Superfluid-Insulator Transition in a Moving System of Interacting Bosons

E. Altman, A. Polkovnikov, E. Demler, B. I. Halperin, and M. D. Lukin

Physics Department, Harvard University, Cambridge, Massachusetts 02138, USA

(Received 2 November 2004; published 6 July 2005)

We analyze the stability of superfluid currents in a system of strongly interacting ultracold atoms in an optical lattice. We show that such a system undergoes a dynamic, irreversible phase transition at a critical phase gradient that depends on the interaction strength between atoms. At commensurate filling, the phase boundary continuously interpolates between the classical modulation instability of a weakly interacting condensate and the equilibrium quantum phase transition into a Mott insulator state at which the critical current vanishes. We argue that quantum fluctuations smear the transition boundary in low dimensional systems. Finally we discuss the implications to realistic experiments.

DOI: 10.1103/PhysRevLett.95.020402 PACS numbers: 03.75.Lm, 03.75.Kk

The quantum phase transition from a superfluid (SF) to a Mott insulator (IN) [1] is an important paradigm of strong correlation physics. Recently this transition was demonstrated in spectacular experiments involving ultracold atoms in an optical lattice [2,3]. An important feature of these systems is that they can be essentially isolated from the environment, opening unique possibilities to study, not only the equilibrium phase diagram, but also quantum dynamics very far from equilibrium [4–10]. In particular, it is now possible to explore a new class of phenomena involving nonequilibrium dynamics in the vicinity of quantum phase transitions.

In this Letter we analyze the stability of superfluid current flow in a system of strongly interacting bosons in a lattice. We show that at the mean-field level such a system undergoes a dynamic phase transition, associated with irreversible decay of the superfluid flow at a critical momentum that depends on the interaction strength. We argue that quantum phase fluctuations play an important role near the phase boundary. In systems of lower dimensionality, they broaden the transition significantly as was indeed observed in recent experiments [11] and numerical simulations [10,12] in one dimensional systems. In three dimensions, by contrast, we predict that the current decay rate exhibits a sharp discontinuity at the mean-field transition. We propose to test this prediction with transport experiments along the lines of Ref. [11], in three dimensional optical lattices.

A well studied effect, closely related to our discussion, is the modulational instability of weakly interacting bosons on a lattice [6,7]. It was experimentally demonstrated [5,13] that such a condensate undergoes a dynamical localization transition, involving onset of chaos, when the phase gradient (or condensate momentum) associated with the flow exceeds $\pi/2$ per lattice unit. The dynamic phase transition described in this Letter interpolates continuously between the classical instability at condensate momentum $\pi/2$ and the quantum phase transition into the Mott state at zero current, thereby establishing a natural connection between the two transitions.

Dependence of the critical momentum on the interaction can be understood as follows. The superfluid current I associated with a condensate moving within the lowest Bloch band is $I(p) \sim \rho_s \sin(p)$, where p is the (quasi)momentum of the condensate measured in the units of inverse lattice constant and ρ_s is the superfluid density. In a weakly interacting condensate ρ_s is independent of p. Thus, the current increases with p up to a maximal value at $p_c = \pi/2$. Beyond this point, the effective mass changes sign and any further increase in p results in decrease of the current, rendering the superfluid unstable [14]. At strong interactions ρ itself is a function of the effective mass and thus also of p. Specifically, ρ decreases as p is increased, such that the maximum of $I(p)$ occurs in general at $p_c < \pi/2$. In particular, close to the Mott insulator, a slight increase in effective mass, and thus also in p, leads to vanishing of ρ. Therefore, p_c tends to zero toward the Mott transition. These considerations include the effect of quantum depletion at the mean-field level, which is effective in all dimensions, and leads to a stability phase diagram (for commensurate filling) depicted in Fig. 1. Smearing of the transition lines by quantum phase slips beyond mean-field theory is effective only in lower dimensions.

Static and dynamic properties of condensates in optical lattices can be described by the Bose Hubbard model (BHM)

$$H = \frac{U}{2}\sum_i n_i(n_i - 1) - J\sum_{\langle ij\rangle}(a_i^\dagger a_j + \text{H.c.}), \qquad (1)$$

where J is the hopping amplitude between the nearest neighbors $\langle ij\rangle$, U is the on-site repulsive interaction, and $n_i = a_i^\dagger a_i$ is the number operator. We denote the average number of bosons per site by N. Provided the system is deep in the superfluid phase ($JN \gg U$), the dynamics can be well approximated by the discrete Gross-Pitaevskii equations (GP)

$$i\frac{d\psi_i}{dt} = -J\sum_{k\in O}\psi_k + U|\psi_i|^2\psi_i, \qquad (2)$$

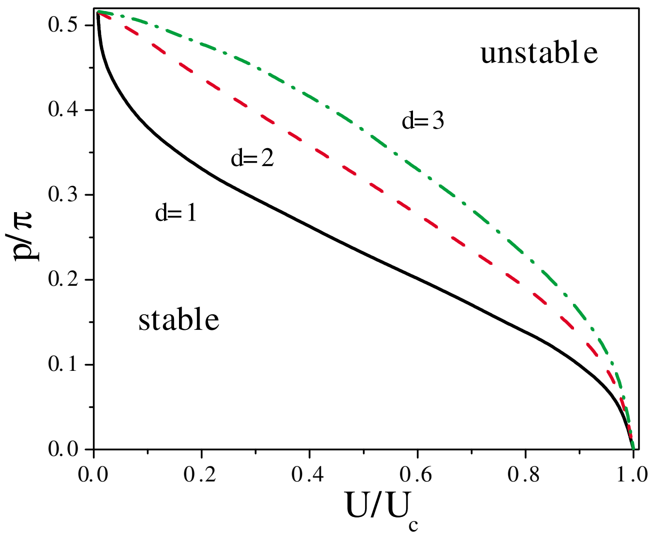

FIG. 1 (color online). Stability phase diagram in the plane of phase twist per bond vs dimensionless interaction for filling of $N = 1$ particle per site found from numerical solution of time dependent Gutzwiller equations (8).

where $\psi_i = \langle a_i \rangle$ is the matter field and the set O contains the nearest neighbors of site i. Linear mode analysis around the stationary current carrying solutions $\psi_i = \sqrt{N}\exp(ipx_i)$ yields the onset of instability at $p = \pi/2$ [6,7].

Close to the Mott transition, increased quantum fluctuations invalidate the GP description. However, one can still use semiclassical order parameter dynamics if one coarse grains the system into blocks of roughly a coherence length ξ, which is related to the superfluid density by a standard scaling form [15]. As in the weak coupling theory, the current should become unstable when the phase change per unit cell exceeds $\pi/2$, with the unit cell now of order ξ. Since the coherence length, ξ, diverges at the transition, we expect p_c to vanish as $1/\xi$, as we indeed find below. The diverging length scale facilitates a continuum description of the dynamics close to the Mott transition, in the form of a time dependent Ginzburg-Landau equation [8,14]

$$\ddot{\psi} = \nabla^2\psi + \psi(\xi^{-2} - |\psi|^2). \tag{3}$$

Within the mean-field approximation, and in the limit of large average occupation $N \gg 1$, $\xi^{-2} = 2d(1-u)$, where $u = U/(8JNd)$ is the dimensionless interaction constant. If N is not too large then Eq. (3) still holds but the expressions for ξ and u are more complicated [14].

We choose the zero of energy at the state with integer filling. Then the deviation from commensurate density is given in terms of the superfluid order parameter ψ by $\delta n = C_d(\psi^*\dot{\psi} - \psi\dot{\psi}^*)/2i$, with $C_d = u^{-1}(2d)^{-3/2}$ and d being the dimensionality of the system. Note that $\int d^d x \delta n$ is a constant of motion under (3). The supercurrent is similarly given by $I = C_d(\psi^*\nabla\psi - \psi\nabla\psi^*)/2i$.

The equation of motion (3) admits uniform solutions $\psi = \rho e^{ipx+i\mu t}$, with $\rho = \sqrt{\xi^{-2} + \mu^2 - p^2}$, which are characterized by a phase gradient p and a relative density

$$\delta n = C_d\mu(\xi^{-2} + \mu^2 - p^2). \tag{4}$$

In particular, at commensurate filling $\mu = 0$ and ψ is time independent. To analyze whether these solutions are stable we find the spectrum of small fluctuations around them. There are two eigenmodes in the superfluid regime ($\xi^{-2} > 0$): a stable gapped mode and a phase (Bogoliubov) mode with linear dispersion at long wavelengths. The dispersion of the latter, for wave vectors parallel to the current, reads:

$$\omega(k) = \frac{2\mu p}{2\mu^2 + \rho^2}k + \frac{\rho}{2\mu^2 + \rho^2}\sqrt{\xi^{-2} + 3\mu^2 - 3p^2}|k|. \tag{5}$$

Here the first term is analogous to the usual Doppler shift and the second describes propagation of the sound waves in the moving reference frame. The onset of imaginary frequencies marking the instability occurs at $p_c^2 - \mu(p_c)^2 = 1/3\xi^2$. Combining this with Eq. (4) we find that for $N \gg 1$

$$p_c = \sqrt{\frac{1}{3\xi^2} + \left(\frac{3\delta n \xi^2}{4C_d}\right)^2}. \tag{6}$$

As argued before on general grounds, in the case of commensurate filling $\delta n = 0$, the critical phase gradient vanishes toward the equilibrium Mott transition ($u = 1$) as $p_c \propto 1/\xi \propto \sqrt{1-u}$. At incommensurate density there is no equilibrium Mott transition. As a result, we do not expect the instability to reach $p = 0$. Indeed, p_c has a minimum at $u < 1$ ($\xi < \infty$) and diverges as $u \to 1$. The divergence simply signals the breakdown of the continuum theory and is cut off by the lattice.

To interpolate between the regimes of weak and strong interactions we employ the Gutzwiller approximation [16]. In this approach, the wave function is assumed to be factorizable:

$$|G\rangle = \prod_j \left[\sum_{n=0}^{\infty} f_{jn}|n\rangle_j\right]. \tag{7}$$

Here j is a site index and n is the site occupation. The ansatz (7) supplemented by self-consistency conditions leads to equations of motion for the variational parameters:

$$-i\dot{f}_{jn} = \frac{U}{2}n(n-1)f_{jn} - Jz(\sqrt{n}f_{j,n-1}\psi_j + \sqrt{n+1}f_{j,n+1}\psi_j^*), \tag{8}$$

where

$$\psi_j \equiv \frac{1}{z}\sum_{i\in O}\langle G|a_i|G\rangle. \tag{9}$$

For actual calculations with $N = 1$ we truncated (7) at five and ten states per site without noticeable differences in the results.

Equations (8) admit uniform current carrying solutions. We numerically check their stability to slight perturbations in the equations of motion. We show the stability boundaries at commensurate filling in Fig. 1. It is evident that the dynamical instability at $\pi/2$ in the GP regime is continuously connected to the equilibrium (zero current) Mott transition. Note that the accuracy by which we determine p_c from the simulation suffers from the fact that the characteristic time scale of the instability diverges as $U \to 0$. This is the reason for the small deviation of p_c from $\pi/2$ in this limit (see Figs. 1 and 2).

We perform a similar analysis at incommensurate filling (Fig. 2). In agreement with the continuum expression (6) we find that the critical momentum p_c reaches a minimum at some $u < 1$. At stronger interactions, p_c increases and saturates at $\pi/2$.

The mean-field transition discussed above ignores the possibility of current decay below the critical momentum due to quantum tunneling out of the metastable state. Such processes are exponentially suppressed by a tunneling action through a barrier. But since the barrier vanishes at the mean-field instability, they can potentially broaden the transition rendering the phase diagrams of Figs. 1 and 2 meaningless. This problem is addressed in full detail in Ref. [14] within the general framework of [17]. Here we describe one important result for the decay rate close to the equilibrium SF-IN transition, i.e., at small critical current. To obtain the tunneling action close to the critical current we expand the GL action associated with (3) around the metastable solution to cubic order in the fluctuations. Then we use a scaling approach similar to the one introduced in Ref. [18] in the context of spinodal decomposition. Since the instability in (5) arises at $\mathbf{k} \to 0$ the barrier vanishes only for a tunneling instanton of diverging (space-time) volume. By dimensional analysis we find $V_{\rm inst} \propto (p_c - p)^{d+1/2}$, while the energy density of the barrier $E_b \propto (p_c - p)^3$. Consequently the instanton action is $S_{\rm inst} \sim E_b \times V_{\rm inst} \propto B_d (p_c - p)^{2.5-d}$. Note that this scaling is different from that derived in Ref. [18], because the field ψ is complex. Thus in one and two dimensions the tunneling action vanishes continuously toward the mean-field transition. Then we expect the transition to become a wide crossover (B_d is calculated in [14] and found to be of order unity). This agrees with recent experiments [11] and numerical simulations [10] in one dimensional traps.

In three dimensions, by contrast, the action of "critical" instantons diverges because of their diverging volume. Currents would then rather decay via noncritical instantons, i.e., ones of finite size that feel a finite energy barrier, and thus cost finite action. We therefore predict that in three dimensions, the decay rate will exhibit a discontinuity at the mean-field transition. A variational calculation [14] yields a rate $\Gamma \propto e^{-4.3}$ in the vicinity of the transition. In this sense the mean-field phase diagram (Fig. 1) is well defined in three dimensions.

In realistic experimental situations condensates are confined in harmonic traps which leads to a nonuniform density distribution in the form of domains with different N. In the weakly interacting regime the critical momentum is $p_c = \pi/2$; i.e., it is insensitive to the spatial density variation induced by the harmonic confinement. By contrast, in the regime of strong interactions the position of the dy-

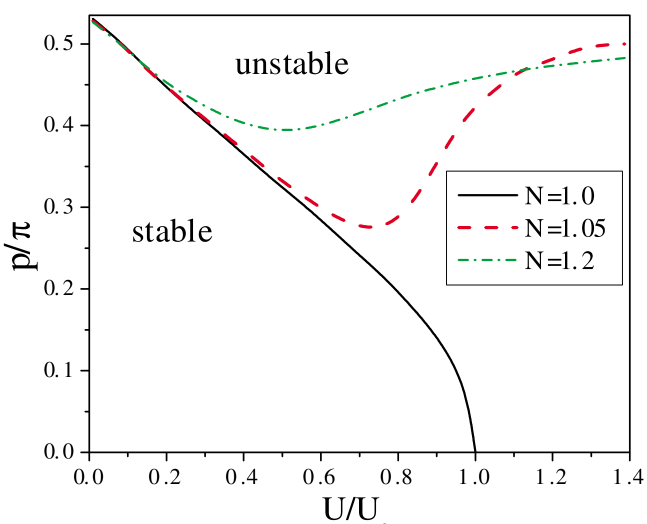

FIG. 2 (color online). Stability phase diagrams for different filling factors in a two-dimensional lattice from numerical solution of the time dependent Gutzwiller equations (8). Away from commensurate filling the critical phase gradient reaches a minimum and climbs back to $\pi/2$.

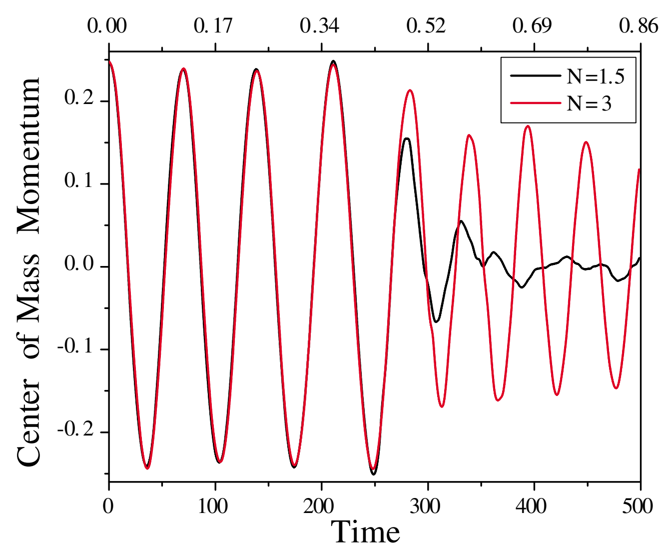

FIG. 3 (color online). Time dependence of the condensate momentum in a two-dimensional harmonic trap with different filling factors per central site. The simulated system is a lattice of dimensions 120×60 with global trapping potential $V(j_x, j_y) = 0.01(j_x^2 + j_y^2)$. We set the hopping amplitude $J = 1$ while increasing the interaction linearly in time: $U(t) = 0.01t$.

namical instability strongly depends on the filling factor N that is directly affected by the density distribution. In particular, the motion first becomes unstable for the smallest integer filling $N = 1$.

In Fig. 3 we plot the time evolution of the condensate momentum (computed within the Gutzwiller approximation) in a trap for two different filling factors. The center of mass motion becomes unstable at approximately the same interaction strength in both cases. But while at smaller filling the condensate motion rapidly becomes chaotic as in the uniform case, damping of oscillations at larger filling occurs much more gradually. These results can be understood by noting that if the phase gradient in the condensate exceeds the critical value corresponding to $N = 1$ these domains become unstable triggering the decay of current. However, when there is high filling of the central sites the overall weight of domains with $N = 1$ is small. Thus the effect of the instability on the total current is reduced.

An important experimental manifestation of these results is the inherently irreversible nature of the phase transition at finite currents. Consider a situation in which a moving condensate is first prepared on a weak lattice. Then, the depth of the periodic potential is increased adiabatically [19], which corresponds to moving along a horizontal line in the parameter space of Fig. 1. Finally, the lattice depth is slowly decreased back to its original state and the visibility of the interference fringes compared to their initial value. If, in this sequence, we pass the instability, then the current will decay into incoherent excitations and heat the condensate. This will result in total loss of current and reduced visibility of the interference fringes at the end of the cycle. Such experiments could be used to probe the nonequilibrium phase diagram (Fig. 1) and to determine the position of the equilibrium Mott transition.

This work was supported by the NSF (Grants No. DMR-01328074, No. DMR-0233773, No. DMR-0231631, No. DMR-0213805, No. PHY-0134776), the Sloan and the Packard Foundations, and by Harvard-MIT CUA.

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