Dynamical Phase Transitions and Instabilities in Open Atomic Many-Body Systems

Sebastian Diehl,1,2 Andrea Tomadin,2,3 Andrea Micheli,1,2 Rosario Fazio,3 and Peter Zoller1,2

1Institute for Theoretical Physics, University of Innsbruck, Technikerstr. 25, A-6020 Innsbruck, Austria
2Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, A-6020 Innsbruck, Austria
3NEST, Scuola Normale Superiore and Istituto Nanoscienze - CNR, Pisa, Italy

We discuss an open driven-dissipative many-body system, in which the competition of unitary Hamiltonian and dissipative Liouvillian dynamics leads to a nonequilibrium phase transition. It shares features of a quantum phase transition in that it is interaction driven, and of a classical phase transition, in that the ordered phase is continuously connected to a thermal state. Within a generalized Gutzwiller approach which includes the description of mixed state density matrices, we characterize the complete phase diagram and the critical behavior at the phase transition approached as a function of time. We find a novel fluctuation induced dynamical instability, which occurs at long wavelength as a consequence of a subtle dissipative renormalization effect on the speed of sound.

PACS numbers: 64.70.Tg,03.75.Kk,67.85.Hj

Experiments with cold atoms provide a unique setting to study nonequilibrium phenomena and dynamics, both in closed systems but also for (driven) open quantum dynamics. This relies on the ability to control the many-body dynamics and to prepare initial states far from the ground state. For closed systems we have seen a plethora of studies of quench dynamics [1][2], thermalization [3][4], and transport [5], and also dynamical studies of crossing in a finite time quantum critical points in the spirit of the Kibble-Zurek mechanism [6][7]. On the other hand, cold atom systems allow to engineer the coupling to an environment and the controlled realization of open driven-dissipative dynamics of many-body systems similarly to studies in quantum optics and mesoscopic physics [8][9].

For a many-body system in thermodynamic equilibrium the competition of two noncommuting parts of a microscopic Hamiltonian \( H = H_1 + gH_2 \) manifests itself as a quantum phase transition (QPT), if the ground states for \( g \ll g_c \) and \( g \gg g_c \) have different symmetries [10]. For temperature \( T = 0 \) the critical value \( g_c \) then separates two distinct quantum phases, while for finite temperature this defines a quantum critical region around \( g_c \) in a \( T \) vs. \( g \) phase diagram. A seminal example in the context of cold atoms in optical lattices is the superfluid–Mott insulator transition in the Bose-Hubbard (BH) model, with Hamiltonian

\[
H = -J \sum_{\ell,\ell'} \hat{b}_\ell^\dagger \hat{b}_{\ell'} - \mu \sum_\ell \hat{n}_\ell + \frac{1}{2} U \sum_\ell \hat{n}_\ell (\hat{n}_\ell - 1),
\]

with \( b_\ell \) bosonic operators annihilating a particle on site \( \ell \), \( \hat{n}_\ell = \hat{b}_\ell^\dagger \hat{b}_\ell \) number operators, \( J \) the hopping amplitude, and \( U \) the onsite interaction strength. For a given chemical potential \( \mu \), chosen to fix a mean particle density \( n \), the critical coupling strength \( g_c = (U/J_2)_{c} \) separates a superfluid \( J_2 \gg U \) from a Mott insulator regime \( J_2 \ll U \) (\( z \) the lattice coordination number).

In contrast, we consider a nonequilibrium situation in which the competition of microscopic quantum mechanical operators results from an interplay of unitary (Hamiltonian) and dissipative (Liouvillian) dynamics. We study cold atom evolution described by a master equation for the many-body density operator

\[
\frac{\partial_t \rho}{\partial t} = -i[H, \rho] + \mathcal{L}[\rho],
\]

where\( \mathcal{L}[\rho] = \frac{1}{2} \kappa \sum_{\ell,\ell'} \left( 2c_{\ell\ell'}^\dagger c_{\ell\ell'} \rho - c_{\ell\ell'}^\dagger c_{\ell\ell'} \rho - c_{\ell\ell'} c_{\ell\ell'}^\dagger \rho \right),
\]

and \( c_{\ell\ell'} = (b_\ell^\dagger + b_{\ell'}^\dagger)(b_\ell - b_{\ell'}) \) are Lindblad “jump operators” acting on adjacent sites \( (\ell, \ell') \). The energy scale \( \kappa \) is the dissipative rate. As shown in [11], such dissipative reservoir couplings can be engineered in a setup where laser driven atoms are coupled to a phonon bath provided by a second condensate. If \( J = U = 0 \), the Liouvillian drives the system into a pure Bose-Einstein condensate (BEC) steady state independently of the initial state [11]. This can be easily understood in momentum space, where the annihilation part of \( c_{\ell\ell'} \) reads \( \sum_{\lambda} (1 - \exp(iq_{\lambda} a)) b_{q_{\lambda}} \) with \( \lambda \) the reciprocal lattice directions and \( a \) the lattice constant. \( c_{\ell\ell'} \) thus feature a (unique) dissipative zero mode at \( q = 0 \) — a many-body “dark state” (BEC) \( \sim b_0^N |\text{vac}\rangle \), into which the system is consequently driven for long wait times. We stress that it is the driven nature of \( \mathcal{L} \) that allows to approach a zero entropy state, similarly to laser cooling [12]. This places the system far away from thermodynamic equilibrium.

A purely kinetic Hamiltonian has \( |\text{BEC}\rangle \) as an eigenstate, making \( J \) an energy scale compatible with dissipation \( \kappa \). However, an onsite interaction \( U \) suppresses off-diagonal order and consequently competes with \( \kappa \). We therefore obtain a nonequilibrium analog to the conventional purely Hamiltonian scenario, in which the competition of unitary and dissipative dynamics is described by the parameter \( u = U/(4\kappa z) \). Dominant dissipation \( u \ll 1 \) has a superfluid steady state, while dominant interaction \( u \gg 1 \) results in a diagonal density matrix.

Our scenario bears some resemblance to a system of Josephson junction arrays coupled to a dissipative bath [14], which suitably chosen can stabilize the supercon-
Nonlinear mean field master equation

In order to solve the master equation we have developed a generalized Gutzwiller approach, expected to hold in sufficiently high spatial dimension, which compared to the standard mean field procedure allows to include density matrices corresponding to mixed states. This is implemented by a product ansatz $\rho = \otimes \rho_i$ for the full density matrix, with the reduced local density operators $\rho_i = Tr_{\xi \neq i} \rho$ obtained by tracing out all the degrees of freedom but those on the $i$th site. The equation of motion (EoM) for the reduced density operator reads

$$\partial_t \rho_i = -i [h_i, \rho_i] + L_i [\rho_i] ,$$

with the local Hamiltonian $h_i = -J \sum_{\langle \ell, \ell' \rangle} \langle \ell | \psi \rangle \langle \psi | \ell' \rangle + \langle \ell | b_i | \ell' \rangle b_i^\dagger \ell' - \mu \ell_i + \frac{1}{2} U \ell \ell_i (\ell_i - 1)$ reproducing the standard form of the Gutzwiller mean field approach and a Liouvillian of the form $L_i [\rho_i] = \kappa \sum_{\langle \ell, \ell' \rangle} \sum_{\sigma=1}^4 \Gamma_{\ell}^{\sigma} \left[ 2 A_i \rho_i A_i^\dagger - A_i^\dagger A_i \rho_i - \rho_i A_i^\dagger A_i^\dagger \right]$. The Liouvillian is constructed with the vector of operators $A_i = (1, b_i, b_i^\dagger, \hat{n}_i)$ and the matrix of correlation functions $\Gamma_{\ell}^{\sigma} = \sigma' \sigma \langle \hat{\sigma}_i \hat{\sigma}^{\dagger}_{\ell} \rangle$ for any $\sigma = (-1, -1, 1, 1)$. The $\rho$-dependent correlation matrix makes the master equation nonlinear in $\rho_i$.

**Dynamical quantum phase transition.**—At $U = 0$ a steady state solution of Eq. (3) is given by the pure state $\rho_i^{\text{(c)}} = |\Psi \rangle \langle \Psi |$ for any $\ell$ together with the choice $\mu = -J z$, where $|\Psi \rangle$ is a coherent state of parameter $n e^{i \theta}$ for any phase $\theta$. In order to understand the effect of a finite interaction $U$, we apply the rotating frame transformation $V(U) = \exp[i U \hat{n}_i (\hat{n}_i - 1)]$ to Eq. (3). This removes the interaction term from the unitary evolution, but the annihilation operators become $V b_i V^{-1} = \sum_m \exp(i m U t) |m \rangle \langle m| b_i$. The effect of a finite $U$ is thus to rotate the phase of each Fock state differently, leading to dephasing of the coherent state $\rho_i^{\text{(c)}}$. Hence, for strong enough $U$, off-diagonal order is suppressed completely and the density matrix becomes diagonal. In this case Eq. (3) reduces precisely to the master equation for a system of bosons coupled to a thermal reservoir with occupation $n$, whose solution is a mixed diagonal thermal state $\rho^{\text{(t)}}$. Interestingly, unlike the standard case of an external heat bath, the strongly interacting system provides its own heat reservoir.

We substantiate the discussion above with the numerical integration of the EoM (3) for a homogeneous system (we drop the index $\ell$). The system is initially in the coherent state and the condensate fraction $|\psi|^2/n$, where $\psi = (b)$, decreases in time depending on the value of the interaction strength $U$. The result is a continuous transition from the coherent state $\rho^{\text{(c)}}$ to the thermal state $\rho^{\text{(t)}}$, shown in Fig. 2 for some typical parameters. The boundary between the thermal and the condensed phase with varying $J, n$ is shown in Fig. 1 with solid lines.

The transition is a smooth crossover for any finite time, but for $t \to \infty$ a sharp nonanalytic point indicating a second order phase transition develops. In the universal vicinity of the critical point, $1/\kappa t$ may be viewed as an irrelevant coupling in the sense of the renormalization group. We may use this attractive irrelevant direction to extract the critical exponent $\alpha$ for the order parameter.
from the identity $n = \langle \delta b^\dagger \delta b \rangle + |\psi_0|^2$. The value of the chemical potential is fixed to remove the driving terms in the equations for $\langle \delta b \rangle$, leading to $\mu = nU$. This is an equilibrium condition similar to the vanishing of the mass of the Goldstone mode in a thermodynamic equilibrium system with spontaneous symmetry breaking. The solution of the equations in steady state yields the condensate fraction

$$|\psi_0|^2 = \frac{2u^2(1 + (j + u)^2)}{1 + u^2 + j(8u + 6j(1 + 2u^2) + 24j^2u + 8j^3)},$$

with dimensionless variable $j = J/(4\kappa)$. Eq. (5) reduces to the simple quadratic expression $1 - 2u^2$ in the limit of zero hopping, with the critical point $U_c(J = 0) = 4\kappa z / \sqrt{2}$. The phase boundary, obtained by setting $\psi_0 = 0$ in Eq. (5), reads $uc = j + \sqrt{1/2 + 2j^2}$. Fig. 1] shows that these compact analytical results (solid red line) match the full numerics for small densities (solid blue line), and also explain the qualitative features of the phase boundary for large densities. We note the absence of distinct commensurability effects for e.g. $n = 1$, tied to the fact that the interaction also plays the role of heating.

**Dynamical instability.**—Numerically integrating the full EoM (3) with site-dependence (in one dimension for simplicity), we observe a dynamical instability, manifesting itself at late times in a long wavelength density wave with growing amplitude, cf. Fig. 3(a). Numerical linearization of Eq. (3) around the homogeneous steady state allows to draw a phase border for the unstable phase (see Fig. 1). The instability is cured by the increase of hopping $J$, which is associated to an operator compatible with dissipation $\kappa$. Furthermore, we note that the thermal state is always dynamically stable against long wavelength perturbations.

The origin of this instability is intriguing and we discuss it analytically within the low-density limit introduced above. We linearize in time the EoM (3), writing the generic connected correlation function as $\langle \hat{O}_\ell(t) \rangle(t) = \langle \hat{O}_\ell \rangle_0 + \delta \langle \hat{O}_\ell \rangle(t)$, where $\langle \hat{O}_\ell \rangle_0$ is evaluated on the homogeneous steady state of the system. The EoM for the time and space dependent fluctuations is then Fourier transformed, resulting in a $7 \times 7$ matrix evolution equation

$$\partial_t \Phi_{q} = M \Phi_q$$

for the correlation functions $\Phi_q = (\langle \delta b \rangle_q, \langle \delta b^\dagger \rangle_q, \langle \delta b^\dagger \delta b \rangle_q, \langle \delta b^2 \rangle_q, \langle \delta b^2 \rangle_q, \langle \delta b^2 \rangle_q, \langle \delta b^2 \rangle_q)$. We note that the fluctuation $\delta \langle \delta b \rangle_q (\delta \langle \delta b^\dagger \rangle_q)$ coincides with the fluctuation of the order parameter $\delta \psi_q (\delta \psi^* q)$. The full matrix $M$ can be easily diagonalized numerically revealing the spectrum in Fig. 3 (we display only the relevant real part $\gamma$ corresponding to damping). The lowest-lying branch gives $\gamma_q < 0$ in a small interval around the origin $q = 0$. This means that the correlation functions grow exponentially $\propto e^{\gamma t}$ in a range of low momenta, resulting e.g. in a long wavelength density wave like in Fig. 3(a).
Due to the scale separation for $\mathbf{q} \to 0$ in the matrix $M$ apparent from Fig. 3(b), we can apply second order perturbation theory twice in a row to integrate out the fast modes $\gamma \propto \kappa$ and $\propto \kappa n$. We then obtain an effective low energy EOM for the fluctuations of the order parameter $(\delta \psi^\dagger, \delta \psi)$, governed by a $2 \times 2$ matrix

$$M_{\text{eff}} = \begin{pmatrix} Un + \epsilon_q - i\kappa_q & Un + 9un\kappa_q \\ -Un - 9un\kappa_q & -Un - \epsilon_q - i\kappa_q \end{pmatrix},$$

where $\epsilon_q = JQ^2$ represents the kinetic contribution and $\kappa_q = 2(2n + 1\kappa\mathbf{q})^2$ is the bare dissipative spectrum. The form of the EOM reflects the structure of the spatial fluctuations which are included in our approach, that may be understood as scattering off the mean fields in opposite directions. We note that a naive a priori restriction to the $2 \times 2$ set corresponding to the subset $(\delta \psi^\dagger, \delta \psi^\ast)$ would be inconsistent, for example destroying the dark state property present in the correct solution $M_{\text{eff}}$. On the other hand, factorizing the correlation functions in the Liouvillian $L_{\text{t}}$ yields a dissipative Gross-Pitaevskii equation but its linearization in time produces a matrix $M_{\text{eff}}$ without the fluctuation induced term $\sim u$ and fails to describe the dynamical instability. Thus, in order to correctly capture the physics of the instability at long wavelength $\mathbf{q} \to 0$, the onsite quantum correlations renormalizing $M_{\text{eff}}$ have to be properly taken into account.

We can make the nature of the instability even more transparent from calculating the lowest eigenvalue of $M_{\text{eff}}$, $\gamma_q \simeq \epsilon |\mathbf{q}| + \kappa_q$, with speed of sound $c = \sqrt{2Un(9Un/(2z)))}$. If the hopping amplitude is smaller than the critical value $J_c = 9Un/(2z)$ the speed of sound turns imaginary and contributes to the dissipative real part of $\gamma_q$. The nonanalytic renormalization contribution $\sim |\mathbf{q}|$ always dominates the bare quadratic piece for low momenta, explaining the shape in the inset of Fig. 3 and rendering the system unstable. The linear slope of the stability border for small $J$ and $U$ is clearly visible from the numerical results in Fig. 1.

**Conclusion.**—We have discussed the steady state phase diagram resulting from a competition of unitary Bose-Hubbard and dissipative dynamics with dark state. The features found in the present model are expected to be generic and representative for a whole class of nonequilibrium models discussed recently in the context of reservoir engineering and dissipative preparation of given long range ordered entangled states of qubits or spins on a lattice and paired fermions. In particular, we emphasize the importance of a compatible energy term for the achievement of stability of driven-dissipative many-body systems in future experiments.

We thank M. Hayn, A. Pelster, S. Kehrein, M. Möckel, and J. V. Porto for interesting discussions. This work was supported by the Austrian Science Foundation through SFB FOQUS, SCALA and by EU Networks. The plots have been produced with the Open Source scpy/numpy/matplotlib packages of the Python programming language.

---


