +1 \) ( \( \Theta \approx -1 \) ) and the \( U_1 \cos kz \) potential is attractive at the even (odd), while repulsive at the odd (even) sites. Therefore Eq. (12) is the proper choice for positive feedback that makes the runaway solution of self-organization possible.

Two more parameters describing spatial order are used later in this work: (i) the “defect ratio”, the ratio of atoms closer to minority sites than majority sites; (ii) the “localization parameter”, the position variance (along the cavity axis and/or the transverse pump)

\[ D_z = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{kz_i}{\pi} \right)^2. \]  

(13)

where \( z_i \) is measured from the nearest antinode of the cavity mode function. A uniform distribution of atoms gives a defect ratio close to 50% and a localization parameter of 1/12. For a self-organized pattern, both parameters approach 0.

### B. Canonical distribution

We suppose that the phase-space distribution of the atoms factorizes to position and momentum dependence, the latter simply given by a thermal distribution with mean energy \( k_B T \). There is no external finite-temperature heat bath to set \( k_B T \), it is instead determined by the dynamics through the equilibrium of the cavity cooling and the Langevin noise terms. This allows for a position- and time-dependent effective temperature, effects neglected in this model. For a far-detuned pump, cavity losses dominate spontaneous emission, and an estimate \( k_B T \approx k_B T \approx \hbar \kappa \) is provided by the Einstein relation. The spatial density of the atoms in the potential \( V(z) \) is then given by a canonical distribution,

\[ \rho(z) = \frac{1}{Z} \exp(-V(z)/(k_B T)), \]  

(14)

with the partition function \( Z = \int \exp(-V(z)/(k_B T)) dz \) ensuring that \( \rho(z) \) is normalized to unity. In our case the potential \( V(z) \) is a function of the density \( \rho(z) \), therefore this equation has to be solved in a self-consistent manner.

A direct approach to solving (14) is to use it iteratively to determine the \( \rho(z) \) for given values of the physical parameters. We set the temperature to the cavity cooling limit \( k_B T = \hbar \kappa \). Note that the temperature parameter \( T \) just rescales the pumping strength \( \eta \), e.g., taking \( k_B T = 2\hbar \kappa \) would correspond to increasing \( \eta \) by a factor of \( \sqrt{2} \). The results thus obtained after 100 iterations of (14) for an experimentally realistic example are shown in Fig. 5 (empty diamonds). There we plot the percentage of atoms near odd sites after 10 (full circles) and 100 (empty diamonds) iterations is shown varying the pumping strength \( \eta \).

![FIG. 5: Numerical iterations of the mean-field approximation. The percentage of atoms near odd sites after 10 (full circles) and 100 (empty diamonds) iterations is shown varying the pumping strength \( \eta \). The vertical line is at \( \eta^* \) of (13). The two insets show two steady-state position distribution functions at two different pumping strengths. Parameters: \( \kappa = \gamma/2, \Delta_A = -500\gamma, \Delta_B^2 = 200\gamma^2 \).](image-url)
unformly, for stronger pumping this symmetry is broken. Two examples of such self-organized position distributions obtained by the iterations are shown in the insets. Note also that the convergence of the iterations is slow near the critical $\eta^*$ (critical slowing down), this is evidenced by plotting the results after 10 iterations (full circles) as well.

The uniform distribution, $\rho(z) = 1/\lambda$ leads to $\Theta = 0$, $\mathcal{B} = 1/2$, which give $V(z) = 0$, thus the distribution fulfills (14) trivially for any values of the physical parameters. To investigate its stability, we add an infinitesimal perturbation to it:

$$\rho^{(0)}(z) = \frac{1}{\lambda} + \epsilon g(z) \frac{1}{\lambda},$$

with $\epsilon$ infinitesimal, and the general $\lambda$-periodic perturbation function

$$g(z) = \sum_{m=1}^{\infty} (A_m \cos(mkz) + B_m \sin(mkz)),$$

$$\sum_{m} A_m^2 + B_m^2 = 1.$$

Since the spatial average of $g(z)$ disappears, $\rho^{(0)}(z)$ is normalized to 1. Iterating (14) once leads to the new density function

$$\rho^{(1)}(z) = \frac{1}{\lambda} - N \epsilon \frac{A_1}{\lambda} \frac{\hbar I_0}{k_B T} (\Delta_C - \frac{N}{2} U_0) \cos(kz) + o(\epsilon^2).$$

To lowest order in $\epsilon$ the only relevant perturbation is that proportional to $\cos(kz)$. Stability requires that the first-order correction in $\epsilon$ be self-contracting. Substituting (12) for the cavity detuning, we have the following instability threshold for the uniform distribution:

$$NI_0 \hbar \left(\frac{N}{2} |U_0| + \kappa\right) > k_B T.$$

For far-detuned atoms $|\Delta_A| \gg N g^2/\kappa$, i.e., when the total cavity mode shift by the atoms is much smaller than the cavity linewidth $N |U_0| \ll \kappa$, this translates to the following threshold on the pumping strength:

$$\eta > \eta^* = \sqrt{\frac{k_B T \kappa |\Delta_A|}{\hbar \sqrt{N g}}}.$$

This approximation of the critical value $\eta^*$ is in good agreement with the simulations shown on Fig. 5 giving $\eta^* = 35.4\gamma$, which differs by less than $\gamma$ from the actual value. To make the physical content more transparent, this condition can be expressed in terms of the transverse pumping power density (energy/unit area/unit time) as

$$P_{in} > k_B T \left(\frac{\Delta_A}{\gamma}\right)^2 \frac{4\kappa^3}{3N/V \gamma}.$$

As shown in the next Section, the condition (19) amounts to requiring that the potential depth along the cavity axis of a self-organized checkerboard pattern exceed significantly the energy scale of thermal fluctuations.

C. Critical exponent

The stability analysis of the uniform distribution of atoms $\rho(z) = 1/\lambda$ has revealed the critical value of the pumping strength $\eta^*$. Moreover, we have seen that for $\eta \approx \eta^*$, the relevant perturbation gives

$$\rho(z) = 1/\lambda + \epsilon \cos(kz)/\lambda.$$

Going beyond first-order perturbations, the above formula allows us to solve Eq. (14) self-consistently.

Pumping the atoms slightly above threshold, $\eta = \eta^*(1 + \delta)$, with $\delta \ll 1$, we expect (21) to give a good approximation of $\rho(z)$, with $\epsilon$ depending nonlinearly on $\delta$. Substituting it into (14) we need to expand the exponential to third order to obtain a solution to lowest order in the small parameters. This analytical calculation yields $\epsilon \propto \delta^{3/2}$, i.e., above the critical value $\epsilon$ increases from 0 as the square root of the dimensionless excess pumping strength. The order parameter $\theta = \epsilon/2$ and the percentage of majority atoms ($2\epsilon/\pi$) both depend linearly on the small parameter $\epsilon$. Therefore, the analytical result shows the critical exponent of this phase transition to be $1/2$.

V. NUMERICAL SIMULATIONS OF THE PHASE TRANSITION

In the mean-field description of the steady state, the number of atoms enters only in the form of the atomic density $N/V \propto Ng^2$. The approximation is expected to be valid in the thermodynamic limit, i.e., $N \to \infty$ with the atomic density and the cavity loss rate constant. Trying to approach this limit in simulations of Eq. (4) we are in for a surprise. In Fig. 6 we show the measured percentage of defect atoms after 4 ms of simulation time as a function of the pumping laser strength. The thermodynamic limit is approached in three steps, $N = 50, 200, \text{ and } 800$. The parameters are the same as in Fig. 5 the atoms had random initial velocities from a thermal distribution with average kinetic energy $\hbar \kappa$. The initial positions were either uniformly distributed (“up”) or at “odd” points of maximal coupling (“down”). In this controlled way we mimic the ramping of the laser power. Although the “down” curves show reasonable agreement with the mean field result, the “up” curves scale anomalously: a hysteresis is observed, whose breadth increases with the atom number.

The hysteresis effect observed in Fig. 6 is absent from the mean-field prediction is due to the long timescales associated with reaching a steady state. In fact, thermal fluctuations do not only alter the equilibrium solution by smoothing out the concentration differences due to the dynamics (this is correctly rendered by the mean field approach), but they can also delay significantly the onset of that equilibrium. This slowing down is effective if the energy scale of thermal fluctuations is at least of the same order as the potential differences due to the statistical fluctuations in the initial positions of the atoms.
The statistical fluctuations for a finite uniformly distributed atomic ensemble lead to \((N - \delta N)/2\) atoms around the \(kz = 2n\pi\) and \((N + \delta N)/2\) atoms are around the \(kz = (2n + 1)\pi\) positions. Taking uniform distributions around the respective antinodes, we have \(\sum \cos(kz_i) \approx 2\delta N/\pi\) and \(\sum \cos^2(kz_i) \approx N/2\). The potential difference then reads

\[
\Delta E = 2 |U_1| = \hbar \frac{8\delta N}{\pi} (\kappa - N|U_0|/2) = \hbar \frac{8\delta N \eta^* g^2}{\kappa \Delta A^2}.
\]

For the final expression in the second line, we considered the far-detuned regime, \(|\Delta A| \gg \gamma \sim \kappa \sim g\), and \(N|U_0|, N\Gamma_0 \ll \kappa\).

The self-organization occurs “instantly” if the trap depth originating from the statistical fluctuations exceeds the average kinetic energy \(k_B T\) of the atoms. Using the expectation value of the finite-size fluctuations, \(\delta N \approx \sqrt{N}\), we obtain

\[
\eta > \eta_\text{I} = \sqrt{\frac{k_B T}{\hbar \kappa} \frac{\kappa |\Delta A|}{N^{1/4}}} \frac{\sqrt{\pi}}{2} \frac{\sqrt{N}}{\eta^*}
\]

Comparison with \((19)\) gives \(\eta_\text{I} = \sqrt{\pi/8} N^{1/4} \eta^*: \) the functional dependence of the two thresholds on the physical parameters are the same, except for the “anomalous” scaling of \(\eta^*\) with \(N\) as the thermodynamic limit is approached.

To check the laboratory timescale threshold for self-organization \((29)\), we performed simulations with the same physical parameters as in Figs. 5 and 6 starting from uniformly distributed atoms, but this time increasing the atom number with \(Ng^4 = \text{const}\). In Fig. 7, the percentage of defect atoms is plotted as a function of the pumping \(\eta\). These numerical results confirm that the threshold depends on \(Ng^4\), moreover, the value \(\eta_\text{I} = 83\gamma\) from \((23)\) with \(k_B T = \hbar \kappa\) is also consistent with the simulations. In the transition regime, there is a remarkable overlap of the curves corresponding to various number of atoms with keeping \(Ng^4\) constant, indicating that the equilibration time also scales with \(Ng^4\).

\[
\eta > \eta_\text{I} = \sqrt{\frac{k_B T}{\hbar \kappa} \frac{\kappa |\Delta A|}{N^{1/4}}} \frac{\sqrt{\pi}}{2} \frac{\sqrt{N}}{\eta^*}
\]

VI. STABLE DEFECT ATOMS

The curve in Fig. 4 corresponding to \(N = 3200\) deviates slightly from the other data and for large pumping strength it converges to a nonzero value of the defect atoms. In fact, for the parameters chosen there, defect atoms can be stably trapped at the minority sites of the checkerboard of maximally coupled points, which presents another important physical element of the system beyond the capabilities of the simple mean-field theory. In the following we discuss the condition for the appearance of defects and the upper limit on their number.
For the analytical treatment of the defect atoms we use the 1D model of Section IV. If the atoms are perfectly self-organized, say, \( k z_j = 2 n_j \pi \) with integer \( n_j \) for every \( j \), then the potential depths of Eqs. (24) scale with the number of atoms as \( U_2 = -N^2 I_0 |U_0| \), and \( U_1 = -N 2 I_0 \kappa \). Thus, for large enough \( N \), the \( \lambda/2 \)-periodic potential is dominant and atoms can be trapped in the minority sites. These stable “defect” atoms reduce the superradiant scattering of the self-organized pattern.

How many defects can stably reside in the pattern? For simplicity, we take \( N - M \) atoms exactly at \( k z = n \pi \) and \( M < N/2 \) “defect” atoms at \( k z = (2n + 1) \pi \), neglecting the position spread. We then obviously have \( \sum \cos(kz_i) = N - 2M \) and \( \sum \cos^2(kz_i) = N \). Substituting this and the prescription (12) for the cavity detuning into (8a) we obtain

\[
U_2 = -(N - 2M)^2 |U_0| \hbar I_0, \quad (24a) \\
U_1 = -2(N - 2M) \hbar I_0 \kappa, \quad (24b) \\
I_0 = \frac{|\eta_{\text{eff}}|^2}{|\kappa + N \Gamma_0|^2 + \kappa^2}. \quad (24c)
\]

Defect atoms can persist if at every \( k z = n \pi \) there is a potential minimum:

\[
0 < |U_2| - |U_1| = 2 \hbar I_0 (N - 2M) [(N - 2M) |U_0| - \kappa],
\]

which entails

\[
\frac{N}{2} - \frac{\kappa}{2 |U_0|} > M. \quad (25)
\]

If some defect atoms appear, the rise in their number is limited by the above inequality. In particular, if the left-hand-side is negative, there can be no stable defects: the condition for the possibility of stable defects reads

\[
N > N_{\text{thr}} = \frac{\kappa}{|U_0|}. \quad (26)
\]

Note that this threshold is independent of the pumping strength. The maximum number of defects is limited by

\[
M < M_{\text{max}} = \frac{N - N_{\text{thr}}}{2}. \quad (27)
\]

Working at large atomic detuning, \( |U_0| \approx g^2/|\Delta_A| \), we find that defects can appear if the total mode frequency shift due to the atoms exceeds the cavity linewidth:

\[
N g^2 > \kappa |\Delta_A|. \quad (28)
\]

This inequality puts a lower bound on the atomic density. Equivalently, it amounts to an upper bound on the atomic detuning \( \Delta_A \): to avoid the occurrence of defects a large detuning can be chosen. This, \( |\Delta_A| \gg N g^2/\kappa \), is exactly the “far-detuned” limit of the previous Sections, used to derive the thresholds \( \eta^*, \eta^f \) and \( \eta^s \). Likewise, none of the curves in Fig. 8 satisfy Eq. (28). On Fig. 8 however, the curve corresponding to \( N = 3200 \) is above the critical density (28).

For comparison to the full solution of the dynamics, we numerically simulated the equations (4) at fixed \( \kappa = \gamma/2 \), \( g = 5\gamma/2 \), \( \Delta_A = -500\gamma \), and \( \eta = 50\gamma \). The number of atoms was varied from 0 to 200, 25 runs with different random seeds were performed for each atom number for a duration of 5 ms. The conditions for self-organization derived in Sects. III and IV give for this parameter setting a threshold atom number \( N > 10-40 \) (for \( k_B T = \hbar \kappa - \gamma \)).

The numerical results presented in Fig. 8 show that the ratio of defect atoms averaged over the 25 trajectories is well below 50%. For small atom numbers this is merely a “finite size” effect compatible with a balanced binomial distribution. For 15 atoms the defect ratio is still about half, for 18 atoms it is only a quarter of that expected from the uniform distribution. The ratio then drops down to the percent range, indicating stable self-organization, for 50 or more atoms. Concerning the appearance of defect atoms, Eq. (26) gives \( N > N_{\text{thr}} \approx 40 \). Due to non-perfect bunching this threshold is shifted to somewhat higher values. The insert of Fig. 8 shows the absolute number of defect atoms after 5 ms, averaged over the runs: the minimum at \( N \approx 60 \) followed by a rise can be identified with the threshold, which is in accordance with the previous, simple estimate.

The transition from the perfectly ordered phase to the one where defect atoms can be present manifests itself in the statistical properties of the system. As discussed in Sect. III the appropriate measure of the thermal excitations is the phase space volume, given by the Heisenberg uncertainty product \( \Delta z \Delta p_z / \hbar \). In Fig. 9, this is plotted as a function of the atom number: both the final phase space volume of individual runs after 5 ms (dots) and the average over these trajectories after 2, 3, 4 and 5 ms (continuous lines) are shown. For very few atoms, the
FIG. 9: The normalized phase space volume of the system. Dots represent the values taken at individual trajectories at 5 ms, the thick solid line is their average. The thin lines correspond to the average over the trajectories at 2, 3, and 4 ms. The physical parameters are the same as in Fig. 8.

FIG. 10: Photon number in the cavity 5 ms after loading. At high atom numbers \((N > 20)\) the simulation results (dots) are fitted well by a quadratic function (black line), indicating that the atoms scatter cooperatively. The physical parameters are the same as in Fig. 8.

VII. COLLECTIVE EFFECTS IN THE SELF-ORGANIZED PHASE

The most direct evidence of cooperative action is superradiance into the resonator mode that can be measured by detecting the power output from the cavity. In the self-organized checkerboard pattern each atom radiates with the same phase, and so the cavity photon number \(|\alpha|^2\) increases quadratically with the number of atoms. This can be observed in the numerical simulations of Eq. (4), gradually increasing the number of atoms as detailed in the previous Section. The cavity photon number is shown on a logarithmic scale in Fig. 10. For many atoms in the cavity \((N > 20)\) the intensity data are well approximated by the fitted quadratic function \(|\alpha|^2 = 0.08N^2\). The steady-state solution of Eq. (4a) reads

\[ |\alpha|^2 = I_0 \left( \cos(kz_j) \cos(kx_j) \right)^2 N^2 \, . \]  

(29)

If all atoms are perfectly at the antinodes \((|\cos(kz_j) \cos(kx_j)|^2 = \Theta = \mathcal{B} = 1)\) this yields a coefficient of 0.125. The value from the simulations is 30% below this: the difference can be attributed to the position spread and to the defect atoms.

The superradiance has important effects on the spatial distribution of the atoms about their respective field antinodes. With increasing number of atoms the trap deepens so that the size of the atomic clouds about the antinodes is compressed, as shown in Fig. 11. We note again the appearance of the shoulder at \(N \approx 60\) due to the transition into the double-well potential with stable defect atoms. Apart from this, the overall decrease of the localization parameter in the range \(N = 10, \ldots, 200\) is proportional to \(1/N\). As we show below, this scaling law can be derived by a careful examination of the self-generated trap potential.

FIG. 11: The localization parameter \(D_z = \sum_i \frac{(kz_i/\pi)^2}{N}\) measured by the simulation (dots) and averaged over runs (continuous black line) shows an overall \(1/N\) dependence as a function of the atom number. The dashed line is the approximation of Eq. (31). The physical parameters are the same as in Fig. 8.
We consider one-dimensional motion of the atoms in the limit where they are strongly localized in the vicinity of the antinodes. In this limit of harmonic oscillation the field amplitude in Eq. (21) is coupled to the atomic positions only through the sum $\sum z_i^2$, i.e., through the localization parameter defined in Eq. (13). It is instructive to introduce new coordinates in the configuration space: the mean radius $r = \sqrt{\sum z_i^2/N}$, and a number of $N-1$ angular coordinates $\varphi_j$ with canonically conjugate momenta $p_{\varphi_j} = Nmr^2\dot{\varphi}_j$, these latter decoupled from the field dynamics. Only the radial motion is damped by the cavity cooling mechanism, the angular ones are not. For the coordinate $r$ the potential is composed of the harmonic attraction $\propto r^2$ and a centrifugal repulsion $\propto 1/r^2$. There is a potential minimum and the radius is damped into it by cavity cooling. For large number of atoms the cloud size at an antinode can be simply estimated by the variance is much smaller than the mean.

For a quasi-stationary field amplitude, the harmonic potential is $mr^2/2$ with vibration frequency

$$\nu = \sqrt{\frac{\hbar k^2}{m} \left( \frac{|U_0|}{g} |\alpha| + 2|U_0||\alpha|^2 \right)}.$$  

The angular kinetic energies are of the form $p_{\varphi_j}^2/(2mN^2)$, $j = 1, \ldots, (N - 1)$. The momenta $p_{\varphi_j}$ can be estimated by their initial value in the unorganized phase, when all degrees of freedom have the same energy $k_BT/2$ and the radius is $r = \lambda/\sqrt{4\pi}$. The potential minimum is just at the radius where the harmonic potential energy equals the sum of the centrifugal energies. Simple algebra leads to the cloud size

$$r^2 \approx \frac{\lambda^2}{8\pi\sqrt{3}} \sqrt{\frac{k_BT}{\hbar|U_0|} \left( \frac{g}{\nu} |\alpha| + 2|\alpha|^2 \right)^{-\frac{1}{2}}}.$$  

and since $|\alpha|^2 \propto N^2$, the $1/N$ law for the localization parameter follows. Altogether, the increase in atom number results in a smaller cloud size in the vicinity of the antinodes, a very important virtue of the collective atomic action. This compression is limited by the dipole-dipole interaction of the atoms near the same antinode, which effect was not taken into account in the present model.

**VIII. CONCLUSION**

A dilute cloud of non-interacting cold atoms in a high-Q cavity can undergo a phase transition if driven from the side by a laser sufficiently red detuned from an atomic resonance. Increasing the laser power above a threshold the atoms self-organize into a lattice so as to scatter most effectively into the cavity mode. In this way the atoms minimize their energy in the optical potential generated from the interference pattern of the cavity and pump field. Under proper conditions the atoms are cooled in this process giving long term stability to the pattern.

The phenomenon has been previously seen in simulations and strong evidence was found in experiments [21], but threshold, scaling and efficiency of the effect with atom number, cavity parameters and system size remained unclear. Here we gave a thorough analytical discussion of the effect. A continuous density approach allowed us to derive analytical formulas for the critical pump power as a function of atom number and cavity volume and showed that the effect should persist if one scales up the volume at fixed atomic density, i.e., $N_0^2 = \text{const}$. Numerical simulations of the evolution for finite durations revealed a hysteresis between the ordered and homogeneous density phase on varying the control parameter, i.e., the pumping strength. This shifts the observable threshold in the pumping strength, which then scales with $N_0^4$. We still have a cooling mechanism for large numbers of any type of optically polarizable particles.

The system is composed of non-interacting atoms that communicate via a commonly coupled, single cavity mode. The cavity component of the system plays a multiple role. First, the binding energy of the ordered phase is stored in the superradiantly enhanced field intensity of this single mode. Next, as an attractive feature of this system, the outcoupled field intensity directly serves as a possibility of time-resolved monitoring of the formation of the ordered phase. Note that in setups without resonator, the uncontrolled scattered field can lead to a binding of micrometer-sized particles in an ordered pattern in liquid [40, 41]. In the cavity scheme, finally, the viscous motion is provided by the dynamically coupled single-mode cavity field. Apart from the geometry, this is also a distinctive feature with respect to CARL.

From the laser cooling point of view, the picture is complicated by the phase transition. The appropriate measure of the cooling efficiency is the phase space volume occupied by the system. The self-organization process reduces this volume below that of a system at the cavity cooling limit with uniform spatial distribution. Moreover, the steady state is established within milliseconds, and this is closely independent of the number of atoms in the cloud (numerical simulations confirm this up to few hundreds of atoms). Collective cooling was previously known only for the stochastic cooling method [12] and for common vibrational modes of trapped particles [13]. The collective behaviour strongly improves the localization, i.e., the size of the atom cloud pieces at the trapping sites is proportional to the inverse of the atom number.

This work could be extended to various directions. First of all, the numerical simulations should confirm some of the statements of the present paper on a larger range of the atom number, or on a longer time scale (e.g., the dependence of the hysteresis on the duration of the evolution). Our prescription for the pump-cavity detuning $\Delta_C$ in Eq. (12) is probably impractical in the limit of large atom numbers, as one has to go closer to
the resonance in order to initiate the self-organization. Next, the maximum achievable densities can not be determined in the present model as some of the limiting factors were omitted, e.g., vacuum-mediated dipole-dipole interaction between the atoms, the eventual superradiant enhancement of the spontaneous scattering into lateral directions, etc. In extremely good cavities, quantum effects in the motion of the atoms begin to play an important role [44, 45], which was not studied here. Finally, the nature of the phase transition is strongly determined by the geometry of the cavity mode: the possible trapping sites are defined by the antinodes of the cavity mode and the transverse pumping field. This situation can be essentially modified in a cavities with different geometry, e.g., ring or confocal resonator.

We thank Walter Rantner for useful discussions and Zoltán Kurucz for reading the manuscript. This work was supported by the National Scientific Fund of Hungary (Contract Nos. T043079, T049234), the Bolyai Program of the Hungarian Academy of Sciences, and by the Austrian FWF SFB P12.