

Oscillating Superfluidity of Bosons in Optical Lattices

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Following a suggestion by Orzel *et al.* [Science **291**, 2386 (2001)], we analyze bosons in an optical lattice undergoing a sudden parameter change from the Mott to superfluid phase. We introduce a modified coherent states path integral to describe both phases. The saddle point theory yields collective oscillations of the uniform superfluid order parameter. We calculate its damping rate by phason pair emission. In two dimensions the overdamped region largely overlaps with the quantum critical region. Measurements of critical dynamics on the Mott side are proposed.

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With recent experimental developments of ultracold atoms in optical lattices, the fascinating phenomena of Bose-Einstein condensation have entered the domain of strong interactions [1,2]. Macroscopic quantum states can be effectively manipulated, and time evolution of order parameters (OP), adiabatic [2] or nonadiabatic [1], can be probed by varying the optical lattice parameters.

In one such experiment, the strength of a three-dimensional optical lattice potential was tuned to induce a quantum phase transition between a Mott insulator and a superfluid of bosons [2]. This phase transition has been extensively analyzed theoretically [3–7] and numerically [8]. The two phases are characterized by markedly different many body states. The Mott phase, at large lattice potential barriers, is well described by definite real space occupation numbers. The compressible superfluid phase, on the other hand, sustains long range phase order. This phase is detected by self-interference patterns after the gas is released from the trap.

In an interesting proposal, Orzel *et al.* [1] suggested the possibility of observing OP time evolution. Basically, the bosons are prepared in the number squeezed Mott state, and then the potential is suddenly reduced into the superfluid phase. The consequent evolution of the superfluid order can be deduced from the intensity of interference patterns appearing when the atoms are released from the trap at sequential times. This would open up exploration of a new regime of *macroscopic quantum dynamics* [9–11]. The initial questions which come to mind are the following: (i) Could coherence oscillations be observed? (ii) What would be the time scale of superfluid OP evolution? (iii) What would be the damping mechanism, and damping rate of such effects?

These are the primary issues addressed in this paper. We derive the effective Hamiltonian of the superfluid OP starting from interacting bosons in a periodic lattice. We find a variational bosonic representation which describes the phase diagram and treats the elementary excitations on both the Mott and superfluid phases. In the Mott phase, the two degenerate gapped excitations become gapless at the transition. The superfluid phase reduces to a relativistic Gross-Pitaevskii action, with one (gapless) phase

mode and one (gapped) amplitude mode. We obtain a semiclassical solution of a macroscopically oscillating superfluid order and calculate its relative damping rate. This provides an estimate of the experimental regime where such oscillations should be visible. In two dimensions this region largely overlaps with the quantum critical region, as we estimate from Ginzburg's criterion. We end by commenting on critical dynamics, and how they might be observed.

The Bose Hubbard model (BHM) describes interacting bosons in an optical lattice,

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

where n_i is the boson occupation on site i . The tunneling J and interaction U are known functions of the microscopic forces [12]. At integer fillings, $\bar{n} = 1, 2, \dots$, the BHM exhibits quantum phase transitions. For large tunneling (weak optical potential barriers) $J\bar{n} \gg U$ the ground state is a superfluid (Bose condensed) with long range phase order. Below a critical tunneling strength $J < J_c(\bar{n})$, bosons are localized in incompressible (integer occupations) Mott phases.

In the vicinity of the Mott phase, number fluctuations are small. An effective Hamiltonian truncated into the subspace of lowest local number states $|\bar{n} - 1\rangle, |\bar{n}\rangle, |\bar{n} + 1\rangle$, captures the essential correlations around the transition. The reduced Hilbert space can be represented by three commuting t bosons $|\bar{n} + \alpha\rangle = t_{\alpha i}^\dagger |0\rangle$, $\alpha = 1, 0, -1$, which obey the holonomic constraint $\sum_\alpha t_{\alpha i}^\dagger t_{\alpha i} = 1$. In this subspace, the bosons of the BHM are represented by $a_i^\dagger = \sqrt{\bar{n}} t_{0i}^\dagger t_{-1i} + \sqrt{\bar{n} + 1} t_{1i}^\dagger t_{0i}$. At large \bar{n} [13], the effective Hamiltonian assumes a particularly simple pseudospin-one form

$$H_{\text{eff}} = \frac{U}{2} \sum_i (S_i^z)^2 - J\bar{n} \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y) - \mu \sum_i S_i^z, \\ S_i^+ = \sqrt{2}(t_{0i}^\dagger t_{-1i} + t_{1i}^\dagger t_{0i}), \quad S_i^z = t_{1i}^\dagger t_{1i} - t_{-1i}^\dagger t_{-1i}. \quad (2)$$

The complex superfluid OP field breaks planar spin symmetry $\Psi(\mathbf{x}_i) = \sqrt{\bar{n}}\langle S_i^+ \rangle$. It is tempting to describe the action of H_{eff} using spin one coherent states [14]. However, the Mott ground state is perturbatively connected to the O(2) rotationally invariant state $\prod_i |S_i^z = 0\rangle$. Thus, it is difficult to describe this phase as a saddle point of a spin coherent states path integral.

Alternatively we can use *modified* coherent states defined by

$$|\Omega(\theta, \eta, \phi, \chi)\rangle = \{\cos(\theta/2)t_0^\dagger + e^{i\eta}\sin(\theta/2) \times [e^{i\phi}\sin(\chi/2)t_1^\dagger + e^{-i\phi}\cos(\chi/2)t_{-1}^\dagger]\}|0\rangle. \quad (3)$$

The *mean field theory* is similar to previous variational approaches [4,5]. A homogeneous variational wave function which captures both phases is $|\Phi_{mf}\rangle = \prod_i |\Omega_i\rangle$. $\theta = 0$ describes the Mott phase, while $\theta > 0$ supports a superfluid OP $\Psi \propto \sqrt{\bar{n}}\sin\theta$. The variational energy per site is

$$e_{\text{var}} = \left(\frac{U}{2} + \mu \cos\chi\right)\sin^2\left(\frac{\theta}{2}\right) - \frac{Jz\bar{n}}{4}\sin^2\theta[1 + \bar{n}^{-1}\sin^2(\chi/2) + \sqrt{1 + \bar{n}^{-1}}\sin\chi\cos 2\eta], \quad (4)$$

where z is the lattice coordination number. The Mott phase boundaries found by minimizing e_{var} are given by

$$\mu_c/U = -\frac{1}{8\bar{n}u} \pm \frac{1}{2}\sqrt{1 - \frac{1}{u}\left(1 + \frac{1}{2\bar{n}}\right) + (4\bar{n}u)^{-2}}, \quad (5)$$

where $u = U/4J\bar{n}z$. For large \bar{n} (and commensurate density) the Mott transition occurs at $\mu = 0$ and $u = 1$. For $\bar{n} = 1$ it occurs at $U = 5.8zJ$.

The error incurred by truncation to three states per site is estimated by comparing (3) with a variational ansatz which includes 11 occupation states. Even for $\bar{n} \ll 1$ we find a wide regime ($u > 0.4$) in which the probability weight of states outside the truncated Hilbert space is less than 1%. The particle number fluctuation $\delta n < 0.6$ in this range and the error in δn is less than 10%.

To keep the presentation simple, we focus on the limit of large occupation numbers. This amounts to treating (2), which we believe retains the correct qualitative dynamics even for low occupations.

Excitations.—Consider the canonical transformation

$$\begin{aligned} b_{0i} &= \cos(\theta/2)t_0 + \sin(\theta/2)(t_{1i} + t_{-1i})/\sqrt{2}, \\ b_{ai} &= \sin(\theta/2)t_0 - \cos(\theta/2)(t_{1i} + t_{-1i})/\sqrt{2}, \\ b_{\phi i} &= (t_{1i} - t_{-1i})/\sqrt{2}, \end{aligned} \quad (6)$$

with local constraints $\sum_m b_{mi}^\dagger b_{mi} = 1$. The mean field variational state is simply the Fock state $|\Phi_{mf}\rangle = \prod_i b_{0i}^\dagger |0\rangle$. The remaining b_α^\dagger and b_ϕ^\dagger bosons create fluctu-

ations about this state. The next step is to apply the constraint in (6), and eliminate b_0 from the Hamiltonian [15]:

$$\begin{aligned} b_m^\dagger b_0 &= b_m^\dagger \sqrt{1 - b_\alpha^\dagger b_\alpha - b_\phi^\dagger b_\phi} \\ &\approx b_m^\dagger \left(1 - \frac{1}{2}b_\alpha^\dagger b_\alpha - \frac{1}{2}b_\phi^\dagger b_\phi \dots\right). \end{aligned} \quad (7)$$

Truncation at quadratic order is valid provided $\langle b_\alpha^\dagger b_\alpha \rangle, \langle b_\phi^\dagger b_\phi \rangle \ll 1$, which can be tested self-consistently in the regime of interest.

Now we can expand Eq. (2) in terms of the fluctuation operators b_α and b_ϕ , to obtain a harmonic Hamiltonian with normal and anomalous terms. It is diagonalized by a standard Bogoliubov transformation to obtain

$$H_{\text{fluc}} = \sum_{m\mathbf{k}} \omega_{m\mathbf{k}} \beta_{m\mathbf{k}}^\dagger \beta_{m\mathbf{k}}, \quad m = 1, 2 \quad (8)$$

In the superfluid phase, there is an amplitude mode and phasons

$$\begin{aligned} \omega_\alpha(\mathbf{k}) &= 2zJ\bar{n}\sqrt{1 - u^2}\gamma_{\mathbf{k}} \approx \sqrt{c^2\mathbf{k}^2 + \Delta^2}, \\ \omega_\phi(\mathbf{k}) &= Jz\bar{n}(1 + u)\sqrt{1 - \gamma_{\mathbf{k}}} \approx c|\mathbf{k}|, \end{aligned} \quad (9)$$

where $\gamma_{\mathbf{k}} = 1/z \sum_{\delta} e^{i\mathbf{k}\cdot\delta}$, $c = J\bar{n}\sqrt{z}(1 + u)$, $\Delta = 2Jz\bar{n}\sqrt{1 - u^2}$. The massive amplitude mode ω_α softens at the Mott transition and becomes degenerate with ω_ϕ . In the Mott phase, the two modes

$$\omega_p = \omega_h = \frac{U}{2}\sqrt{1 - u^{-1}\gamma_{\mathbf{k}}} \quad (10)$$

are gapped, representing particle and hole excitations. The local density of fluctuations is found to be relatively small $\langle b_{mi}^\dagger b_{mi} \rangle < 0.08$ even at the critical point. This measures the accuracy of the variational state (3) at least for the short wavelength correlations. In the critical region, which will be estimated later, we do not expect this mean field theory to yield correct exponents for the vanishing of the gap or the long wavelength correlations.

Using the modified coherent states $|\Omega\rangle$, we can construct a path integral for the evolution operator as follows. A resolution of identity is found to be of the form

$$\int_0^\pi d\theta \int_0^\pi d\chi \int_0^{2\pi} d\phi \int_{-\pi/2}^{\pi/2} d\eta \mathcal{M}(\theta) |\Omega\rangle \langle \Omega| = I, \quad (11)$$

with the invariant measure $\mathcal{M}(\theta) = C \cos\theta(3 \cos\theta - 1)$. It is also straightforward to calculate the kinetic term

$$\langle \Omega | \frac{d}{dt} | \Omega \rangle = i \sin^2(\theta/2) (\dot{\eta} - \cos\chi \dot{\phi}) \equiv -iY(t). \quad (12)$$

Equations (11) and (12) are the necessary ingredients for the path integral

$$\mathcal{U}(t) = \int \mathcal{D}\Omega \mathcal{M}(\theta) \exp\left\{i \int_0^t dt' [Y(t') - H(t')]\right\}. \quad (13)$$

We now focus on the commensurate case $\mu = 0$. An action in terms of $\Psi = \sqrt{\bar{n}} \sin\theta e^{-i\varphi}$ is obtained by integrating over the massive fields η and χ . Expanding to fourth order in $|\Psi|$ and taking the continuum limit, we arrive at a “relativistic” Gross-Pitaevskii action

$$S = \frac{1}{8Jz\bar{n}^2} \int_0^t dt' \int d^d r \{ |\dot{\Psi}|^2 - (2J\bar{n})^2 z |\nabla\Psi|^2 - (2J\bar{n}z)^2 (u-1) |\Psi|^2 - (Jz)^2 \bar{n} u |\Psi|^4 \}. \quad (14)$$

This derivation is valid to second order in the dimensionless distance to the critical point $|1-u|$.

Saddle point collective oscillations.—The time evolution of the system after a sudden change of parameters from the Mott to the superfluid state is determined by the saddle point of the action (14). The equation of motion for the OP, rescaled by its equilibrium value, $|\Psi_0| = \sqrt{2\bar{n}(1-u)/u}$ is given by

$$\ddot{\Psi} = c^2 \nabla^2 \Psi + \frac{1}{2} \Delta^2 \Psi (1 - |\Psi|^2). \quad (15)$$

The constants $\Delta = 2\sqrt{2}Jz\bar{n}\sqrt{1-u}$ and $c = 2J\bar{n}\sqrt{z}$ are identical to the expressions below (9) to leading order in $|1-u|$. For a uniform field configuration (15) is readily integrated to give the nonlinear oscillations shown in Fig. 1(b) whose time scale is set by Δ . Figure 1(a) shows the motion of the OP on the potential landscape.

Restriction to a uniform field is not justified *a priori*. In particular, topological defects may be trapped by the so-called Kibble-Zurek mechanism [16]. However, the number of trapped vortices can be diminished. If the initial Mott state is close to the transition, a large correlation length ξ_M determines the distance between seed vortices. If, on the other hand, we start deep in the Mott phase, we should consider initially zero OP with small random fluctuations, uncorrelated on the scale of a lattice constant. This amounts to a seed vortex on almost every plaquette. However, we argue that only a few will survive the first stage of evolution. To describe the initial growth of the OP, consider the linearized version of (15) around $\Psi = 0$, whose eigenmodes are easily found to be $\omega(\mathbf{k}) =$

$$S = \frac{1}{8Jz\bar{n}^2} \int dt' d^d x \{ \dot{\alpha}^2 - c^2 (\nabla\alpha)^2 - \Delta^2 \alpha^2 + (|\Psi_0|^2 + 2|\Psi_0|\alpha) [\dot{\varphi}^2 - c^2 (\nabla\varphi)^2] \}, \quad (16)$$

where $\alpha = |\Psi| - |\Psi_0|$ is the linearized amplitude mode and $c = 2\sqrt{z}J\bar{n}$. In order to compute the damping rate of the oscillating field α , it is convenient to recast the continuum theory in operator form, using the amplitude and phason operators of Eq. (8)

$$\alpha_{\mathbf{q}=0} = \sqrt{\frac{2Jz\bar{n}^2}{\Delta}} (\beta_{1,\mathbf{q}=0} + \beta_{1,\mathbf{q}=0}^\dagger), \quad (17)$$

$$\varphi_{\mathbf{k}} = \sqrt{\frac{2Jz\bar{n}^2}{ck|\Psi_0|^2}} (\beta_{2,\mathbf{k}} + \beta_{2,\mathbf{k}}^\dagger).$$

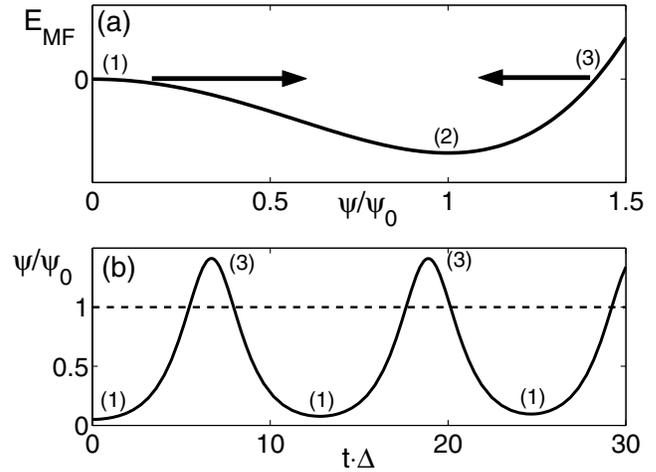


FIG. 1. Oscillations of the superfluid OP Ψ in a system prepared in the Mott state. (a) Mean field energy, where the equilibrium ground state is marked by point (2). (b) Solutions of the saddle point Eq. (15), which exhibits macroscopic oscillations. The dashed line indicates the superfluid OP in the ground state (2).

$\sqrt{(ck)^2 - \frac{1}{2}\Delta^2}$. Since it is the fastest growing, the uniform $k = 0$ mode will dominate the development of an OP. Moreover, fluctuations with $k > 1/(\xi\sqrt{2})$ do not grow at all. This implies that defects with the same topological charge must be separated by at least $\xi \equiv c/\Delta$, a large distance in the regime of interest, not far from the transition point. The impact of the few remaining vortices on the evolution is an interesting open issue which deserves further study.

Damping of the oscillations.—The collective oscillations in Fig. 1 are, in fact, a macroscopic occupation (in a coherent state) of the zero wave vector amplitude mode $\omega_a(\mathbf{k} = 0)$. Since this mode is coupled anharmonically to the low energy phasons, we expect a finite damping of the oscillations due to phason pair emission.

Expanding the action in Eq. (14), up to the harmonic and cubic interactions, we obtain

Phason pair creation is dominated by the vertex

$$H_{\text{int}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} V_{\mathbf{k}} (\beta_{1,0} \beta_{2,\mathbf{k}}^\dagger \beta_{2,-\mathbf{k}}^\dagger + \text{H.c.}). \quad (18)$$

By Fermi's golden rule, the damping rate is

$$\Gamma = \frac{N}{(2\pi)^{d-1}} \int d^d k V(\mathbf{k})^2 \delta(2ck - \Delta). \quad (19)$$

At wave vector $|\mathbf{k}| = \Delta/(2c)$, the vertex coupling constant is given by

$$V_{\mathbf{k}}^2 = \frac{(2J\bar{n}z)^2}{N\sqrt{2}} u(1-u)^{-1/2}. \quad (20)$$

Consequently, the relative damping rate diverges in one and two dimensions as

$$Q_d \equiv \frac{\Gamma_d}{\Delta} = \frac{u}{\sqrt{2}} (1-u)^{(d-3)/2}. \quad (21)$$

Oscillations could be observable for $\Gamma/\Delta < 1$ which implies $u < 0.59$ for $d = 1$ and $u < 0.73$ for $d = 2$. In three dimensions, Q_d is finite at the transition.

The damping ratio (21) can also be derived from the one loop correction to the longitudinal susceptibility [17]. Higher order terms can be resummed using a large N or renormalization group approach to obtain expressions valid in the critical region [17–19].

We comment that emitted phasons will eventually thermalize, bringing the system to a new, finite temperature, equilibrium. However, we are concerned with the shorter time transient of the system, regardless of its ultimate equilibrium fate.

Critical phenomena.—Time dependent experiments such as those proposed in Ref. [1] could potentially measure quantum critical fluctuations directly. By our mean field theory, the collective oscillation frequency, $\omega_1(k=0)$, vanishes at the transition as $(1-u)^{1/2}$ according to Eq. (9). We can estimate the quantum critical region below the critical dimension $d = 3$, using Ginzburg's criterion for the $(d+1)$ -dimensional action (14). For $d = 2$, we have obtained $|1-u| \leq 0.15$, which overlaps with the overdamped region of the critical amplitude oscillations.

In the critical region, the mean field gap exponents as read from (9) and (10) should be modified. To leading order in $\epsilon = 3-d$ the gap exponent is given in Ref. [19] by $\nu = \frac{1}{2} + 0.1\epsilon$.

Experimental parameters for the boson Hubbard model extracted from Ref. [1] can be translated into $\bar{n} \approx 50$, $2\pi\hbar/2Jz\bar{n} \approx 0.7$ ms. The oscillation period is therefore larger than this time scale by a factor of $1/\sqrt{1-u^2}$.

In summary, we have described the dynamics of bosons in an optical lattice using a modified coherent states path integral. This affords a unified description of both the superfluid and Mott phases. A system prepared in the unstable Mott state, is expected to exhibit macroscopic oscillations of the superfluid OP, with damping which increases towards the transition in one and two dimensions. It would be very interesting to investigate superfluid oscillations on the Mott side of the transition, where

there are no low energy phason modes to cause damping. Close to the transition, this would provide direct measurement of the dynamical critical exponents.

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Note added.—After completing this paper, we received a preprint by Polkovnikov *et al.* addressing a similar Mott to SF transition, using a dynamical rotator representation [20].

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