Winding Up of the Wave-Function Phase by an Insulator-to-Superfluid Transition in a Ring of Coupled Bose-Einstein Condensates

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We study phase transition from the Mott insulator to superfluid in a periodic optical lattice. Kibble-Zurek mechanism predicts buildup of winding number through random walk of BEC phases, with the step size scaling as a third root of transition rate. We confirm this and demonstrate that this scaling accounts for the net winding number after the transition.

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Introduction.—In a second order phase transition, the critical point is characterized by divergences in the correlation length and in the relaxation time. This critical slowing down implies that no matter how slowly a system is driven through the transition, its evolution cannot be adiabatic close to the critical point [1]. As a result, the state after the transition is not perfectly ordered: it is a mosaic of domains whose size depends on the rate of the transition. This scenario was first described in the cosmological setting by Kibble [2] who appealed to relativistic causality to set an upper bound on domain size. The dynamical mechanism that determines domain size in second order phase transitions was proposed by one of us [1]. It is based on the universality of critical slowing down, and predicts that average size of the ordered domains $\hat{\xi}$ scales with the transition time τ_Q as $\hat{\xi} \sim \tau_Q^w$, where w is a combination of critical exponents. This Kibble-Zurek mechanism (KZM) for second order thermodynamic phase transitions was confirmed by numerical simulations [3] and tested by experiments in liquid crystals [4], superfluid helium 3 [5], both high-T_c [6] and low-T_c [7] superconductors, and even in nonequilibrium systems [8]. With the exception of superfluid ^{4}He—where the situation remains unclear [9], experimental results are consistent with KZM (see [10] for a review). Spontaneous appearance of vorticity during Bose-Einstein condensation driven by evaporative cooling was recently reported [11]. This confirms KZM predictions [12] and is further elucidated by numerical studies of BEC formation [13].

Our goal is to study dynamics of a quantum phase transition in a simple yet nontrivial example that can be implemented experimentally. Quantum phase transitions we consider differ qualitatively from finite temperature transitions. Most importantly, evolution is unitary, so there is no damping and no thermal fluctuations to initiate symmetry breaking. Recent work on the dynamics of quantum phase transitions is mostly theoretical [14–23], but there is one possible exception: Reference [24] on the transition in a spin-1 BEC. Generic outcome of that experiment is a mosaic of ferromagnetic domains whose origin was attrib-

uted to a sudden quench limit of KZM. This explanation is supported by theory [25].

Model.—Bose-Hubbard model is a paradigmatic example of a nonintegrable quantum critical system. It describes cold bosonic atoms in an optical lattice [26]. In dimensionless variables, its Hamiltonian reads

$$H = -J \sum_{s=1}^{N} (a_{s+1}^\dagger a_s + \text{h.c.}) + \frac{1}{2n} \sum_{i=1}^{N} a_s^\dagger a_s^\dagger a_s a_s. \quad (1)$$

Here, N is the number of lattice sites, and n is an average number of atoms per site. This model with periodic boundary conditions (which we assume) should be directly experimentally accessible in a ring-shaped optical lattice [27]. For an integer n, the transition from the Mott insulator (small J) to the superfluid phase (large J) is located at $J_c \simeq n^{-2}$ [28].

We drive the system through its critical point by a linear quench with a quench time scale τ_Q:

$$J(t) = t/\tau_Q. \quad (2)$$

In an experiment, one can increase Josephson coupling J by turning off the optical lattice potential as in [26]. The initial state is the Mott insulator ground state at $J = 0$,

$$|n, n, n, \ldots, n\rangle, \quad (3)$$

with the same atom number at each site. We assume $n \gg 1$: This large density limit is accessible experimentally.

Numerical approach.—We replace annihilation operators a_s by complex field ϕ_s, $a_s \approx \sqrt{n}\phi_s$, which is normalized, $\sum_{s=1}^{N} |\phi_s|^2 = N$, and evolves with the time-dependent Gross-Pitaevskii equation

$$i\frac{d\phi_s}{dt} = -J(\phi_{s+1} + \phi_{s-1} - 2\phi_s) + |\phi_s|^2\phi_s. \quad (4)$$

These approximations are accurate for $n \rightarrow \infty$, when the critical point $J_c \simeq n^{-2} \rightarrow 0$.

In the truncated Wigner method we employ, quantum expectation values are given by the averages over stochastic realizations of the field $\phi_s(t)$ [13,29,30]. For example,

the correlation function becomes

$$C_R = \frac{\langle a_s^\dagger a_{s+R} \rangle}{n} \approx \overline{\phi_s^* \phi_{s+R}}. \tag{5}$$

Here, $\langle \ldots \rangle$ means quantum expectation value while the overline is an average over realizations. All realizations of $\phi_s(t)$ evolve with the same deterministic Gross-Pitaevskii equation (4), but they start from different random initial conditions which come from a probability distribution depending on an initial quantum state. The initial Mott state (3) corresponds to initial fields

$$\phi_s(0) = e^{i\theta_s} \tag{6}$$

with independent random phases $\theta_s \in [0, 2\pi)$: The Mott state has the same number of n particles at each site [i.e., $|\phi_s(0)| = 1$], and, hence, indeterminate phases that translate into random θ_s.

Kibble-Zurek mechanism.—In an optical lattice with BEC pools that become gradually connected with Josephson couplings in accord with Eq. (2), it is natural to rephrase KZM: Rather than seek distance $\hat{\xi}$ over which phase remains more or less the same, we compute size $\Delta\theta_s$ of a typical phase step between neighboring sites. One could use it to deduce the size of domains $\hat{\xi}$ over which winding number changes by one, and get the accumulated phase from square root of circumference of the whole ring of BEC pools measured in units of $\hat{\xi}$, as in [1]. However, the same result obtains from a random walk between neighboring sites, with the corresponding step size $\Delta\theta_s$. We now compute $\Delta\theta_s$ as a function of τ_Q.

The Gross-Pitaevski equation (4) can be linearized in small fluctuations $\delta\phi_s$ around uniform large background, $\phi_s = 1 + \delta\phi_s$, and $\delta\phi_s$ can be expanded in Bogoliubov modes as $\delta\phi_s = \sum_k (b_k u_k e^{iks} + b_k^* v_k^* e^{-iks})$ with pseudo-momentum k. For constant J, we have $b_k(t) = b_k(0)e^{-i\omega_k t}$ with $\omega_k = 2\sqrt{J(1-\cos k)[1 + J(1-\cos k)]}$ and stationary Bogoliubov modes $u_k = -\mathcal{N}_k[1 + 2J(1-\cos k) + \omega_k]$, $v_k = \mathcal{N}_k$ where $\mathcal{N}_k$ are such that $u_k^2 - v_k^2 = 1$. In the Josephson regime, when $J \ll 1$, we have $v_k \approx -u_k$ so that purely imaginary $\delta\phi_s$ in $\phi_s = 1 + \delta\phi_s$ is a phase fluctuation. However, for our random initial conditions (6), this linearization is justified only for short wavelength modes of ϕ_s, with $k \approx \pm\pi$, for whom the modes with longer wavelength are a *locally* uniform large background. From now on, we focus on the short wavelength modes because they determine variance of the nearest-neighbor $\Delta\theta_s$.

When $k \approx \pm\pi$ and $J \ll 1$, then $\omega_k \approx 2\sqrt{2J}$. Early in the linear quench (2), this ω_k is small so that early evolution of the short wavelength modes is approximately impulse, i.e., their magnitude remains the same as in the initial Mott state and, consequently, $\overline{\Delta\theta_s^2} \simeq 1$ in this impulse stage. The impulse approximation breaks down at $\hat{J}$ ([1]) when the transition rate $\dot{\omega}_k/\omega_k$ equals ω_k,

$$\dot{\omega}_k/\omega_k \simeq \omega_k, \tag{7}$$

and evolution becomes adiabatic. Equation (7) leads to

$$\hat{J} \simeq \tau_Q^{-2/3} \tag{8}$$

which is consistent with $J \ll 1$ when $\tau_Q \gg 1$.

The crossover from impulse to adiabatic evolution at $\hat{J}$ is the key ingredient of KZM. In the following adiabatic evolution after $\hat{J}$, but before $J \approx 1$, short wavelength phase fluctuations scale as $\delta\phi_s \sim J^{-1/4}$ because the mode amplitudes $|b_k|$ do not change, but u_k and v_k follow stationary Bogoliubov modes $u_k \approx -v_k \approx -\frac{1}{2}(2J)^{1/4}$. Consequently, $\Delta\theta_s$ has variance scaling as $\overline{\Delta\theta_s^2}|_J \simeq \overline{|\delta\phi_s|^2} \sim J^{-1/2}$. Given the boundary condition at $\hat{J}$ that $\overline{\Delta\theta_s^2}|_{\hat{J}} \simeq 1$, phase fluctuations must shrink as $\overline{\Delta\theta_s^2}|_J \simeq \overline{\Delta\theta_s^2}|_{\hat{J}}(J/\hat{J})^{-1/2} \simeq \tau_Q^{-1/3}J^{-1/2}$ while $J \ll 1$.

On the other hand, when $J \gg 1$, then stationary modes $u_k \approx 1$ and $v_k \approx 0$ do not depend on J and $\overline{\Delta\theta_s^2}$ does not depend on J either. This means that $\overline{\Delta\theta_s^2}$ must stabilize between the regimes of $J \ll 1$ and $J \gg 1$, i.e., around $J \simeq 1$ where it takes its final value

$$\overline{\Delta\theta_s^2}|_{J \gg 1} \approx \overline{\Delta\theta_s^2}|_{J \simeq 1} \simeq \tau_Q^{-1/3} \tag{9}$$

which scales with a power of $w = 1/3$.

This variance determines, e.g., the correlator C_1 in

$$K_1 = 1 - C_1 = 1 - \overline{\cos\Delta\theta_s} \simeq \tau_Q^{-1/3}, \tag{10}$$

for $\tau_Q \gg 1$. Kinetic hopping energy per particle K_1 is expected to stabilize for $J \gg 1$, when the hopping term dominates over the nonlinearity in Eq. (4) and K_1 becomes an approximate constant of motion, see Fig. 1.

Key ingredients of KZM are confirmed by our simulations: Phase performs a random walk that is Markovian to a good approximation. Moreover—as seen in Fig. 1—its size is consistent with the above predictions.

Winding number.—Condensate wave function is single-valued. Therefore, phase accumulated Θ_R after $R = N$ steps defines integer winding number

$$W_N = \frac{1}{2\pi} \sum_{s=1}^{N} \text{Arg}(\phi_{s+1}\phi_s^*), \tag{11}$$

where $\text{Arg}(\ldots) \in (-\pi, \pi]$. A random walk of phase, with the variance of nearest-neighbor phase differences scaling as in Eq. (9), gives winding numbers with variance

$$\overline{W_N^2} \simeq N\tau_Q^{-1/3}. \tag{12}$$

There are two limits where this scaling is bound to fail. For very fast quenches with $\tau_Q \ll 1$, phases are completely random between neighboring sites, so $\overline{\Delta\theta_s^2} = \pi^2/3$, and $\overline{W_N^2} = N/12$. For quenches so slow that $\overline{W_N^2} < 1$, the nature of the problem changes, leading to steeper falloff of $\overline{W_N^2}$ with τ_Q [7,16]. Between these two limits, the $\frac{1}{3}$-scaling in Eq. (12) for the winding number is confirmed by our numerical results in Fig. 2.
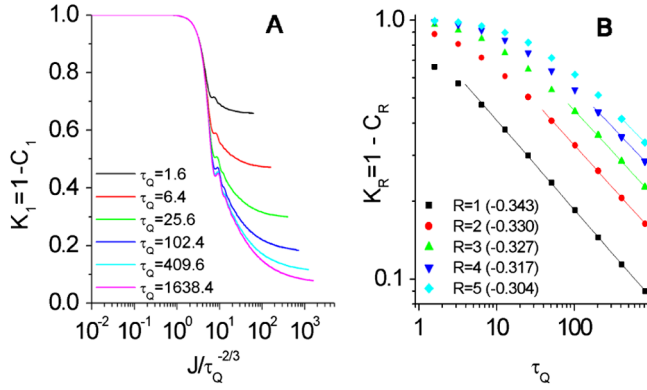
FIG. 1 (color online). Kinetic hopping energy $K_1 = 1 - C_1 \approx \overline{1 - \cos\Delta\theta_s} \approx \frac{1}{2}\overline{\Delta\theta_s^2}$ as a function of rescaled $J/\hat{J}$ for different τ_Q is seen in (a). When $J \ll 1$, all the plots overlap demonstrating that $\hat{J} = \tau_Q^{-2/3}$ is the relevant scale for $J \ll 1$. Individual plots depart from this small-J "common bundle" at $J \simeq 1$, or $J/\tau_Q^{-2/3} \simeq \tau_Q^{2/3}$, when $K_1 = 1 - C_1$ is expected to stabilize. In (b), we show $K_R \equiv 1 - C_R$ at $J = 10$ as a function of τ_Q for $R = 1, \ldots, 5$. Data points for each R were fitted with lines, their slopes giving exponents close to the $\frac{1}{3}$-scaling predicted in Eq. (10) with error bars on their last digits. Size of typical phase step can be estimated as $\overline{\Delta\theta_s^2} \simeq K_R/R$ when $K_R \ll 1$, and already this rough estimate yields a good approximation of winding numbers shown in Fig. 2.

Correlation function.—Constant amplitude and Gaussian distribution of phase Θ_R after R steps imply

$$C_R \simeq \int_{-\infty}^{\infty} \frac{d\Theta_R \cos\Theta_R}{\sqrt{2\pi\sigma_R^2}} e^{-\Theta_R^2/2\sigma_R^2} = e^{-\sigma_R^2/2}, \quad (13)$$

where σ_R is dispersion of $\Theta_R = \sum_{s=1}^{R} \mathrm{Arg}(\phi_{s+1}\phi_s^*)$ which after $R = N$ steps becomes the winding number in Eq. (11), i.e., $W_N = \Theta_N/2\pi$. For a random walk, $\sigma_R^2 = R\overline{\Delta\theta_s^2}$, which leads one to expect

$$C_R \simeq \exp(-R\overline{\Delta\theta_s^2}/2) \equiv \exp(-R/\xi). \quad (14)$$

Using Eq. (9), we would expect scaling $\xi \simeq \tau_Q^{1/3}$.

Numerical simulations confirm exponential correlations, see Fig. 3, but correlation lengths ξ measured at $J = 10$ are better fitted by $\xi \simeq \tau_Q^{0.45}$. On the other hand, early on in the quench, for smaller values of $J \ll 1$, correlation length exhibits $\xi \simeq \tau_Q^{1/3}$. It seems that intermediate scales are subject to phase ordering between the freeze-out at $\hat{J} \simeq \tau_Q^{-2/3}$ and the final $J = 10$. Similar post-transition phase ordering was observed in the integrable quantum Ising chain [21].

On the other hand, winding number continues to scale with $\tau_Q^{-1/3}$, see Fig. 2. It is not too surprising that it is insensitive to phase ordering: While in our simulations winding number is not really stable following the freeze-out, it changes much less frequently than smaller scale excitations, as its topological nature leads one to expect.
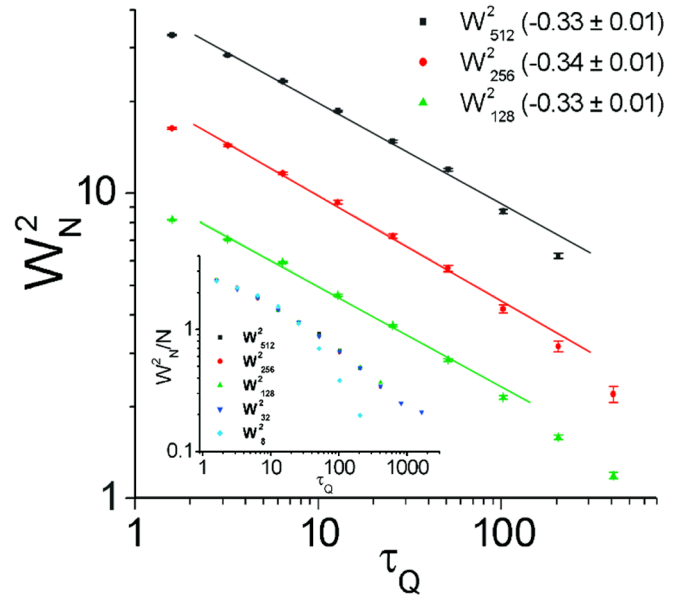

FIG. 2 (color online). Variance of winding number $\overline{W_N^2}$ measured at $J = 10$ as a function of τ_Q for lattice sizes $N = 512$, 256, 128. Here, point sizes equal error bars. The data points with $\tau_Q > 2$ and $\overline{W_N^2} > 2$ were fitted with the solid lines giving slopes close to the predicted $-\frac{1}{3}$ in Eq. (12). $\overline{W_N^2}$ is shown over a wider range of τ_Q to show the saturation for nearly instantaneous quenches, when $\tau_Q < 2$, and the crossover to steeper slope when $\overline{W_N^2} < 2$. In the inset, we show a rescaled $\overline{W_N^2}/N$ for $N = 512$, 256, 128, 32, 8 to demonstrate that $\overline{W_N^2} \sim N$ in the KZM regime of $\tau_Q > 2$ and $\overline{W_N^2} > 2$.

Summary.—We have investigated the process making a single condensate wave function out of many—N—independent BEC pools. We conclude that, in the ring geometry, the overall winding number W_N (which will set up persistent current) can be predicted using simple idea of a random walk in phase between the initially independent BEC fragments [1]. For very quick quenches, this leads to saturation at $W_N = N/12$. Slower quenches lead to scaling of W_N with the rate of reconnection that can be inferred from the Kibble-Zurek mechanism.

Correlation functions also exhibit behavior consistent with a random walk in phase. Initially, correlations scale in a way that is directly related to healing length at the instant when dynamics of the system becomes faster than the rate of change of its Hamiltonian [1]. However, while winding number "remembers" this scaling as Josephson couplings increase, correlations on smaller scales evolve. In thermodynamic transitions, similar phase ordering associated with diffusion is responsible for the post-transition smoothing of the order parameter structure so that—eventually—only topological defects still "remember" initial state of the system. In our model, evolution is completely reversible. Therefore, diffusion cannot smooth out small-scale structures. However, evolution itself appears to redistribute energy between the excitations. This may be regarded as a quantum analogue of phase ordering.
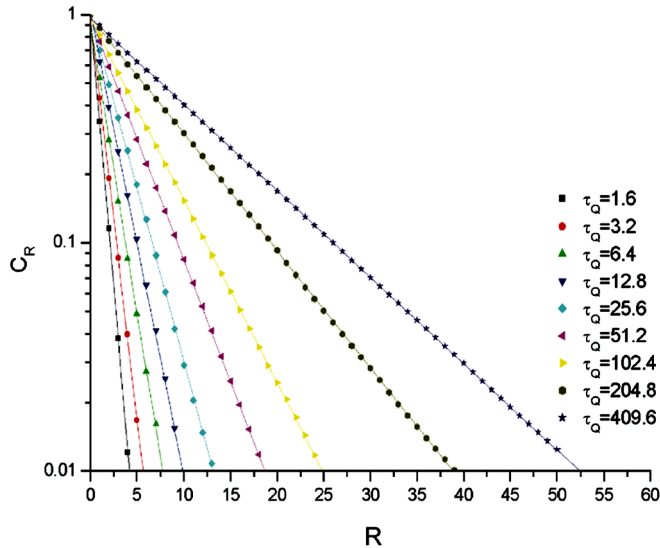
FIG. 3 (color online).   Correlation function C_R for different τ_Q measured at $J = 10$ on a lattice of $N = 512$ sites. This logarithmic plot demonstrates that C_R is exponential in R.

Correlations on intermediate scales change, but (as was also the case in thermodynamic phase transitions) small-scale evolution does not affect the topologically protected winding number W_N.

Our model ignores decoherence and damping that are likely to intervene in the laboratory experiments with, say, gaseous BECs. It is relatively easy to modify equations and introduce damping "by hand." There is however no unique prescription for it (although one could appeal to presence of a dilute thermal cloud, as in simple models of BEC decoherence [31]). In experiments, dissipation and decoherence are inevitable. We expect dissipation to affect small scales, but leave the topologically conserved W_N intact. This is based on a limited number of simulations we have conducted where different models of dissipation were tried out. Above all, this is corroborated by the experiment [11] where sudden reconnection of $N = 3$ uncorrelated condensates led to relaxation to a condensate with stable vortices—stable winding number. It is also consistent with the recent numerical results [32].

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