# Quantum phases of incommensurate optical lattices due to cavity backaction

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Ultracold bosonic atoms are confined by an optical lattice inside an optical resonator and interact with a cavity mode whose wavelength is incommensurate with the spatial periodicity of the confining potential. We predict that the intracavity photon number can be significantly different from zero when the atoms are driven by a transverse laser whose intensity exceeds a threshold value and whose frequency is suitably detuned from the cavity and the atomic transition frequency. In this parameter regime the atoms form clusters in which they emit in phase into the cavity. The clusters are phase locked, thereby maximizing the intracavity photon number. These predictions are based on a Bose-Hubbard model, whose derivation is reported here in detail. The Bose-Hubbard Hamiltonian has coefficients which are due to the cavity field and depend on the atomic density at all lattice sites. The corresponding phase diagram is evaluated using quantum Monte Carlo simulations in one dimension and mean-field calculations in two dimensions. Where the intracavity photon number is large, the ground state of the atomic gas lacks superfluidity and possesses finite compressibility, typical of a Bose glass.

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# I. INTRODUCTION

Self-organization of interacting systems of photons and atoms in cavities is a remarkable example of pattern formation in the quantum world. The structures which are formed are due to the nonlinear dependence of the atomic potential on the atomic density: The field scattered into the cavity depends on and determines the atomic density distribution by means of the mechanical effects of atom-photon interactions [1]. Features related to these dynamics were already predicted and then observed in atomic gases confined by optical lattices in free space [2-4]. In a high-finesse cavity the effect is significantly enhanced due to the strong coupling one can achieve between atoms and light at the single-photon level. Here, spatial ordering [5-8], collective-atom recoil lasing [9,10], synchronization [11], and motion-induced bistability [12-15] have been observed in gases of laser-cooled atoms inside a high-finesse cavity, when either the cavity or the atoms are driven by an external laser. These phenomena typically occur when the laser intensity exceeds a threshold value and can be revealed by the light transmitted by the resonator's mirrors

In recent theoretical studies it was argued that ultracold atoms in cavity quantum electrodynamics setups offer a novel setting to study disorder and glassiness [16,17]. Along a similar line, in a recent work we analyzed self-organization of atoms trapped by an external optical lattice and interacting with the standing-wave field of a cavity whose periodicity is incommensurate with the lattice periodicity. A sketch of the setup is shown in Fig. 1. In this situation we showed that scattering of light into the resonator generates an optical lattice which is incommensurate with the one confining the atoms and whose intensity depends on the atomic density at all lattice sites [18]. This global potential is a feature of cavity quantum electrodynamics setups, where the cavity photons undergo multiple scattering and give rise to an effective atomic potential which is long ranged. It is important to note that this potential would not be generated if the atoms were pointlike particles located at the minima of the classical lattice: in this case there is no coherent scattering into the cavity mode [19]. Density fluctuations here favor elastic scattering of photons into the cavity field, giving rise to the formation of patterns which maximize the intracavity field and which can exhibit finite compressibility with no long-range coherence. The latter feature is typical of disordered systems and corresponds to a Bose-glass (BG) phase for sufficiently deep potentials [20–22]. Here, it emerges due to the nonlocal quantum potential of the cavity field.

The purpose of the present paper is to provide the details of the analytical and numerical derivation at the basis of Ref. [18]. We discuss in detail the statistical features which emerge from the interaction with the cavity field, which induces an interparticle potential whose range is as large as the system size. We compare our results with numerical studies, in which the quantum ground-state properties of bosonic atoms in a classical bichromatic potential are analyzed. We also report in detail the experimental parameter regimes where these dynamics can be found making reference to the setup in Ref. [7].

This paper is organized as follows. In Sec. II the theoretical model is introduced. Here, the Bose-Hubbard Hamiltonian is derived, which includes the infinitely ranged cavity potential and is at the basis of the numerical simulations. The results for the ground-state properties of the Bose-Hubbard model are reported in Sec. III: In Sec. III A we show the results of quantum Monte Carlo (QMC) simulations for the one-dimensional (1D) lattice, while in Sec. III B the phase diagrams for the two-dimensional (2D) case are discussed, which are obtained using a mean-field approach. The limits of validity of the model and the experimental parameter are analyzed in Sec. IV. Conclusions are drawn in Sec. V, while the Appendices report

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FIG. 1. (Color online) Ultracold atoms are tightly confined by an optical lattice of periodicity  $\lambda_0/2$ . They are driven by a weak transverse laser at Rabi frequency  $\Omega$  and strongly couple to the mode of a standing-wave cavity, both at wavelength  $\lambda$ . Since  $\lambda$  and  $\lambda_0$  are incommensurate, one would expect no coherent scattering into the cavity mode. The mechanical effects due to multiphoton scattering, however, give rise to an incommensurate quantum potential, which mediates an effective long-range interaction between the atoms and modifies the properties of the quantum ground state. As a result, the intracavity photon number can be large. The corresponding ground state can show features typical of a Bose glass.

details at the basis of the derivation of the Bose-Hubbard model in Sec. II and of the numerical results in Sec. III A.

# **II. THEORETICAL MODEL**

The system we consider is composed of N ultracold identical atoms of mass m which obey Bose-Einstein statistics. The atoms are tightly confined by a 2D optical lattice of wave number  $k_0 = 2\pi/\lambda_0$ , with  $\lambda_0$  the wavelength, such that the spatial periodicity is  $d_0 = \lambda_0/2$ . An optical dipole transition of the atoms is driven by a laser and scatters photons into a mode of a high-finesse resonator, according to the geometry shown in Fig. 1. The resonator field is a standing wave of wavelength  $\lambda$ , which is incommensurate with the wavelength  $\lambda_0$  of the external potential confining the atoms. When quantum fluctuations can be neglected, i.e., deep in the Mott-insulator (MI) phase of the external potential, the cavity field is in the vacuum [19]. Density fluctuations, on the other hand, induce photon scattering into the cavity field, giving rise to the formation of patterns which maximize scattering into the cavity mode.

In order to provide an appropriate description we consider the Hamiltonian of the system in second quantization. We derive an effective model for the dynamics of the atomic external degrees of freedom, from which we obtain a Bose-Hubbard Hamiltonian. This Bose-Hubbard Hamiltonian is the starting point of the numerical investigations in Sec. III.

### A. Coherent dynamics

The atoms are prepared in an electronic stable state which we denote  $|1\rangle$ . They are confined on the *x*-*z* plane by an external potential, while the motion along the *y* axis is here assumed to be frozen out. For an atom at position  $\mathbf{r} = (x,z)$ 

the external potential reads

$$V_{\rm cl}(\mathbf{r}) = V_0 \{\cos^2(k_0 z) + \beta \cos^2(k_0 x)\},\tag{1}$$

where  $V_0$  is the potential depth along the *z* direction and  $\beta V_0$  the potential depth along *x*. The atoms are at ultralow temperature *T* and tightly bound to the potential minima. The quantum gas density also spatially overlaps with the field of an optical resonator: An atomic dipole transition with ground state  $|1\rangle$  and excited state  $|2\rangle$  at frequency  $\omega_0$  couples strongly with a cavity mode at frequency  $\omega_c$ , wavelength  $\lambda$ , and wave number  $k = 2\pi/\lambda$  such that the wave vector is along the *z* axis. The intracavity field is pumped by the photons that the atoms scatter, when these are driven by a transverse laser at frequency  $\omega_L$  close to  $\omega_c$ , such that it has effectively the same wavelength  $\lambda$  as the cavity mode. The setup is shown in Fig. 1.

The coherent dynamics of the cavity field and the atomic internal and external degrees of freedom is governed by Hamiltonian  $\hat{\mathcal{H}}$ , which we decompose into the sum of the Hamiltonian for the cavity, the atoms, and their mutual interaction:

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_C + \hat{\mathcal{H}}_A + \hat{\mathcal{H}}_{\text{int}}.$$

The Hamiltonian for the cavity mode reads

$$\hat{\mathcal{H}}_C = \hbar \omega_c \hat{a}^{\dagger} \hat{a}, \qquad (2)$$

where  $\hat{a}$  and  $\hat{a}^{\dagger}$  are the annihilation and creation operators of a cavity photon, respectively, and obey the commutation relation  $[\hat{a}, \hat{a}^{\dagger}] = 1$ .

The Hamiltonian for the atomic degrees of freedom  $\hat{\mathcal{H}}_A$  (in the absence of the resonator) takes the form

$$\hat{\mathcal{H}}_{A} = \sum_{j=1,2} \int d^{2}\mathbf{r} \,\hat{\Psi}_{j}^{\dagger}(\mathbf{r}) \hat{\mathcal{H}}_{j}(\mathbf{r}) \hat{\Psi}_{j}(\mathbf{r}) + 2U_{12} \int d^{2}\mathbf{r} \,\hat{\Psi}_{1}^{\dagger}(\mathbf{r}) \hat{\Psi}_{2}^{\dagger}(\mathbf{r}) \hat{\Psi}_{2}(\mathbf{r}) \hat{\Psi}_{1}(\mathbf{r})$$
(3)

and is written in terms of the atomic field operator  $\hat{\Psi}_j(\mathbf{r},t)$ , which destroys an atom in the internal state  $|j = 1,2\rangle$  at position **r** and time *t*, and obeys the commutation relations  $[\hat{\Psi}_i(\mathbf{r},t), \hat{\Psi}_i^{\dagger}(\mathbf{r}',t)] = \delta_{ij} \,\delta(\mathbf{r} - \mathbf{r}')$ . Here,

$$\hat{H}_{j}(\mathbf{r}) = -\frac{\hbar^{2}\nabla^{2}}{2m} + V_{cl}^{(j)}(\mathbf{r}) + \frac{U_{jj}}{2}\hat{\Psi}_{j}^{\dagger}(\mathbf{r})\hat{\Psi}_{j}(\mathbf{r}) + \hbar\omega_{0}\delta_{j,2},$$
(4)

where  $V_{cl}^{(j)}(\mathbf{r})$  is the optical potential of the atoms in state j = 1, 2, which for the ground state, j = 1, coincides with  $V_{cl}$  in Eq. (1),  $\delta_{j,2}$  is the Kronecker  $\delta$ , and  $U_{j,l}$  is the strength of the contact interaction between atoms in state j and atoms in state l, with j, l = 1, 2.

Finally, the Hamiltonian describing the interaction between the atomic dipoles and the electric fields reads

$$\hat{\mathcal{H}}_{\text{int}} = \hbar g_0 \int d^2 \mathbf{r} \cos{(kz)} [\hat{\Psi}_2^{\dagger}(\mathbf{r}) \hat{\Psi}_1(\mathbf{r}) \hat{a} + \text{H.c.}] + \hbar \Omega \int d^2 \mathbf{r} \cos{(kx)} (\hat{\Psi}_2^{\dagger}(\mathbf{r}) \hat{\Psi}_1(\mathbf{r}) e^{-i\omega_L t} + \text{H.c.}),$$
(5)

where  $g_0$  is the cavity vacuum Rabi frequency and the term in the second line describes the coherent coupling between the dipolar transition and a standing-wave laser along the x direction with Rabi frequency  $\Omega$ .

## B. Heisenberg-Langevin equation and weak excitation limit

Throughout this paper we assume that the photon scattering processes are elastic. This regime is based on assuming that the detuning between fields and atoms is much larger than the strength with which they are mutually coupled. The large parameter is the detuning,

$$\Delta_a = \omega_L - \omega_0, \tag{6}$$

between the pump and the atomic transition frequency, which is chosen so that  $|\Delta_a| \gg \gamma$ , where  $\gamma$  is the radiative line width of the excited state, and so that  $|\Delta_a| \gg \Omega$ ,  $g_0 \sqrt{n_{cav}}$ , namely, the detuning is much larger than the strength of the coupling between the ground and the excited state, where  $n_{cav} = \langle \hat{a}^{\dagger} \hat{a} \rangle$ is the intracavity photon number. In this regime the population of the excited state is neglected.

Photons are elastically scattered into the resonator when the laser is quasiresonant with the cavity field, which here requires that  $|\Delta_a| \gg |\delta_c|$  with

$$\delta_c = \omega_L - \omega_c. \tag{7}$$

In this limit the field operator  $\hat{\Psi}_2(\mathbf{r},t)$  is a function of the cavity field operator  $\hat{a}$  and of the atomic field operator  $\hat{\Psi}_1(\mathbf{r},t)$  at the same instant of time according to the relation [23,24]

$$\hat{\Psi}_{2}(\mathbf{r},t) = \frac{g_{0}}{\Delta_{a}} \cos(kz) \hat{\Psi}_{1}(\mathbf{r},t) \hat{a}(t) + \frac{\Omega}{\Delta_{a}} \cos(kx) \hat{\Psi}_{1}(\mathbf{r},t),$$
(8)

which is given here to lowest order in the expansion in  $1/|\Delta_a|$ . Using Eq. (8) in the Heisenberg equation of motion for the field operator  $\hat{\Psi}_1(\mathbf{r},t)$  results in the equation

$$\dot{\hat{\Psi}}_{1} = -\frac{i}{\hbar} [\hat{\Psi}_{1}, \hat{\mathcal{H}}_{A}] - i \frac{\Omega^{2}}{\Delta_{a}} \cos^{2}(kx) \hat{\Psi}_{1} - i U_{0} \cos^{2}(kz) \hat{a}^{\dagger} \hat{\Psi}_{1} \hat{a} - i S_{0} \cos(kz) \cos(kx) (\hat{a}^{\dagger} \hat{\Psi}_{1} + \hat{\Psi}_{1} \hat{a}), \qquad (9)$$

which determines the dynamics of the system together with the Heisenberg-Langevin equation for the cavity field:

$$\dot{\hat{a}} = -\kappa \hat{a} + i(\delta_c - U_0 \hat{\mathcal{Y}})\hat{a} - iS_0 \hat{\mathcal{Z}} + \sqrt{2\kappa} \hat{a}_{\rm in}, \quad (10)$$

where  $\kappa$  is the cavity line width and  $\hat{a}_{in}(t)$  is the input noise operator, with  $\langle \hat{a}_{in}(t) \rangle = 0$  and  $\langle \hat{a}_{in}(t) \hat{a}_{in}^{\dagger}(t') \rangle = \delta(t - t')$  [25]. The other parameters are the frequency  $U_0 = g_0^2 / \Delta_a$ , which scales the depth of the intracavity potential generated by a single photon, and the frequency  $S_0 = g_0 \Omega / \Delta_a$ , which is the Raman scattering amplitude with which a single photon is scattered by a single atom between the cavity and the laser mode [26]. Moreover, in Eq. (10) we have introduced the operators

$$\hat{\mathcal{Z}} = \int d^2 \mathbf{r} \cos(kz) \cos(kx) \,\hat{n}(\mathbf{r}) \,,$$

$$\hat{\mathcal{Y}} = \int d^2 \mathbf{r} \cos^2(kz) \,\hat{n}(\mathbf{r}),$$
(11)

where

$$\hat{n}(\mathbf{r}) = \hat{\Psi}_1^{\dagger}(\mathbf{r})\hat{\Psi}_1(\mathbf{r})$$
(12)

is the atomic density. The two operators in Eq. (11) are the spatial integrals of the atomic density weighted by the fields spatial-mode function and space-dependent intensity, respectively. In the limit in which the atoms can be considered pointlike, then  $\hat{n}(\mathbf{r}) \approx n_{cl}(\mathbf{r}) = \sum_{j} \delta(\mathbf{r} - \mathbf{r}_{j})$  and  $Z_{cl} = \sum_{j} \cos(kz_{j}) \cos(kx_{j})$ ,  $\mathcal{Y}_{cl} = \sum_{j} \cos^{2}(kz_{j})$ . Hence, when the atoms are randomly distributed in the cavity field potential, then  $Z_{cl} \rightarrow 0$ . In this case, thus, no photon is elastically scattered into the cavity mode and the cavity field is in the vacuum. This behavior can also be found in the situation we consider in this work, where the atoms are ordered in an array with periodicity which is incommensurate with the periodicity of the pump and cavity standing wave. The focus of this work is to analyze the effect of quantum fluctuations on this behavior.

### C. Adiabatic elimination of the cavity field

We now derive an effective Hamiltonian governing the motion of the atoms inside the resonator by eliminating the cavity degrees of freedom from the atomic dynamics. This is performed by assuming that the cavity field follows adiabatically the atomic motion. Formally, this consists in a time-scale separation. We identify the time scale  $\Delta t$  over which the atomic motion does not significantly evolve while the cavity field has relaxed to a state which depends on the atomic density at the given interval of time. This requires that  $|\delta_c + i\kappa|\Delta t \gg 1$  while  $\kappa_B T \ll \hbar/\Delta t$ , with  $k_B$  the Boltzmann constant [23]. Moreover, the coupling strengths between atoms and fields, which determine the time scale of the evolution due to the mechanical effects of the interaction with the light, are much smaller than  $1/\Delta t$ . In this limit, we identify the field operator  $\hat{a}_{st}$ , which is defined by the equation

$$\int_t^{t+\Delta t} \hat{a}(\tau) d\tau / \Delta t \approx \hat{a}_{\rm st},$$

such that  $\int_{t}^{t+\Delta t} \dot{a}_{st}(\tau) d\tau = 0$ , with  $\dot{a}$  given in Eq. (10). The "stationary" cavity field is a function of the atomic operators at the same (coarse-grained) time and, in particular, takes the form

$$\hat{a}_{\rm st} = \frac{S_0 \hat{\mathcal{Z}}}{(\delta_c - U_0 \hat{\mathcal{Y}}) + i\kappa} + \frac{i\sqrt{2\kappa}\hat{a}_{\rm in}}{(\delta_c - U_0 \hat{\mathcal{Y}}) + i\kappa},\qquad(13)$$

with  $\bar{a}_{in}$  the input noise averaged over  $\Delta t$ . The quantum noise term can be neglected when the mean intracavity photon number is larger than its fluctuations, which corresponds to taking  $|S_0\langle \hat{Z} \rangle| \gg \kappa$ . In this limit, the field at the cavity output,

$$\hat{a}_{\rm out} = \sqrt{2\kappa}\hat{a}_{\rm st} - \bar{\hat{a}}_{\rm in},\tag{14}$$

allows one to monitor the state of the atoms [19,25,27]. Using Eq. (13) in place of the field  $\hat{a}$  in Eq. (9) leads to an equation of motion for the atomic field operator which depends solely on the atomic variables [23,24].

#### D. Bose-Hubbard model

Denoting the number of lattice sites K, a well-defined thermodynamic limit is identified assuming the scaling of the cavity parameters with K according to the relations  $S_0 = s_0/\sqrt{K}$  and  $U_0 = u_0/K$  [23,28]. Under the assumption that the atoms are tightly bound by the external periodic

potential in Eq. (1), we apply the single-band approximation and perform the Wannier decomposition of the atomic field operator [29,30],

$$\hat{\Psi}_1(\mathbf{r}) = \sum_{i,j} w_{i,j}(\mathbf{r}) \hat{b}_{i,j},\tag{15}$$

with the Wannier function  $w_{i,j}(\mathbf{r})$  centered at a lattice site with coordinate  $(x_i, z_j)$  (with  $x_i = id_0, z_j = jd_0$ , and  $d_0 = \lambda_0/2$  the lattice periodicity), while  $\hat{b}_{i,j}$  and  $\hat{b}_{i,j}^{\dagger}$  are the bosonic operators annihilating and creating, respectively, a particle at the corresponding lattice site. The decomposition is performed starting from the equation of motion of the atomic field operator, obtained from Eq. (9) with the substitution  $\hat{a} \rightarrow \hat{a}_{st}$ , Eq. (13). The details of the procedure are reported in Refs. [23,24] and are summarized in Appendix A. We remark that  $w_{i,j}(\mathbf{r})$  are the Wannier functions obtained for the dynamics of single atoms in a classical optical lattice, Eq. (1). Their properties are summarized, for instance, in Ref. [31].

The resulting Bose-Hubbard Hamiltonian reads [18]

$$\begin{aligned} \hat{\mathcal{H}}_{BH} &= -\sum_{\langle i'j',ij \rangle} \hat{t}_{ij,i'j'} (\hat{b}_{i,j}^{\dagger} \hat{b}_{i',j'} + \hat{b}_{i',j'}^{\dagger} \hat{b}_{i,j}) \\ &+ \frac{U}{2} \sum_{i,j} \hat{n}_{i,j} (\hat{n}_{i,j} - 1) + \sum_{i,j} \hat{\epsilon}_{i,j} \hat{n}_{i,j}, \end{aligned}$$
(16)

where the  $\langle i'j', ij \rangle$  in the sum denotes the nearest neighbors of the corresponding lattice site. The on-site interaction, the on-site energy, and the tunneling rate are defined as

$$U = U_{11} \int d^2 \mathbf{r} \, w_{i,j}(\mathbf{r})^4, \qquad (17)$$

$$\hat{\epsilon}_{i,j} = \epsilon^{(0)} + \delta \hat{\epsilon}_{i,j}, \quad \hat{t}_{ij,i'j'} = t^{(0)} + \delta \hat{t}_{ij,i'j'}.$$
 (18)

In particular, the on-site energy (tunneling rate) is the sum of a term which is constant,  $\epsilon^{(0)}(t^{(0)})$ , and of a term which depends on the lattice site and is due to the cavity field. In detail, the constant terms read

$$\epsilon^{(0)} = E_0 + V_0 X_0, \quad t^{(0)} = -E_1 - V_0 X_1,$$

with

$$X_{s} = \int d^{2}\mathbf{r} \, w_{i,j}(\mathbf{r}) [\cos^{2}(k_{0}x) + \beta \cos^{2}(k_{0}z)] w_{i',j'}(\mathbf{r}), \quad (19)$$

$$E_s = -\frac{\hbar^2}{2m} \int d^2 \mathbf{r} \, w_{i,j}(\mathbf{r}) \nabla^2 w_{i',j'}(\mathbf{r}), \qquad (20)$$

such that for s = 0, then (i, j) = (i', j'), while for s = 1, then (i', j') is a nearest-neighbor site. These terms are due to the dynamics in the absence of a cavity field. In Appendix A we show that the site-dependent term of the tunneling coefficient,  $\delta \hat{t}_{ij,i'j'}$  is negligible, so that  $\hat{t}_{ij,i'j'} \sim t^{(0)}$ . The site-dependent part of the coefficient  $\epsilon_{i,j}$  proves, instead, to be relevant and reads

$$\delta\hat{\epsilon}_{i,j} = V_1 J_0^{(i,j)} + \frac{\hbar s_0^2}{\hat{\delta}_{\text{eff}}^2 + \kappa^2} \hat{\Phi} \hat{\delta}_{\text{eff}} Z_{0,0}^{(i,j)}, \qquad (21)$$

where the various terms of the sum on the right-hand side (r.h.s.) have different physical origins (note that  $\langle \delta \hat{\epsilon}_{i,j} \rangle$  is real-valued under the assumption that  $\langle \hat{\delta}_{eff} \rangle \gg \kappa$ , as we assume in what follows). The first term on the r.h.s. is due to the standing

wave of the classical transverse pump, with  $V_1 = \Omega^2 / \Delta_a$  and

$$J_0^{(i,j)} = \int d^2 \mathbf{r} \, w_{i,j}(\mathbf{r}) \cos^2(k \, x) \, w_{i,j}(\mathbf{r}).$$
(22)

This coefficient is site dependent along the *x* direction, namely, in the direction of propagation of the transverse field, while it is constant along the *z* direction when *x* is fixed. The other term on the r.h.s. of Eq. (21) is due to the cavity field. In particular, it depends on the operator

$$\hat{\delta}_{\text{eff}} = \delta_c - u_0 \sum_{i,j} Y_0^{(i,j)} \hat{n}_{i,j} / K, \qquad (23)$$

whose mean value gives the shift of the cavity resonance due to the atomic distribution [24], while the coefficients

$$Y_{0}^{(i,j)} = \int d^{2}\mathbf{r} \, w_{i,j}(\mathbf{r}) \cos^{2}(kz) \, w_{i,j}(\mathbf{r}),$$

$$Z_{0,0}^{(i,j)} = \int d^{2}\mathbf{r} \, w_{i,j}(\mathbf{r}) \cos(kz) \cos(kx) \, w_{i,j}(\mathbf{r})$$
(24)

are the overlap integrals due to the cavity optical lattice and the mechanical potential associated with the scattering of cavity photons, respectively. Finally, this term is multiplied by the operator

$$\hat{\Phi} = \sum_{i,j} Z_{0,0}^{(i,j)} \hat{n}_{i,j} / K, \qquad (25)$$

which is the sum of the atomic density over the lattice mediated by the Raman scattering amplitude.

### E. Discussion

When the pump is off,  $\Omega = 0$ , the Hamiltonian we have derived reduces to the typical Bose-Hubbard model as it occurs in systems of ultracold atoms confined by optical lattices [29,30]. The latter exhibits a superfluid (SF)–MI quantum phase transition which is controlled either by changing the potential depth  $V_0$ , and hence the hopping coefficient t, or by the on-site interaction strength U [29,30]. In this paper we assume U to be constant and vary t by varying the potential depth  $V_0$ .

When the transverse laser drives the cavity field by means of elastic scattering processes, the Hamiltonian depends on the nonlocal operator, (25), which originates from the long-range interaction between the atoms mediated by the cavity field. The physical observable which is associated with this operator is the cavity-field amplitude,

$$\hat{a}_{\rm st} \approx \frac{S_0 K \hat{\Phi}}{\hat{\delta}_{\rm eff} + i\kappa},$$
 (26)

as is visible by using Eq. (25) in Eq. (13), and after discarding the noise term, assuming this is small. It can be measured by homodyne detection of the field at the cavity output [32]. The intracavity photon number,  $\hat{n}_{cav} = \hat{a}_{st}^{\dagger} \hat{a}_{st}$ , reads

$$\hat{n}_{\rm cav} \approx \frac{S_0^2 K^2}{\hat{\delta}_{\rm eff}^2 + \kappa^2} \hat{\Phi}^2 \equiv K \frac{s_0^2}{\hat{\delta}_{\rm eff}^2 + \kappa^2} \hat{\Phi}^2, \tag{27}$$

and the intensity of the field at the cavity output provides a measurement of the operator  $\hat{\Phi}^2$ , where the second expression on the r.h.s. uses the chosen scaling of the cavity parameters with the number of sites. The intracavity photon number

vanishes when the atomic gas forms an MI state: In this case  $\langle \hat{\Phi}^2 \rangle_{\text{MI}} \propto (\sum_{i,j} Z_0^{(i,j)})^2 = 0$ , since there is no coherent scattering into the cavity mode. Also, deep in the SF phase  $\langle \hat{\Phi}^2 \rangle_{\text{SF}} \rightarrow 0$ , as one can verify using Eq. (25).

It is interesting to note that, using definitions (25) and (23), Hamiltonian (16) can be cast in the form

$$\begin{aligned} \hat{\mathcal{H}}_{\rm BH} &= -\sum_{\langle i'j',ij\rangle} t\,(\hat{b}_{i,j}^{\dagger}\hat{b}_{i',j'} + \hat{b}_{i',j'}^{\dagger}\hat{b}_{i,j}) + \frac{U}{2}\sum_{i,j}\hat{n}_{i,j}(\hat{n}_{i,j} - 1) \\ &+ \epsilon^{(0)}\hat{N} + V_1\sum_{i,j}J_0^{(i,j)}\hat{n}_{i,j} + \frac{\hbar s_0^2}{\hat{\delta}_{\rm eff}^2 + \kappa^2}K\hat{\Phi}^2\hat{\delta}_{\rm eff}, \end{aligned}$$

$$(28)$$

where we have neglected the site dependence of the tunneling parameter (the validity of this approximation is discussed in Appendix A). In this form the Bose-Hubbard Hamiltonian depends explicitly on the operator corresponding to the number of intracavity photons [see Eq. (27)], showing the long-range interacting potential due to the cavity field. This potential either decreases or increases the total energy, depending on the sign of  $\langle \hat{\delta}_{eff} \rangle$ : When  $\langle \hat{\delta}_{eff} \rangle < 0$ , "disordered" (i.e., aperiodic) density distributions are expected when the mean density is fractional. Its sign hence critically determines whether disordered density distributions are energetically favorable. A similar behavior has been identified in the dynamics of self-organization in periodic potentials [28,33,34]. The dependence of the chemical potential on the operator  $\hat{\Phi}$  is a peculiar property of our model, which makes it different from the case of a bichromatic optical lattice [22,35], in which the strength of the incommensurate potential is an external parameter, independent of the phase of the ultracold atomic gas.

We further remark that interesting dynamics could be observed for density distributions such that  $\langle \hat{\delta}_{eff} \rangle = 0$ . In this regime, bistability due to the quantum motion is expected [13,14,24,36,37]. In this work we focus on the regime in which the system is far away from this situation, so that  $|\langle \hat{\delta}_{eff} \rangle| \gg \kappa$ .

## **III. RESULTS**

The Bose-Hubbard model of Eq. (16) is at the basis of the results of this section. We first consider a 1D lattice along the cavity axis by taking the aspect ratio  $\beta \gg 1$  in  $V_{cl}(\mathbf{r})$  and study the phase diagram by means of Monte Carlo simulation. We then analyze the situation where the atoms are ordered in a 2D optical lattice inside the cavity and determine the phase diagram using a mean-field approach. In both cases, the phase diagram is found by evaluating the ground state  $|\phi_G\rangle$  of the free energy, such that it fulfills the relation

$$\min\{\langle \phi_G | \hat{\mathcal{H}}_{BH} - \mu \hat{N} | \phi_G \rangle\},\tag{29}$$

where  $\mu$  is the chemical potential.

In the following the ratio between the typical interparticle distance  $d_0$  and the wavelength of the cavity is chosen to be  $d_0/\lambda = 83/157$ , which is close to 1/2. Although this ratio is a rational number, nevertheless, for sufficiently small system sizes (here about 300 sites per axis) the emerging dynamics simulates the incommensurate behavior. We remark that, for the chosen number of sites, the number of intracavity photons is 0 for pointlike scatterers when the density is uniform. We

refer the reader to Refs. [38–40], where the phase diagram of bichromatic potentials in systems of finite size is discussed.

The parameters of the cavity field, which determine the coefficients of the Bose-Hubbard Hamiltonian in Eq. (16), are extracted from the experimental values  $g_0/2\pi = 14.1$  MHz,  $\kappa/2\pi = 1.3$  MHz, and  $\gamma/2\pi = 3$  MHz for <sup>87</sup>Rb atoms [7,14]. From these values, after fixing the size of the lattice we get  $u_0$  and the range of parameters within which we vary the rescaled pump strength  $s_0$ . Finally, the on-site interaction in the 1D case is  $U/\hbar \sim 50$  Hz ( $U_{11}/\hbar = 6.4 \times 10^{-6}$  Hz m) and has been taken from Ref. [41]. For the 2D optical lattice,  $U/\hbar$  varies between 1 and 3 kHz ( $U_{11}/\hbar = 5.5 \times 10^{-11}$  Hz m<sup>2</sup>) (see Ref. [42]). A detailed discussion on the validity of Eq. (16) for this choice of parameters is reported in Sec. IV.

# A. One-dimensional lattice

We focus here on atoms confined in the lowest band of a 1D lattice along the cavity axis. For this geometry the first term on the r.h.s. of Eq. (21) is a constant energy shift along the cavity axis and can be reabsorbed in the chemical potential; that is,  $\mu \rightarrow \mu - \epsilon^{(0)} - V_1 J_0$ . The 1D Hamiltonian can thus be written as

$$\hat{\mathcal{H}}_{\rm BH}^{\rm (1D)} = -\sum_{i} t \, (\hat{b}_{i}^{\dagger} \hat{b}_{i+1} + \hat{b}_{i+1}^{\dagger} \hat{b}_{i}) + \frac{U}{2} \sum_{i} \hat{n}_{i} (\hat{n}_{i} - 1) \\ + \frac{\hbar s_{0}^{2}}{\hat{\delta}_{\rm eff}^{2} + \kappa^{2}} K \, \hat{\Phi}^{2} \hat{\delta}_{\rm eff},$$
(30)

where *i* labels the lattice site along the lattice and  $J_0$  is the value of integral (22) at the considered string. Here, the on-site energy term depends on the sites only through cavity QED effects.

## 1. Tunneling coefficient $t \rightarrow 0$

We first analyze the case in which the tunneling  $t \rightarrow 0$ , where the atoms are classical pointlike particles localized at the minima of the external potential. We determine the mean density  $\bar{n} = \sum_{i=1}^{K} \langle \hat{n}_i \rangle / K$  as a function of the chemical potential  $\mu$  and evaluated over the ground state, which is found by diagonalizing Hamiltonian (30) after setting t = 0 [43]. The  $\mu$  dependency of the density is shown in Fig. 2 for different values of the laser-cavity detuning  $\delta_c = \omega_L - \omega_c$ . The derivative of the curve gives the compressibility  $\chi = \partial \bar{n} / \partial \mu$ . The two curves in Fig. 2 correspond to two behaviors that are determined by the sign of the coefficient  $C = \langle \hat{\delta}_{eff} \rangle$  in Eq. (21). For the parameters we choose this sign is controlled by the sign of the detuning  $\delta_c$ , Eq. (6), namely, by whether the laser frequency is tuned to the red or to the blue of the cavity frequency (the parameter choice is discussed in Sec. IV). When  $\delta_c > 0$ , for a finite intracavity photon number the cavityinduced interaction energy is positive: The configurations minimizing the energy are thus the ones for which  $\langle \hat{n}_{cav} \rangle = 0$ , for which Hamiltonian (30) reduces to the Bose-Hubbard model for atoms in a periodic potential.

For  $\delta_c < 0$ , on the other hand, the cavity-induced interaction energy is negative: In this case an arrangement of the atoms that maximizes the intracavity field is energetically favorable. Concomitantly the incompressible phase at  $\overline{n} = 1$  shrinks, while for fractional densities the compressibility becomes



FIG. 2. (Color online) Mean density  $\bar{n}$  as a function of the chemical  $\mu$  (in units of U) at t = 0 in a 1D lattice. Curves were obtained by an exact diagonalization of Hamiltonian (30) for  $\delta_c = 5\kappa$  (dashed line) and  $\delta_c = -5\kappa$  (solid line), both for K = 100. Other parameters are  $s_0 = 0.006\kappa$  (with  $\kappa = 2\pi \times 1.3$  MHz),  $u_0 = 0.8\kappa$ , and  $U/\hbar =$ 50 Hz. Here, the chemical potential is reported without the constant shift, i.e.,  $\mu \rightarrow \mu - \epsilon^{(0)} - V_1 J_0$ . The dash-dotted line was evaluated for the same parameters as the solid line, except with K = 200. It shows that the results remain invariant as the system size is scaled up.

nonzero and the intracavity field is significantly different from 0. For incommensurate densities the quantum ground state is twofold degenerate. Figure 3 displays the two corresponding density profiles (i.e., the local boson occupation numbers  $n_i$ as a function of the lattice site index i) for the case  $\delta_c < 0$ and  $\mu = 0$ , for which  $\bar{n} < 1$ . One configuration corresponds to particle occupation,  $n_i = 1$ , at sites with  $Z_0^{(i,j)} > 0$  (hence  $\Phi > 0$ ) and  $n_i = 0$  for the other sites; the other configuration, to particle occupation at sites with  $Z_0^{(i,j)} < 0$  (hence  $\Phi < 0$ ). The two configurations correspond to two phases of the cavity field which differ by  $\pi$ . This behavior is analogous to that encountered in the self-organization of ultracold atoms in optical potentials [6,44]. Nevertheless, it must be noted that, whereas in the system of Ref. [44] the atomic patterns are periodic and maximize scattering into the resonator, here scattering into the cavity is maximized by aperiodic density distributions.

Clearly, even in the presence of finite intracavity fields, the mean value of the amplitude vanishes because of this



FIG. 3. (Color online) Boson occupation number,  $n_i$ , as a function of the site *i* for the two distributions corresponding to the two ground states at  $\delta_c = -5\kappa$  and  $\mu = 0$ . Other parameters are the same as in the caption of Fig. 2. Filled bars correspond to  $\langle \hat{n}_i \rangle = 1$ ; white bars, to  $\langle \hat{n}_i \rangle = 0$ .



FIG. 4. (Color online) Mean density  $\bar{n}$  as a function of  $\mu$  (in units of U) for a 1D lattice of K = 100 sites for t = 0,  $\delta_c = -5\kappa$ ,  $u_0 = 0.8\kappa$ ,  $U/\hbar = 50$  Hz (with  $\kappa/2\pi = 1.3$  MHz), while the values of  $s_0$  are reported in the legend. (a) Curves were evaluated by diagonalizing Eq. (30) after setting  $\langle \hat{\Phi} \rangle = 1/4$  (i.e., by artificially removing cavity backaction). (b) Curves were found for the corresponding parameters by diagonalizing the full quantum model of Eq. (30). Other parameters are as described in the caption to Fig. 2.

degeneracy. Therefore, when analyzing the intracavity-field amplitude we plot the mean value of operator  $|\hat{\Phi}|$ . In the rest of this article  $\langle \hat{\Phi} \rangle \equiv \langle |\hat{\Phi}| \rangle$  and can be either 0 or a positive real number.

It is interesting to compare the results for our system with the predictions for a 1D bichromatic lattice with incommensurate wavelengths [38-40]. For this purpose we substitute the operator  $\hat{\Phi}$  in Eq. (30) with a scalar  $\hat{\Phi} \rightarrow 1/4$ . This choice is made in order to obtain similar curves at commensurate densities  $\bar{n} = 0, 1, 2$  for  $s_0 = 0.004\kappa$ . Figure 4(a) displays the resulting density as a function of the chemical potential for different strengths of the cavity field and  $\delta_c < 0$ . We observe that, by increasing  $s_0$  in the model where  $\hat{\Phi}$  is a scalar, the parameter regions for which the particle density is constant, and hence the gas is incompressible, rapidly shrink [45]. This trend is significantly slower for the case in which cavity backaction is taken into account, as shown in Fig. 4(b). In addition, in the presence of cavity backaction, discontinuities in the values of the compressibility are encountered and seem to correspond to the first-order phase transition [46]. This



FIG. 5. (Color online) (a) Mean density  $\bar{n}$  and (b) expectation value  $\langle \hat{\Phi} \rangle$  versus the chemical potential  $\mu$  (in units of U) for a 1D lattice at different tunneling values, t/U = 0.014, 0.053, 0.096, 0.216. Other parameters are the same as for the black line at  $s_0 = 0.008\kappa$  in Fig. 4(b). Curves were evaluated by means of a QMC program described in Appendix B. Dotted vertical lines indicate the values of  $\mu$  in Fig. 6.

behavior qualitatively differs from that encountered when artificially removing the effect of the cavity, as shown in Fig. 4(a). For the largest value of the laser intensity considered here,  $s_0 = 0.008\kappa$ , the incompressible phases disappear.

### 2. Phase diagram for t > 0

In the following we discuss our results for t > 0, which we obtained with a QMC approach [47,48], whose details are reported in Appendix B. Figure 5(a) displays the averaged density versus chemical potential for  $s_0/\kappa = 0.008$  and increasing values of the tunneling rate. For  $t \to 0$  one recovers the black curve in Fig. 4(b), while as t grows the curve is increasingly shifted towards negative values of  $\mu$  and tends to a more smooth curve at larger values of  $\mu$ . The discontinuities in the mean density and in the cavity-field amplitude observable in Fig. 5 lead to a steplike dependency of the compressibility from  $\mu$ . The three vertical bars for t = 0.096U indicate the three values of  $\mu/U$  which we choose for plotting the density profile,  $\langle n_i \rangle$  vs. *i*, in Fig. 6. Here, we observe that as  $\mu$  is increased the amplitude of the density oscillations increases. The appearance of clusters where the density has periodicity  $\lambda_0 = 2d_0$  is due to the fact that  $\lambda \sim 2d_0$ : These oscillations locally maximize the value of  $\langle \hat{\Phi} \rangle$ . Since the ratio  $\lambda/d_0$  is incommensurate (for the system size we consider), this pattern can only exist locally: The size of the clusters is in fact limited by the beating between the two spatial periodicities. In particular, after a number of sites of the order of the length scale of the beating signal, the density fluctuations increase and allow the atomic distribution to reorganize in the external potential. In this way, the fields emitted by the atoms add up coherently and the intracavity field is maximized. In all cases considered the on-site energies exceeds the on-site repulsion.

Figures 7(a) and 7(b) display  $\bar{n}$  and  $\langle \hat{\Phi} \rangle$ , which is proportional to the cavity-field amplitude, as a function of  $\mu$ . Curves are evaluated at t = 0.053U and for two different values of  $s_0$ , such that the on-site energy is typically smaller than the on-site repulsion. The case corresponding to the typical Bose-Hubbard model, which is found here by setting  $s_0 = 0$  (i.e., the pump laser is off), is reported for comparison. In the presence of a laser incompressible phases are still found. For the corresponding values of the chemical potential the cavity field vanishes. We observe, in addition, jumps in the density between commensurate values of  $\bar{n}$  for which the intracavity photon number is different from 0. Figure 7(d)reports the Fourier transform of the pseudocurrent-current correlation function  $J(\omega)$  [47,48] for three points in the phase diagram, which are indicated by the arrows in Fig. 7(c)(details of the procedure are reported in Appendix B). The SF density is obtained by the extrapolated value at zero frequency,  $\omega = 0$ . In the whole parameter region where the cavity field is different from 0, we observe that the SF density vanishes. This behavior, together with the nonvanishing compressibility, is characteristic of a BG phase. Outside this region the gas is SF.

The density profile,  $\langle n_i \rangle$  versus *i*, is shown in Fig. 8 for the three values of  $\mu$  indicated in Fig. 7(c). In the left plot, corresponding to the vanishing SF fraction, we observe a density modulation and thus localized density fluctuations. These become less localized for  $\mu = 0.04$ , while in the SF region, where the number of photons is 0, the density is uniform along the lattice.

The phase diagram is extrapolated by tracking the behavior of the density  $\bar{n}$  versus the chemical potential for different tunneling values. Figure 9 displays the resulting phase diagram in the  $\mu$ -t parameter plane. Gray regions indicate the MI states at densities  $\bar{n} = 0, 1, 2$ ; blue regions, a compressible phase with vanishing SF density, where the number of intracavity photons is large, while outside these shaded regions the phase is SF. The effect of cavity backaction is evident at low tunneling, where  $\langle \hat{\Phi} \rangle > 0$ : Here the size of the MI regions is reduced and one observes a direct transition between the MI and the BG phases. At larger tunneling a direct MI-SF transition occurs and the MI-SF phase boundary merges with the one found for  $s_0 = 0$ : In fact, for larger quantum fluctuations  $\langle \hat{\Phi} \rangle \rightarrow 0$  in the thermodynamic limit. This feature is strikingly different from the situation in which the incommensurate potential is classical [38–40], where the MI lobes shrink at all values of t with respect to the pure case. Before we conclude this section, some remarks regarding the determination of the phase diagram must be made. In fact, we have used the grand-canonical ensemble to obtain the phase diagram in the presence of cavity backaction. In the absence of cavity backaction ( $\Phi \rightarrow 0$ ) we have used the canonical approach for QMC simulation, which allows us to accurately determine the transition borders.

### **B.** Two-dimensional lattice

We now analyze the phase diagram of a 2D lattice of which one axis coincides with the cavity axis, while in the perpendicular direction the atoms are pumped by the standing-wave laser, which is quasiresonant with the cavity field. In this situation, hence, the site-dependent term proportional to the laser intensity  $(V_1)$  in Eq. (21) is relevant. The presence of this classical field, in fact, significantly affects the phase diagram even in the absence of the cavity, since its wavelength is taken



FIG. 6. (Color online) Upper row: On-site density distribution  $\langle \hat{n}_i \rangle$  and local density fluctuations  $\langle \hat{n}_i^2 \rangle - \langle \hat{n}_i \rangle^2$  as a function of the site *i*. The line connecting the points serves as a guide for the eyes. Lower row: On-site energy due to the cavity field,  $\delta \epsilon_i$  (in units of *U*). Curves were evaluated for the parameters of the curve in Fig. 5 with t = 0.096U and  $s_0 = 0.008\kappa$ . Plots correspond to  $\mu/U = 0.2, 0.7, \text{ and } 1.2$  (from left to right).

to be incommensurate with the periodicity of the confining optical lattice.

Before we discuss the results, some consideration of the parameters is in order. For the parameters we take that the effect of the classical incommensurate potential proportional to  $V_1$  dominates over the cavity incommensurate field in determining the value of the on-site energy, Eq. (21). In particular, the sign of the coefficient  $V_1$  is determined by the detuning  $\Delta_a$ . The size of the lattice is fixed to vary about the value  $K \sim 300 \times 300$ , then the expectation value of operator  $\hat{\delta}_{\text{eff}}$  in Eq. (23) is such that it can be approximated by  $\hat{\delta}_{\text{eff}} \sim -u_0 \sum_{i,j} Y_0^{(i,j)} \hat{n}_{i,j}/K$ . This property shows that the sign of the cavity-induced potential in the Bose-Hubbard Hamiltonian, Eq. (28), is controlled by the sign of  $u_0$  and, thus, of the detuning  $\Delta_a$  between atom and pump. A simple check of the sign of the coefficients in Eq. (28) shows that the formation of finite intracavity potentials is energetically favored when  $\Delta_a > 0$ .

We first analyze the behavior of the mean density as a function of the chemical potential for  $t \rightarrow 0$  for opposite signs of  $\Delta_a$ , which is found by determining the ground state of the 2D Hamiltonian in Eq. (28) after setting the tunneling coefficient t = 0. The results are displayed in Fig. 10. For the set of

parameters considered we observe the appearance of incompressible phases. To a very good approximation they are in the interval of values determined by the classical incommensurate potential  $V_1$ , which takes either positive or negative values depending on whether  $\Delta_a$  is positive or negative. For commensurate density  $\bar{n} = 1$  and  $\Delta_a < 0$ , for instance, an incompressible phase is found in the interval  $0 \leq 1$  $\mu \leq \mu_1 < U$ , where  $\mu_1$  depends on  $V_1$ . For  $\Delta_a > 0$ , instead, the incompressible phase is in the interval  $0 < \mu_1 \leq \mu \leq 1$ . Differently from the 1D case, the incommensurate phase shrinks only on one side due to the effect of the classical pump (while the cavity potential is a small correction). The dominant effect of the classical field is also visible when analyzing the curve in the parameter regime where the phase is compressible: The inset in Fig. 10 shows a zoom of the curve for  $\Delta_a > 0$ , which exhibits various discontinuities in the compressibility. The finite compressibility is mostly due to the classical field. The jump of the density at  $\mu'$  (with  $-0.05 < \mu' < 0$ ) corresponds to the region in which an intracavity potential is built and is thus due to cavity backaction. Note that this discontinuity is observed at a shifted value of  $\mu$  when  $\Delta_a < 0$ .

We now determine the behavior at finite *t* for the 2D lattice taking  $\Delta_a > 0$  by means of a local mean-field calculation.



FIG. 7. (Color online) Results of QMC simulations for a 1D lattice with 74 sites and t = 0.053 with periodic boundary conditions. (a) Mean density  $\bar{n}$  and (b) modulus of the mean intracavity-field amplitude  $\langle \hat{\Phi} \rangle$  versus  $\mu$  (in units of U) for  $s_0 = 0.003\kappa$  (triangles), for  $s_0 = 0.004\kappa$  (circles), and in the absence of the pump laser  $s_0 = 0$  (squares). (c) Zoom of mean density in the region of parameters with  $-0.18 \leq \mu \leq 0.18$ . (d) Fourier transform of the pseudocurrent-current correlation function  $\tilde{J}(\omega)$  for the values of  $\mu/U$  indicated by the arrows in (c) for  $s_0 = 0.003\kappa$ . Simulation parameters used are L = 128 and  $\Delta \tau = 1$ . Lines show cubic interpolations of the data. The extrapolated value at zero frequency is the estimation of the SF density. Other parameters are the same as in Fig. 5.

This is performed by setting  $\hat{b}_{i,j} = \psi_{i,j} + \delta \hat{b}_{i,j}$ , where  $\psi_{i,j} = \langle \hat{b}_{i,j} \rangle$  is a scalar giving the local SF order parameter and  $\delta \hat{b}_{i,j}$  are the fluctuations with zero mean value. The new form is substituted in Eq. (16) and the second-order fluctuations of the hopping term, namely, the terms  $\delta \hat{b}_{i,j} \delta \hat{b}_{i',j'}$ , are discarded [49]. The resulting Bose-Hubbard Hamiltonian in the mean-field approximation takes the form  $\hat{\mathcal{H}}_{BH}^{(MF)} = \sum_{i,j} \hat{\mathcal{H}}_{i,j}$ , where

$$\hat{\mathcal{H}}_{i,j} = -t\eta_{i,j} \left( \hat{b}_{i,j}^{\dagger} - \frac{\psi_{i,j}^{*}}{2} \right) + \text{H.c.} + \frac{U}{2} \hat{n}_{i,j} (\hat{n}_{i,j} - 1) \\ + \hat{\epsilon}_{i,j} \hat{n}_{i,j},$$
(31)

and  $\eta_{i,j} = \psi_{i+1,j} + \psi_{i-1,j} + \psi_{i,j+1} + \psi_{i,j-1}$  is the sum of the local SF parameters of the neighboring sites. We remark that cavity backaction makes Hamiltonian  $\hat{\mathcal{H}}_{i,j}$  in (31) nonlocal in the density, since it depends on the collective operator  $\hat{\Phi}$  appearing in  $\hat{\epsilon}_{i,j}$ . The local SF order parameters  $\psi_{i,j}$  are found by solving the coupled set of self-consistency equations  $\psi_{i,j} = \langle \phi_G^{(\mathrm{MF})} | \hat{b}_{i,j} | \phi_G^{(\mathrm{MF})} \rangle$ , where  $| \phi_G^{(\mathrm{MF})} \rangle = \bigotimes_{i,j=1}^K | \phi_{i,j} \rangle$  is the ground state in the mean-field approximation. It is thus the direct product of the single-site states  $| \phi_{i,j} \rangle$ , defined as

$$|\phi_{i,j}\rangle = \sum_{n=0}^{\infty} \alpha_n^{(i,j)} |n\rangle_{i,j}, \qquad (32)$$

in which  $|n\rangle_{i,j}$  is the state of *n* bosons at a lattice site with  $(x_i, z_j)$ , and  $\sum_{i,j} |\alpha_n^{(i,j)}|^2 = 1$ . In our numerical implementation the evaluation of the ground state is repeated till the averaged SF order parameter  $\psi = \sum_{i,j} \psi_{i,j}/K$  converges up to a tolerance of 0.005. The recursive calculation of the ground states of the self-consistent Hamiltonian  $\hat{\mathcal{H}}_{BH}^{(MF)}$  is terminated once the value of  $\bar{n}$  converges with an accuracy of  $2 \times 10^{-4}$ .

Figure 11 displays the mean density as a function of the chemical potential for the same parameters as the solid curve in Fig. 10 but for t = 0.01U. The zoom-in on the region of parameters where the compressibility is different from 0 shows that also at finite t the curve is discontinuous. The jumps indicate the interval of values in which there is an intracavity field (see crosses). The inset displays the corresponding curve when the pump is far detuned from the cavity field: The compressibility does not present jumps in the compressible phase and the mean intracavity field is at least three orders of magnitude smaller.

Figure 12(a) displays the mean SF order parameter in the  $\mu$ -*t* plane and for density  $\bar{n} \leq 1$ . Here, the dotted lines identify the regions where the order parameter takes values below 0.02. The solid curve indicates where the gap in the spectrum is different from 0, corresponding to vanishing density fluctuations  $\Delta \rho = (\bar{n^2} - \bar{n}^2)^{1/2}$ , where  $\bar{n} = \sum_{i,j} \langle \hat{n}_{i,j} \rangle / K$ and  $\bar{n^2} = \sum_{i,j} \langle \hat{n}_{i,j}^2 \rangle / K$  (the threshold is set at 0.02). For comparison, Fig. 12(b) displays the corresponding diagram when the cavity is pumped far off-resonance, so that the effect of cavity backaction is very small and practically negligible. We note that the curve delimiting the MI phase has a very similar behavior in the presence and in the absence of cavity backaction, showing that for the parameters considered the existence of incompressible phases is determined by the transverse optical lattice. The behavior of the compressible



FIG. 8. (Color online) Upper row: On-site density distribution  $\langle \hat{n}_i \rangle$  and local density fluctuation  $\langle \hat{n}_i^2 \rangle - \langle \hat{n}_i \rangle^2$  as a function of the site *i*. The line connecting the points serves as a guide for the eyes. Lower row: Mean on-site energy  $\langle \delta \hat{\epsilon}_i \rangle$  (in units of *U*). Curves were evaluated for the parameters of the (red) curve with triangles in Figs. 7(a)–7(c) with t = 0.053U and  $s_0 = 0.003\kappa$ . Plots correspond to  $\mu/U = 0$ , 0.04, and 0.08 (from left to right).

phase with vanishing order parameter, which we here denote the BG phase, instead varies significantly in the presence of



FIG. 9. (Color online) The phase diagram obtained by QMC calculation for a 1D lattice with 74 sites for  $s_0 = 0.004\kappa$ . Other parameters are as in Fig. 7. Results are compared with the pure case (dotted curves).



FIG. 10. (Color online) Mean density  $\bar{n}$  versus  $\mu$  (in units of U) for a 2D lattice. The curve was evaluated by exact diagonalization of Hamiltonian (16) for t = 0,  $K = 70 \times 70$ , and  $\Delta_a < 0$  (dashed line) and for t = 0,  $K = 70 \times 70$ , and  $\Delta_a > 0$  (solid line). Parameters are  $|\Delta_a| = 2\pi \times 58$  GHz,  $s_0 = 0.15\kappa$ ,  $\delta_c = -5\kappa$ ,  $u_0 = 237\kappa$  ( $\kappa = 2\pi \times 1.3$  MHz). Inset: Zoom of the curve at  $K = 70 \times 70$  and  $\Delta_a > 0$  in the compressible phase. The dashed-dotted line for  $K = 100 \times 100$  and  $\Delta_a > 0$  shows, compared with the solid line, that the qualitative behavior of the curves remains invariant as the system size is scaled up.



FIG. 11. (Color online) Mean density  $\bar{n}$  [upper (blue) line] and  $\langle \hat{\Phi} \rangle$  [lower (green) line with crosses] versus  $\mu$  (in units of U) for a 2D lattice. Curves were evaluated using the local mean field for t = 0.01U and  $K = 70 \times 70$ . Parameters are  $\Delta_a = 2\pi \times 58$  GHz,  $s_0 = 0.15\kappa$ ,  $\delta_c = -5\kappa$ ,  $u_0 = 237\kappa$  ( $\kappa = 2\pi \times 1.3$  MHz). Inset: Same curves, but for  $\delta_c = -300\kappa$ . Note that the maximum value of  $\langle \hat{\Phi} \rangle$  is almost five orders of magnitude smaller than for  $\delta_c = -5\kappa$ .

the cavity potential, as one can observe by comparing Figs. 12(a) and 12(b). We, finally, point out the region delimited by the dashed line, which appears only in Fig. 12(a): This indicates the parameters for which the mean value of  $\hat{\Phi}$  is at least two orders of magnitude larger than outside. In this region there is an intracavity field, which is due to coherent scattering by the atoms.

The typical onsite density encountered in this parameter region, in particular, for the parameters indicated by the white square in Fig. 12(a), is shown in Fig. 12(c). We compare it with the case without cavity backaction: the density corresponding to the white square in Fig. 12(b) is displayed in Fig. 12(d). Without cavity backaction one observes dark stripes along the vertical direction at which the density is minimum. The stripes are almost regularly distributed and are due to the classical incommensurate potential along the x axis. When cavity backaction becomes relevant, an incommensurate potential also appears along the z direction. This intracavity potential is associated with the appearance of clusters within which the density exhibits a checkerboard distribution, as shown in Fig. 12(c). These clusters are the 2D analogy of the density-wave-like behavior observed in one dimension: they maximize scattering into the cavity field and their size is determined by the length due to the beating between the lattice wavelength and the incommensurate cavity potential.

Since a finite intracavity field is associated with certain atomic density distributions and, vice versa, such distributions are due to the backaction of the cavity field, the signal at the cavity output contains the information on the quantum ground state of the system and permits us to monitor its properties. This situation is quite different from the one encountered when light is used to measure the state of a quantum gas [50,51]: There, the mechanical effects of the scattered photons heat the atom and significantly perturb the state. In our case, instead, the mechanical effects of the cavity photons trap the atoms in the BG phase. Cavity losses do not significantly perturb the quantum state of the atoms for the parameter



FIG. 12. (Color online) (a,b) Order parameters in the  $\mu$ -t plane (in units of U) obtained by the mean-field calculation for a 70 lattice with periodic boundary conditions. Dotted lines separate the region with vanishing order parameters, while the solid line identifies the border for the incompressible MI state at density  $\bar{n}$ . Regions with finite compressibility and vanishing order parameters correspond to BG phases. The dashed line separates the region where the photon number is two orders of magnitude larger than outside. Parameters are  $s_0 = 0.15\kappa$ ,  $u_0 = 237\kappa$ ,  $\Delta_a = 2\pi \times 58$  GHz, whereas (a)  $\delta_c = -5\kappa$ and (b)  $\delta_c = -300\kappa$ . In the latter case the effect of the cavity potential is expected to be small. Local densities  $\langle \hat{n}_{i,j} \rangle$  of the phase diagram at  $\mu = 0.1U$  and  $t = 0.01\kappa$  are shown (c) for  $\delta_c = -5\kappa$  and  $\bar{n} = 0.57$ [white square in (a)] and (d) for  $\delta_c = -300\kappa$  and  $\bar{n} = 0.47$  [white square in (b)].

regimes we choose, in which photon number fluctuations can be neglected. We now analyze the signal at the cavity output as a function of the tunneling coefficient at a fixed, fractional density. The corresponding intensity is evaluated by calculating  $n_{out} = \langle \hat{a}_{out}^{\dagger} \hat{a}_{out} \rangle$ , where  $\hat{a}_{out}$  is given in Eq. (14). The intensity as a function of the tunneling coefficient *t* is reported in Fig. 13(a): Upon increasing the trapping potential depth  $V_0$  (decreasing the tunneling), a sudden increase in the intracavity photon number is observed. This corresponds to the



FIG. 13. (Color online) (a) Intensity at the cavity output,  $n_{out} = \langle a_{out}^{\dagger} a_{out} \rangle$ , as a function of *t* (in units of *U*) for the parameters in Fig. 12(a) and by fixing  $\bar{n} = 0.5$ . Here,  $n_{out}$  is in units of  $n_{out}^{(0)} = \kappa n_{cav}^{(max)}$ , where  $n_{cav}^{(max)} = s_0^2 K / (\delta_{eff}^2 + \kappa^2)$  is the maximum number of intracavity photons, obtained when all atoms scatter in phase into the cavity mode. The curve with circles (right *y* axis) gives the corresponding order parameter. (b) Contour plot of the local density distributions at point (I) in (a), where t = 0.034U,  $\mu = 0.106U$ ,  $\langle \hat{\Phi} \rangle = 0.136$ . (c) Local density distributions at point (II) in (a), where t = 0.039U,  $\mu = 0.122U$ , and  $\langle \hat{\Phi} \rangle \simeq 0$ . (d) Local density  $\langle \hat{n}_{i,j} \rangle$  as a function of the site numbers along *z* for lattice site 20 along *x*. The (blue) squares correspond to parameters in (b); (red) circles, to parameters in (c).

transition to density distributions according to checkerboard clusters, as Figs. 13(b)-13(d) show in detail. Before this sudden increase the density distribution is almost flat along the cavity axis: The atoms delocalize over the lattice sites and there is no coherent scattering of photons into the resonator.

# **IV. EXPERIMENTAL PARAMETERS**

The Bose-Hubbard Hamiltonian in Eq. (16) was derived by performing a series of approximations which have been discussed in detail in the previous section. In this section we show that existing experimental setups, like the ones in Refs. [7,14], allow observation of the phases predicted by Eq. (16). Moreover, we identify here the parameters which are then used in the numerical plots presented in Sec. III.

The parameters for the cavity field, which determine the coefficients of the Bose-Hubbard Hamiltonian in Eq. (16), are

extracted from the experimental values  $g_0/2\pi = 14.1$  MHz,  $\kappa/2\pi = 1.3$  MHz, and  $\gamma/2\pi = 3$  MHz for <sup>87</sup>Rb atoms [7,14]. The detuning between atoms and the cavity mode at wavelength  $\lambda = 780$  nm is about  $\Delta_a/2\pi = 58$  GHz. For these parameters  $U_0/\pi \approx 3.4$  kHz. The corresponding value of  $S_0$ depends on the Rabi frequency of the transverse laser. For instance, for  $\Omega/2\pi = 3.08$  MHz, then  $S_0/2\pi = 0.74$  kHz. An external optical lattice trapping the atoms such that the ratio  $d_0/\lambda \simeq 83/157$  is realized can be made by pumping a cavity mode at wavelength 737.7 nm. Other ratios can be considered as well, depending on the cavity setup and the atoms.

# 1. Parameters

We now check that these values are consistent with the approximations we made in deriving Eq. (16). For this purpose we must fix the number of sites, and thus the number of atoms N, since the total shift and the total scattering amplitude must be properly rescaled by N. Let K be the number of sites, such that for densities  $\bar{n} = 1$  the number of sites is equal to the number of atoms. For a 1D lattice with  $K \simeq 300$ sites one finds  $u_0/2\pi = U_0 K/2\pi \approx 1.02$  MHz and  $s_0/2\pi =$  $S_0\sqrt{K/2\pi} \approx 0.013$  kHz or, alternatively,  $u_0 \simeq 0.8\kappa$  and  $s_0 =$  $0.01\kappa$ . Other values are obtained by accordingly changing the Rabi frequency  $\Omega$ . We set  $|\delta_c| = 5\kappa$  and observe that for this value  $|\delta_c - u_0| \approx |\delta_c|$ . We now check the order of magnitude of the coefficients of the Bose-Hubbard model for these parameters. Here,  $s_0^2 K |\delta_c| / (\delta_c^2 + \kappa^2) \simeq 0.0045 \kappa \simeq 2\pi \times 5.75$  kHz. For these parameters the on-site energy due to the cavity field exceeds the MI gap when  $\langle \hat{\Phi}^2 \rangle \ge 10^{-3}$ . For a 2D lattice with  $K = 300 \times 300$  sites, then  $u_0 = U_0 K \simeq 2\pi \times 308.5$  MHz or, alternatively,  $u_0 = 237\kappa$ . For  $\Omega/2\pi = 2.6$  MHz, for instance, then  $s_0 = S_0 \sqrt{K} \simeq 0.15 \kappa$  and  $V_1 = \Omega^2 / \Delta_a \simeq 0.78$  kHz. For these parameters, typical values of the density distribution give  $|\delta_{\rm eff}| \simeq 88\kappa \gg \kappa$ , such that  $s_0^2 K \delta_{\rm eff} / (\delta_{\rm eff}^2 + \kappa^2) = 23\kappa$ . Here, already for  $\langle \hat{\Phi}^2 \rangle \ge 10^{-5}$  cavity backaction has a significant effect.

#### 2. Spontaneous emission rate

Both in the 1D and in the 2D case, the parameters give a very small occupation of the excited state: The probability that an atom is excited scales with  $P_{\text{exc}} \sim K \max(g_0^2 n_{\text{cav}}, \Omega^2) / \Delta_a^2$ , where  $n_{\text{cav}}$  is the mean intracavity photon number. For the parameters considered  $P_{\text{exc}} \lesssim 10^{-3} \ll$ 1. The corresponding spontaneous emission rate following an excitation due to the cavity field reads  $\gamma'_c = \gamma g_0^2 n_{\text{cav}} / \Delta_a^2 \simeq 2\pi \times 0.17 n_{\text{cav}}$  Hz, while spontaneous decay after an excitation due to the transverse laser scales with  $\gamma'_L = \gamma \Omega^2 / \Delta_a^2 \simeq 2\pi \times 0.08$  Hz.

### 3. Adiabatic elimination of the cavity mode

We now check the conditions for adiabatic elimination of the cavity mode for a 1D lattice with 300 sites. The adiabatic elimination of the cavity field from the atomic equations of motion requires that one neglect the coupling with the atoms over the time scale over which the cavity reaches a "stationary" value, which depends on the instantaneous density distribution. This introduces a time scale  $\Delta t = 1/|\delta_c + i\kappa|$ , for which the inequalities shall be fulfilled,  $S_0 \sqrt{n_{cav}} \Delta t \ll 1$  and  $U_0 n_{\text{cav}} \Delta t \ll 1$ . These relations are satisfied for the typical numbers of intracavity photons we encounter. In addition, since the atoms must move slowly over this time scale, their kinetic energy (temperature) must be such that  $k_B T \ll \hbar/\Delta t$ , where  $k_B$  is the Boltzmann constant. The latter condition is satisfied for atoms at  $T \simeq 1 \,\mu\text{K}$ , which is achieved in Bose-Einstein condensates.

## 4. Neglecting quantum noise

Quantum noise in Eq. (13) can be neglected when  $Ks_0^2\langle \hat{\Phi}^2 \rangle \gg \kappa^2$ , which corresponds to a depth of the lattice created by photon scattering that is much larger than single-photon fluctuations. For the parameters discussed here one needs a lattice with sites  $K \gg 10^4$ , which corresponds to the 2D situation we analyze. The 1D lattice we consider numerically contains  $K \simeq 100$  sites, however, the scaling of the behavior with the number of particles shows that our predictions remain valid for larger numbers, where one can discard fluctuations in the intracavity photon number.

# 5. Single-band approximation

In the derivation of the Bose-Hubbard Hamiltonian in Eq. (16) we have performed an expansion of the field operator, (15), into Wannier functions of the lowest band of the external lattice. Discarding the higher bands is correct as long as the energy gap between the lowest and the first excited Bloch band  $\Delta E = \sqrt{4E_R|V_0|}$  is much larger than the interaction energy  $V_{\text{int}}$ , which here is  $V_{\text{int}} = U + \max |\delta \epsilon_{i,j}|$  between the particles [52], where  $E_R = \hbar^2 k_0^2 / 2m$  is the recoil energy. Figure 14 displays the ratio  $\Delta E / V_{\text{int}}$  in the limit of zero tunneling  $t \rightarrow 0$ . We have checked that this ratio remains lower than unity for the parameters chosen here. Increasing the laser amplitude  $\Omega$ , i.e., increasing  $s_0$  (and hence  $\delta \hat{\epsilon}$ ) leads to an increase in  $V_{\text{int}}$  and thus forces one to take into account higher Bloch bands.



FIG. 14. (Color online) Ratio of the energy gap between the two Bloch bands,  $\Delta E = \sqrt{4E_R|V_0|}$ , and the interaction energy,  $V_{int} = U + \max |\delta \epsilon_{i,j}|$ , as a function of the chemical potential  $\mu$  (in units of U) and at zero tunneling. The single-band approximation is valid,  $\Delta E / V_{int} \gg 1$ . The (green) curve with crosses shows the maximum values of  $\langle \delta \hat{\epsilon}_{i,j} \rangle$  at the corresponding values of  $\mu / U$ . Parameters are the same as in Fig. 12(a).

### 6. External harmonic trap

In our treatment we have assumed that the atoms are confined by an external optical lattice. In several experimental situations [14], however, the atoms are additionally confined by a harmonic trap potential. This gives rise to a smooth position-dependent on-site energy, which will act as the bias field, removing the degeneracy between the two ground-state configurations we identify. Moreover, it can lead to the observation of the characteristic wedding-cake form [29,53]. The influence of cavity backaction on such structures shall be analyzed in future works.

## V. CONCLUSION AND OUTLOOK

Ultracold atoms confined in tight classical lattices and strongly coupled with a standing-wave cavity mode selforganize in order to maximize the number of intracavity photons. This self-organization takes place when the atoms are driven by a transverse laser field which is quasiresonant with the cavity mode and whose intensity exceeds a threshold value. In this paper we have studied the quantum ground state when the cavity mode has a wavelength which is incommensurate with the interparticle distance  $d_0$  due to the external lattice. We have shown that the atomic density rearranges in clusters, within which the atoms form density waves, then locally maximize, scattering into the cavity mode. The clusters have a mean size corresponding to the beating wavelength between the two overlapping fields and are phase locked with one another, so that the intracavity field is maximum. These quantum phases are often characterized by vanishing order parameter and finite compressibility, so that they share several analogies with a BG phase.

In our theoretical model, the atomic dynamics are described by a Bose-Hubbard-type Hamiltonian, where the effect of the cavity field enters by means of a nonlocal term, which depends on the density at all sites. This term is the cavitymediated potential, which depends on the atomic distribution. In particular, its sign is determined by the detunings between atoms and fields, which thus controls whether self-organized structures are energetically favorable. When the sign of the detuning is appropriately chosen, the cavity field gives rise to a long-range interaction between the atoms and to new phases, where the atomic densities self-organize in order to maximize the intracavity photon number. We remark that this system constitutes a setting where quantum fluctuations give rise to effects usually associated with disorder.

An attractive feature of the setup we consider is the possibility it offers to measure the state of matter by detecting the cavity light at the output in a nondestructive way. We have shown that the intensity of the light at the cavity output provides a signature of the formation of clusters. An open question is whether and how the quantum phase can be fully characterized by photodetection, thus providing an alternative route to other experimental methods [22,54–56]. In this context we mention that the spectrum of the scattered light can allow one to determine the quantum phase of atoms across the MI-SF phase transition [50,51] and give the fingerprint of a BG phase [57]. Reference [58] reports how to measure the condensate fraction by photodetection. These concepts shall be revisited

and further extended to this setup for the purpose of developing a full quantum state tomography of the self-organized state by measuring the light emitted by the resonator.

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# APPENDIX A: DERIVATION OF THE BOSE-HUBBARD HAMILTONIAN

In this Appendix we report the basic steps which lead to the derivation of the Bose-Hubbard Hamiltonian in Eq. (16). The steps follow methods we developed in Refs. [23,24], We first substitute the cavity-field operator, (13), after neglecting the quantum noise term, into the equation for the quantum-field operator in Eq. (9). Using the Wannier decomposition, we obtain the equations of motion for operators  $\hat{b}_{l,m}$ , which read

$$\dot{\hat{b}}_{l,m} = \frac{1}{i\hbar} [\hat{b}_{l,m}, \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_p] - i\hat{\mathcal{C}}_{l,m}, \qquad (A1)$$

where, for  $\beta = 0, 1$ ,

$$\hat{\mathcal{H}}_{0} = \frac{U}{2} \sum_{i,j} \hat{n}_{i,j} (\hat{n}_{i,j} - 1) + (E_0 + V_0 X_0) \hat{N} + (E_1 + V_0 X_1) \hat{B}$$
(A2)

is the Bose-Hubbard Hamiltonian in the absence of a cavity field and of a transverse laser, with  $E_s$  and  $X_s$  given in Eqs. (19), while U is defined in Eq. (17). Here,  $\hat{B} = \hat{B}^x + \hat{B}^z$ is the hopping term, where  $\hat{B}^x = \sum_{i,j} (\hat{b}_{i+1,j}^{\dagger} \hat{b}_{i,j} + \hat{b}_{i,j}^{\dagger} \hat{b}_{i+1,j})$ describes tunneling between neighboring sites of the lattice along x, and  $\hat{B}^z = \sum_{i,j} (\hat{b}_{i,j+1}^{\dagger} \hat{b}_{i,j} + \hat{b}_{i,j}^{\dagger} \hat{b}_{i,j+1})$  describes tunneling between neighboring sites of the lattice along z. The Hamiltonian  $\hat{\mathcal{H}}_p$  contains the terms due to the pumping laser propagating along the x direction and reads

$$\hat{\mathcal{H}}_p = V_1 \sum_{i,j} J_0^{(i,j)} \, \hat{n}_{i,j} + V_1 \sum_{i,j} J_1^{(i,j)} \hat{B}_{i,j}^x, \qquad (A3)$$

with  $V_1 = \hbar \Omega^2 / \Delta_a$ , while  $J_0^{(i,j)}$  is defined in Eq. (22) and

$$J_1^{(i,j)} = \int d^2 \mathbf{r} \, w_{i,j}(\mathbf{r}) \cos^2(k \, x) \, w_{i+1,j}(\mathbf{r}).$$

Finally, operator  $\hat{C}_{l,m}$  in Eq. (A1) is due to the coupling with the cavity field and reads

$$\hat{\mathcal{C}}_{l,m} = S_0 \left( \frac{S_0 \hat{\mathcal{Z}}}{\hat{D}^{\dagger}} \hat{\mathcal{P}}_{l,m} + \hat{\mathcal{P}}_{l,m} \frac{S_0 \hat{\mathcal{Z}}}{\hat{D}} \right) + U_0 \left( S_0^2 \frac{\hat{\mathcal{Z}}}{\hat{D}^{\dagger}} \hat{\mathcal{Q}}_{l,m} \frac{\hat{\mathcal{Z}}}{\hat{D}} \right),$$
(A4)

where we have introduced the operators  $\hat{D} = (\delta_c - U_0 \hat{\mathcal{Y}}) + i\kappa$ and

$$\begin{aligned} \hat{\mathcal{P}}_{l,m} &= [\hat{b}_{l,m}, \hat{\mathcal{Z}}] \\ &\approx Z_{0,0}^{(l,m)} \hat{b}_{l,m} + Z_{0,1}^{(l,m)} \hat{b}_{l,m+1} + Z_{1,0}^{(l,m)} \hat{b}_{l+1,m} \\ &+ Z_{1,0}^{(l-1,m)} \hat{b}_{l-1,m} + Z_{0,1}^{(l,m-1)} \hat{b}_{l,m-1}, \\ \hat{\mathcal{Q}}_{l,m} &= [\hat{b}_{l,m}, \hat{\mathcal{Y}}] \\ &\approx Y_{0}^{(l,m)} \hat{b}_{l,m} + Y_{1}^{(l,m)} \hat{b}_{l,m+1} + Y_{1}^{(l,m-1)} \hat{b}_{l,m-1}. \end{aligned}$$
(A5)

Operator  $\hat{C}_{l,m}$  cannot be generally written in the form of the commutator between  $\hat{b}_{l,m}$  and a Hermitian operator. However, in the thermodynamic limit we have chosen, operator (A4) can be cast in the form  $\hat{C}_{l,m} = [\hat{b}_{l,m}, \hat{\mathcal{H}}_{BH}^{(1)}]$  (for details see [24]), where the operator

$$\hat{\mathcal{H}}_{\rm BH}^{(1)} = \sum_{i,j} \left( \delta \hat{\epsilon}_{i,j} \hat{n}_{i,j} + \delta \hat{t}_{i,j}^x \hat{B}_{i,j}^x + \delta \hat{t}_{i,j}^z \hat{B}_{i,j}^z \right) \tag{A6}$$

is different from 0 when the pump laser is on,  $\Omega > 0$ . Due to the incommensurate wavelength of the laser and cavity mode with respect to the lattice spacing, the coefficients of the Hamiltonian are site dependent and read

$$\delta\hat{\epsilon}_{i,j} = V_1 J_0^{(i,j)} + \frac{\hbar s_0^2}{\hat{\delta}_{\text{eff}}^2 + \kappa^2} \hat{\Phi} \hat{\delta}_{\text{eff}} Z_{0,0}^{(i,j)}.$$
 (A7)

Here, the collective operator  $\hat{\Phi} = 1/K \sum_{i,j} Z_{0,0}^{(i,j)} \hat{n}_{i,j}$  appears in the site-dependent parameters. The site-dependent tunneling terms read

$$\delta \hat{t}_{i,j}^{x} = -2\hbar \frac{s_{0}^{2} \delta_{\text{eff}}}{\hat{\delta}_{\text{eff}}^{2} + \kappa^{2}} \hat{\Phi} Z_{1,0}^{(i,j)} - V_{1} J_{1}^{(i,j)},$$

$$\delta \hat{t}_{i,j}^{z} = -2 \frac{\hbar s_{0}^{2}}{\hat{\delta}_{\text{eff}}^{2} + \kappa^{2}} \hat{\Phi} \hat{\delta}_{\text{eff}} Z_{0,1}^{(i,j)}.$$
(A8)

In the regime of the parameters we consider (see Sec. IV) for which max  $|\langle \delta \hat{\epsilon}_{i,j} \rangle| \sim U$  and  $|V_0| \gg \max |\langle \delta \hat{\epsilon}_{i,j} \rangle|$  (hence the validity of a single-band approximation),  $|\delta t^x|$  and  $|\delta t^z|$  are at least eight orders of magnitude smaller than  $t^{(0)}$  and are therefore neglected. Thus in our model, only the coefficient  $\hat{\epsilon}_{i,j}$  can depend on the lattice sites in a relevant way.

# APPENDIX B: DETAILS OF THE QMC CALCULATION

For the convenience of the reader, first, we recapitulate the basics of the discrete imaginary time world-line algorithm [48] which we use to obtain the 1D results. Next, we describe how we treat the particular long-range term of our model numerically.

In order to estimate the equilibrium properties of the system, the partition function is decomposed at first by

$$Z = \mathrm{Tr}e^{-\beta\mathcal{H}_{\mathrm{BH}}} = \mathrm{Tr}(e^{-\Delta\tau\mathcal{H}_{\mathrm{BH}}})^{L}, \qquad (B1)$$

where  $\Delta \tau = \beta/L$ . In the 1D case, the Bose-Hubbard Hamiltonian can be written as a sum of pair Hamiltonians  $\mathcal{H}_{BH}^{1d} = \sum_{i=0}^{K-1} \mathcal{H}_{i,i+1}$ , with

$$\mathcal{H}_{i,i+1} = \frac{1}{4} U[\hat{n}_i(\hat{n}_i+1) + \hat{n}_{i+1}(\hat{n}_{i+1}+1)] - t(\hat{b}_i^{\dagger} \hat{b}_{i+1} + \hat{b}_{i+1}^{\dagger} \hat{b}_i).$$
(B2)

In the second step, the Hamiltonian is typically divided into a part of even site labels, which interact with their subsequent odd-labeled sites, and a complementary odd part, which contains the remaining interactions ( $\mathcal{H}_{BH}^{1d} = \mathcal{H}_{even} + \mathcal{H}_{odd}$ ):

$$\mathcal{H}_{\text{even}} = \sum_{i=0}^{K/2-1} \mathcal{H}_{2i,2i+1},$$
(B3)

$$\mathcal{H}_{\text{odd}} = \sum_{i=0}^{K/2-1} \mathcal{H}_{2i+1,2i+2}.$$
 (B4)

At this stage, the Suzuki-Trotter [59,60] formula can be applied:

$$Z \approx \text{Tr}(e^{-\Delta\tau \mathcal{H}_{\text{even}}} e^{-\Delta\tau \mathcal{H}_{\text{odd}}})^L, \tag{B5}$$

which involves an error of the order of  $O(\Delta \tau^3)$  [61]. Finally, 2*L* sets of occupation number states are inserted between each exponential leading to the effective 2D imaginary time path integral representation of the system:

$$Z \approx \sum_{\{n^l\}} \prod_{l=0}^{L-1} \langle n^{2l+2} | e^{-\Delta \tau \mathcal{H}_{\text{even}}} | n^{2l+1} \rangle \langle n^{2l+1} | e^{-\Delta \tau \mathcal{H}_{\text{odd}}} | n^{2l} \rangle,$$
(B6)

in which the bosons are described by world lines (Fig. 15). The system is now described by 2L matrix elements, which consist of easy calculable two-site problems. The Monte Carlo process enters now by sampling the world lines via local updates,



FIG. 15. Path integral representation of the system. The horizontal expansion displays the spatial dimension whereas the vertical slices represents the evolution in imaginary time. One valid configuration is described by a set of particle paths (world-lines) that obey periodic boundary conditions in spatial and temporal direction and particle conservation in each slice. World-lines can either exhibit a closed connection from bottom to top (dash line) with so-called winding number W = 0 or winded around the system [here with W = +1 (solid line)]. The shaded squares of the checkerboard pattern indicates the plaquettes, where  $\mathcal{H}_{i,i+1}$  acts and hence hopping can occur.

where the thermodynamical weights of only four plaquettes are involved, and optionally global updates, which are needed to insert and delete straight world lines in the system for the grand-canonical simulation [47,48].

The quantities, which are diagonal in the occupationnumber representation, like the density (B8) and the local density fluctuation (B9), can now estimated easily by averaging the occupation numbers n(i,l) over all slices after reaching equilibrium:

$$\langle \hat{n}_i \rangle = \frac{1}{2L} \sum_{l=0}^{2L-1} \langle n(i,l) \rangle, \tag{B7}$$

$$\bar{n} = \frac{1}{K} \sum_{i=0}^{K-1} \langle \hat{n}_i \rangle, \tag{B8}$$

$$\kappa_i = \langle \hat{n}_i^2 \rangle - \langle \hat{n}_i \rangle^2, \tag{B9}$$

where  $\langle \cdots \rangle$  denotes the Monte Carlo average. Characterizing the superfluidity is a bit more cumbersome. It has been discussed in Refs. [48,62] that the SF density is related to the mean square of the winding number  $\langle W^2 \rangle$  by

$$\rho_s = \frac{\langle W^2 \rangle}{2\beta t} K, \tag{B10}$$

whereas the winding number is defined as the number of world lines that are wound along the lattice due to the periodic boundary conditions (see Fig. 15). In order to determine  $\rho_s$ , one commonly defines the pseudocurrent, which counts the number of particles that moves to the right minus the number of particles moving to the left for every time slice l = [0, 2L - 1]:

$$j(l) = \frac{1}{2} \sum_{i=0}^{K-1} [n(i,l) - n(i+1,l)] - [n(i,l+1) - n(i+1,l+1)].$$
(B11)

The mean-square winding number can now computed via  $\langle W^2 \rangle = \frac{1}{K^2} \sum_{l,l'=0}^{2L-1} \langle j(l)j(l') \rangle$ . Due to the fact that the applied (local and global) Monte Carlo updates conserve the winding number at every step, *W* is technically restricted to 0. In order to determine  $\langle W^2 \rangle$  anyway, one computes the correlator  $J(l) = \langle j(l)j(0) \rangle$  during the simulation and its Fourier transform  $\tilde{J}(\omega_n) = \sum_l e^{i l\omega_n} J(l)$  afterwards. The value at 0 obeys

$$\tilde{J}(0) = \left\langle \sum_{l} j(l)j(0) \right\rangle = \frac{K^2}{2L} \langle W^2 \rangle, \qquad (B12)$$

which enables the determination of the SF density by means of Eqs. (B12), (B10), and  $\beta = \Delta \tau L$  via the extrapolation:

$$\rho_s = \lim_{\omega_n \to 0} \frac{\tilde{J}(\omega_n)}{t \,\Delta \tau \, K}.\tag{B13}$$

In our particular model, (30), the long-range interaction term

$$\hat{V} = \frac{\hbar s_0^2}{\hat{\delta}_{\text{eff}}^2 + \kappa^2} K \hat{\Phi}^2 \hat{\delta}_{\text{eff}}$$
(B14)

occurs and has to be treated additionally. We decided to distribute this term equally to both the even and the odd parts of the Hamiltonian, namely,  $\mathcal{H}_s = \hat{U}_s + \hat{T}_s + \hat{V}/2$ , where  $s = \{\text{even}, \text{odd}\}$ . The (symmetric) Trotter decomposition of the matrix element of slice *l* is then given by

$$\langle n^{l+1} | e^{-\Delta \tau \mathcal{H}_s} | n^l \rangle \approx \langle n^{l+1} | e^{-\frac{\Delta \tau}{4} \hat{V}} e^{-\frac{\Delta \tau}{2} \hat{U}_s}$$
$$\times (1 - \Delta \tau \hat{T}_s) e^{-\frac{\Delta \tau}{2} \hat{U}_s} e^{-\frac{\Delta \tau}{4} \hat{V}} | n^l \rangle.$$
(B15)

Since  $\hat{V}$  is diagonal in the occupation-number representation, one can trace the matrix element, (B15), back to the common case of the short-range Bose-Hubbard model:

$$\langle n^{l+1} | e^{-\Delta \tau \mathcal{H}_s} | n^l \rangle \approx e^{-\frac{\Delta \tau}{4} (V(\{n^{l+1}\}) + V(\{n^l\}))} \\ \times \prod_{\substack{i \text{ even} \\ (i \text{ odd})}} \langle n_i^{l+1} n_{i+1}^{l+1} | \mathcal{H}_{i,i+1} | n_i^l n_{i+1}^l \rangle.$$
 (B16)

Within the Monte Carlo sampling, the ratios of these matrix elements have to be evaluated efficiently. In the present model, one make use of the fact that the interaction is a function of only two accumulative quantities, which depends linearly on the occupation numbers:

$$\langle n|\hat{V}|n\rangle = V(\{n\}) = f\left(\frac{1}{K}\sum_{i}Z_{0}^{(i)}n_{i}, \frac{1}{K}\sum_{i}Y_{0}^{(i)}n_{i}\right),$$
(B17)

where the (nonlinear) function is

$$f(\Phi, \Psi) = \frac{\hbar s_0^2}{(\delta_c - u_0 \Psi)^2 + \kappa^2} K \Phi^2(\delta_c - u_0 \Psi).$$
(B18)

For the case of single-particle updates, each of these quantities can be evaluated in constant computer time, if one uses the auxillary variables  $\Phi = \frac{1}{K} \sum_{i} Z_0^{(i)} n_i$  and  $\Psi = \frac{1}{K} \sum_{i} Y_0^{(i)} n_i$ and only tracks the differences caused by the update. For an update, e.g.,  $|n_l, n_{l+1}\rangle \rightarrow |n'_l, n'_{l+1}\rangle = |n_l + 1, n_{l+1} - 1\rangle$ , one has to compute

$$\Phi' = \Phi + \left( Z_0^{(l)} - Z_0^{(l+1)} \right) / K, \tag{B19}$$

$$\Psi' = \Psi + \left(Y_0^{(l)} - Y_0^{(l+1)}\right) / K.$$
 (B20)

The desired matrix element  $\langle n' | \hat{V} | n' \rangle$  can now be calculated by applying the new auxillary variable in the function  $f(\Phi', \Psi')$ . The auxillary variable has to be allocated for each time slice separately.

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- [46] To analyze these jumps from the incompressible phase to fractional filling, we performed a canonical QMC simulation, in which the chemical potential is calculated by the difference between the internal energies  $\mu = (E(N + 1) E(N))K/U$  of two simulations with N and N + 1 particles. We found regions with negative compressibility (i.e., negative slope in the  $\bar{n}$ - $\mu$  plot). We then evaluated the grand potential  $E \bar{n}\mu/U$  calculated from the internal energy per site *E*, whose minimum is a criterion for the stability of the system state for temperature T = 0: We found that the region with negative compressibility of the simulations with the canonical ensemble are associated with meta-stable branches. In contrast, the grand-canonical simulation does follow the stable branch, which results in a kink of the grand potential, which is typical for a system undergoing a first-order phase transition.
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