Commensurate-Incommensurate Transition of Cold Atoms in an Optical Lattice

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An atomic gas subject to a commensurate periodic potential generated by an optical lattice undergoes a superfluid-Mott insulator transition. Confining a strongly interacting gas to one dimension generates an instability where an arbitrary weak potential is sufficient to pin the atoms into the Mott state; here, we derive the corresponding phase diagram. The commensurate pinned state may be detected via its finite excitation gap and the Bragg peaks in the static structure factor.

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Ultracold atomic gases are developing into a perfectly tunable laboratory system allowing one to study complex quantum phenomena [1]. Recently, subjecting an atomic Bose-Einstein condensate to an optical lattice, Greiner *et al.* [2] have succeeded in tuning the system through a quantum phase transition separating a superfluid (S) from a Mott insulating (MI) phase. The superfluid is phase coherent and exhibits a soundlike excitation spectrum; there are strong fluctuations in the occupation number of any particular lattice site [3]. In turn, the Mott insulator is commensurate with the optical lattice, incompressible, and has a gapped spectrum. The transition involves weakly interacting bosons and is well understood within the Bose-Hubbard description [4,5]: the system turns insulating when the on-site interaction energy U becomes of the order of the hopping energy J. This strong coupling transition is a result of quenching the kinetic energy by a deep lattice potential. Remarkably, by confining the atomic gas to one dimension (1D), the strong coupling limit can be reached *without* the optical lattice: in 1D, the ratio γ between the interaction and kinetic energies per particle scales inversely with the density n and thus it is the *low*-density limit which is interacting strongly (Tonks gas) [6]. A new instability then appears in the strongly interacting 1D quantum gas at $\gamma \gg 1$: the superfluid ground state of the homogeneous system turns insulating in the presence of an arbitrarily weak commensurate optical lattice, i.e., a lattice accommodating an integer number of atoms per site. The transition to the superfluid state then is exclusively triggered by changing the boson density away from the commensurate density; hence the S-MI transition turns into a transition of the incommensurate-commensurate type. In this Letter, we analyze this new instability and derive the phase diagram for the S-MI transition in the limits of both weakly and strongly interacting gases. Remarkably, this goal can be achieved by a mapping to two classic problems, the Bose-Hubbard model introduced by Jaksch *et al.* [5] and the sine-Gordon problem describing the weakly and the strongly interacting limits of the atomic gas, respectively.

We start with interacting bosons subject to a strong transverse confining potential with frequency $\omega_\perp \gg \mu/\hbar$ (μ the chemical potential); the effective Hamiltonian becomes 1D and takes the form

$$H = \int_{-\infty}^{\infty} dx \psi^+(x)\Big(-\frac{\hbar^2}{2m}\Delta + V(x)\Big)\psi(x) + \frac{g}{2}\int_{-\infty}^{\infty} dx \psi^+(x)\psi^+(x)\psi(x)\psi(x) \qquad (1)$$

with $\psi(x)$ the bosonic field operator. The potential $V(x) = V\sin^2(kx)$ accounts for the optical lattice with wave vector $k = 2\pi/\lambda$ and may also include a harmonic confining potential. The constant g denotes the strength of the δ-function interaction potential; g is related to the 3D scattering length a_s and the transverse confining frequency $\omega_\perp$ via $g = 2\hbar\omega_\perp a_s$ [7]. It is convenient to introduce the dimensionless interaction strength $\gamma = mg/\hbar^2 n$ defined as the ratio between interaction and kinetic energies; n denotes the density and m the mass of the bosons. Obviously, in 1D the strongly interacting limit can now be reached by decreasing the density n, and for $\gamma \gg 1$ the system behaves as a gas of impenetrable bosons.

We first focus on the weakly interacting atomic gas ($\gamma \ll 1$) in a strong optical lattice $V \gg E_r$ ($E_r = \hbar^2 k^2/2m$ is the recoil energy). With all the atoms in the lowest vibrational state at each potential well, the bosonic field operator $\psi(x) = \sum_i w(x - x_i) b_i$ can be expressed in terms of the Wannier functions $w(x)$ at site i, and the Hamiltonian (1) reduces to the Bose-Hubbard model [5]

$$H_{\rm BH} = -J\sum_{\langle i,j\rangle} b_i^+ b_j + U/2\sum_i b_i^+ b_i^+ b_i b_i. \qquad (2)$$

In this tight-binding approximation, the hopping amplitude $J(V)$ derives from the exactly known width $4J = (16/\sqrt{\pi})E_r(V/E_r)^{3/4}\exp[-2(V/E_r)^{1/2}]$ of the lowest band in the 1D Mathieu equation, while the on-site interaction energy $U(V,\gamma)$ becomes $U = \sqrt{2\pi}(g/\lambda)(V/E_r)^{1/4}$ [5].

The zero temperature μ-(J/U) phase diagram of the Bose-Hubbard model is well known [4] and involves insulating Mott states at small J/U embedded in a superfluid phase. The Mott states are characterized by commensurate densities $n = 2i/\lambda$ with i particles per lattice site and the presence of an excitation gap. In 1D, the transition to the lowest Mott lobe with $i = 1$ appears at the critical value $U/J|_{\text{S-MI}} = 2C \approx 3.85$ [8], where strong fluctuations have been properly accounted for. Using the above expressions for U and J, this result translates into the γ-V phase diagram describing the atomic gas at the commensurate density $n = 2/\lambda$; the critical potential strength $V_c(\gamma)$ is obtained from the implicit equation

$$4V/E_r = \ln^2[4\sqrt{2}\pi C(V/E_r)^{1/2}/\gamma] \tag{3}$$

and is shown in Fig. 1. Consistency requires the restriction to weak coupling $\gamma \ll 1$ and large critical potential strength $V_c \gg E_r$.

Next, we turn to the limit of a weak optical lattice $V \ll E_r$. Then the above description of the atomic gas in terms of the Bose-Hubbard model breaks down, since the atoms now occupy several vibrational states in each well. In the limit where the optical lattice is only a small perturbation, the natural choice is to start from a hydrodynamic description of the homogeneous system (1). In this hydrodynamic approach, one expresses the bosonic field operator $\psi(x) \sim \sqrt{n + \partial_x\theta/\pi}\exp(i\phi)$ in terms of the long-wavelength density and phase fields θ and ϕ obeying the standard commutation relation $[\partial_x\theta(x), \phi(y)] = i\pi\delta(x - y)$. In the absence of the optical lattice, the Hamiltonian (1) reduces to the low-energy quadratic form [9]

$$H_0 = \frac{\hbar}{2\pi}\int_{-\infty}^{\infty} dx[v_J(\partial_x\phi)^2 + v_N(\partial_x\theta)^2]. \tag{4}$$

Here, the first term accounts for the kinetic energy of the bosons with $v_J = \pi\hbar n/m$, while the second term derives from the interaction energy with $v_N = \partial_n\mu/\pi\hbar$ determined by the inverse compressibility. The sound velocity

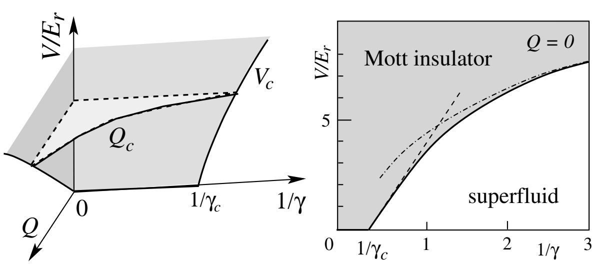

FIG. 1. Left: Schematic phase diagram illustrating the superfluid and Mott insulating phases versus parameters γ (interaction), V (optical potential), and Q (commensuration). Right: Critical amplitude V_c versus interaction $1/\gamma$ for the commensurate situation with $Q = 0$. Below $1/\gamma_c$, an arbitrary weak potential V drives the superfluid into the pinned insulating state. The dashed line denotes the asymptotic behavior near the critical point $1/\gamma_c$ as determined from the sine-Gordon model, while the dash-dotted line derives from the Bose-Hubbard criterion $U/J|_{\text{S-MI}} \approx 3.84$; the solid line interpolates between these two limits.

$v_s = \sqrt{v_J v_N}$ is consistent with the standard thermodynamic relation $mv_s^2 = n\partial_n\mu$. The Hamiltonian (4) with its linear spectrum $\omega = v_s k$ is valid only below a momentum cutoff $1/a \sim \pi n$ [10]; the choice of the length scale a fixes the energy scale of H_0. The dimensionless parameter $K = \sqrt{v_J/v_N}$ determines the quasi-long-range order of the bosonic field operator $\langle\psi^+(x)\psi(x')\rangle \sim |x - x'|^{-1/2K}$ for $|x - x'| \to \infty$; the Hamiltonian (4) describes bosonic particles with a superfluid ground state at zero temperature. The effect of interactions arising from scales smaller then a is properly accounted for by a renormalization of the inverse compressibility $\partial_n\mu(\gamma)$ [9]; the stiffness v_J remains unrenormalized. The renormalization derives from the exact solution of the Hamiltonian (1) in the absence of a periodic potential by Lieb and Liniger [10]. Then the dimensionless parameter K is a monotonically decreasing function of γ; the limiting behavior for small values of γ

$$K(\gamma \to 0) = \pi[\gamma - (1/2\pi)\gamma^{3/2}]^{-1/2} \tag{5}$$

follows from the Bogoliubov approximation in 1D. Surprisingly, this result remains quantitatively correct for γ values up to 10 [10]. At large $\gamma > 10$, the asymptotic behavior is $K(\gamma \to \infty) = (1 + 2/\gamma)^2$.

Adding now an optical lattice, it is necessary to go beyond the hydrodynamic approximation. The particle density operator has to be modified in order to account for the discrete nature of the bosons [9]

$$n(x) = \left[n + \frac{1}{\pi}\partial_x\theta\right]\left[1 + 2\sum_{l=1}^{\infty}\cos(l\theta + l\pi n x)\right]. \tag{6}$$

The periodic potential $V(x)$ in Eq. (1) gives rise to the perturbation

$$H_V = \frac{V}{2}\int_{-\infty}^{\infty} dx n(x)\cos\frac{4\pi x}{\lambda}. \tag{7}$$

Insertion of the Fourier expansion (6) in (7) generates terms of the type appearing in the quantum (1 + 1)-dimensional sine-Gordon theory [11,12]. In the following, we consider particle densities $n \approx 2/\lambda$ close to commensurability, i.e., about one boson per unit cell of the periodic lattice, and define the parameter $Q = 2\pi(n - 2/\lambda)$ as a measure of the deviation from commensurability. Then, the dominant term in Eq. (7) arising from the lowest harmonic in (6) has the conventional sine-Gordon form [4]

$$H_V = \frac{Vn}{2}\int_{-\infty}^{\infty} dx\cos[2\theta + Qx]. \tag{8}$$

The strength of the nonlinear $\cos 2\theta$ perturbation is conveniently expressed through the dimensionless parameter $u = \pi a^2 nV/2\hbar v_s$ which naturally involves the cutoff parameter a [13]. The twist Q vanishes at commensurability; away from commensurability, the finite twist Q is preferably incorporated into the free Hamiltonian (4) via the replacement $\partial_x\theta \to \partial_x\theta - Q/2$ and acts as a shift $\delta\mu = \hbar v_s Q/(2K)$ in the chemical potential for excitations.

The Hamiltonian $H_0 + H_V$ takes the form of the $(1+1)$-dimensional quantum sine-Gordon model, and is the proper low-energy description of the Hamiltonian (1) for a weak optical lattice $u \ll 1$. The quantum sine-Gordon model has been discussed in the context of the commensurate-incommensurate transition of adsorbates on a periodic substrate [14]; it defines an exactly solvable quantum field theory and has been extensively studied in the past [11–13,15]. In the following, we make use of the results pertinent to the description of the phase diagram. We first consider the evolution of the system with changing interaction γ at commensurate density $Q = 0$ and keeping the potential V fixed; see Fig. 1.

A perturbative calculation (see Ref. [12] for a review) shows that the weak optical lattice described by H_V is irrelevant for $K > K_c = 2$ and hence is unable to pin the bosons. The ground-state properties then are determined by H_0 alone and the bosons remain superfluid with a linear excitation spectrum. Using the relation $K(\gamma)$, the critical value $K_c = 2$ translates to $\gamma_c \approx 3.5$ in the γ-V phase diagram. In the strong coupling regime $K < K_c$, the perturbation H_V is relevant, and the atoms are locked to the lattice even for an arbitrary weak potential strength V. In this Mott insulating state, the excitation spectrum takes the form $E_q = \sqrt{(\hbar v_s q)^2 + \Delta^2}$ and exhibits the excitation gap Δ.

The dependence of the gap Δ on u can be obtained from a recent nonperturbative renormalization group analysis of the quantum sine-Gordon model by Kehrein [13]; for small values u and K away from $K_c = 2$ one finds $\Delta = (\hbar v_s/2a)[u/(2-K)]^{1/(2-K)}$; for $K \to 1$ this takes the simple form $\Delta \to \hbar v_s u/2a$. With K approaching $K_c = 2$ the gap vanishes exponentially; see [13] and Fig. 2(a). Exploiting the equivalence between strongly interacting bosons and free fermions in 1D [16] the opening of such a gap is easily understood in the Tonks gas limit $K = 1$. The ground-state wave function of the bosons coincides with that of free fermions [16]; at commensurate filling with one particle per unit cell, the fermions form a band insulator with a single-particle band gap $2\Delta = V/2$ at the Fermi energy. Comparing this result with the above expression $2\Delta(K=1) = \hbar v_s u/a$ fixes the cutoff at the value $1/a = \pi n$ at $K = 1$ and we obtain $u = KV/4E_r$. In the following, we ignore small corrections arising due to a possible modification in the cutoff away from $K = 1$ and arrive at the final form for the gap

$$\Delta = \frac{E_r}{K}\left[\frac{KV}{(2-K)4E_r}\right]^{1/(2-K)}. \tag{9}$$

As a result of the strong interaction between the bosons the excitations obey Fermi statistics.

Increasing the periodic potential strength V, the transition line separating the superfluid from the Mott insulator may be obtained from the Kosterlitz-Thouless nature of the scaling flow near $K_c = 2$: to lowest order in u, $K_c(u) = 2(1+u)$. Combining this result with (5) it is straightforward to determine the line $V_c(\gamma) \approx E_r(\gamma^{-1} - \gamma_c^{-1})/5.5$ in the γ-V phase diagram; see Fig. 1.

Next, we turn away from commensurability and concentrate on the stability of the Mott insulator at fixed V and $\gamma > \gamma_c(V)$, but finite twist $Q \neq 0$. Then, for an arbitrary weak potential V, the transition is of the commensurate-incommensurate type as studied by Pokrovsky and Talapov [14]. The quantum sine-Gordon model describes the competition between the preferred average interparticle distance $1/n$ at given density due to the repulsive interaction and the period $\lambda/2$ imposed by the external potential. The atoms remain locked to the weak periodic potential as long as the shift $\delta\mu$ in the chemical potential induced by the twist Q remains smaller than the single-particle energy $K\Delta$ necessary for the addition of a boson; note that the above solitonic excitations involve $1/K$ bosons [15] and therefore the required energy for an additional boson is $K\Delta$. This condition then translates into the critical twist $Q_c(\gamma, V) = 2K^2\Delta/\hbar v_s$; beyond Q_c the system develops a finite density of excitations, which interpolate between minima of the external potential, thus relieving the frustration present at incommensurate densities $Q \neq 0$.

In order to analyze the consequences of the commensurate-incommensurate transition for cold atoms in a trap, we consider a 1D Bose gas in the presence of a weak longitudinal confining potential $V(x) = m\omega^2 x^2/2$. Provided the associated oscillator length $l = (\hbar/m\omega)^{1/2}$ is much larger than the interparticle distance, the density profile in this inhomogeneous situation may be obtained from the Thomas-Fermi approximation [17]

$$\mu[n(x)] + V(x) = \mu[n(0)], \tag{10}$$

where $\mu[n]$ is the chemical potential of the homogeneous system. The central density $n(0)$ and the associated radius $R = (2\mu[n(0)]/m\omega^2)^{1/2}$ of the cloud are obtained from the normalization condition

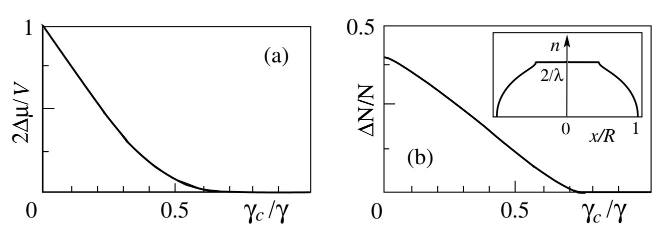

FIG. 2. (a) Size of the gap $\Delta\mu = 2K\Delta$ versus interaction strength γ for a fixed amplitude $V = E_r/2$. For $\gamma \to \infty$ the gap assumes the free fermion limit $V/2$, while it vanishes exponentially for $\gamma \to \gamma_c$. (b) Fraction of atoms in the Mott insulating phase. The inset shows the density distribution $n(x)$ with the Mott phase characterized by a locked commensurate density in the trap center, surrounded by a superfluid region.

$$N = \int_{-R}^{R} dx n(x) = 2R \int_0^{n(0)} dn \sqrt{1 - \frac{\mu[n]}{\mu[n(0)]}} \quad (11)$$

with N the particle number, provided the relation $\mu[n]$ is known explicitly. In the absence of an optical lattice the density profile is a smooth function of the coupling γ. In the limit $\gamma \gg 1$, $\mu[n] \to \mu_F[n] = (\hbar\pi n)^2/2m$ approaches the expression for the Fermi energy of an ideal Fermi gas with density n [17], resulting in a profile $n(x) = (2N/\pi R)\sqrt{1-(x/R)^2}$ with radius $R = (2N)^{1/2} l$.

Adding an optical lattice, the chemical potential $\mu[n]$ as a function of density n jumps by $\Delta\mu = 2K\Delta$ at the commensurate density $n = 2/\lambda$

$$\mu[n] = \mu_F[n] + \frac{\Delta\mu}{2} f\left(\frac{4KE_r}{\Delta\mu}\frac{\delta n}{n_c}\right) \quad (12)$$

with $\delta n = n - n_c$ ($n_c = 2/\lambda$) and

$$f(z) = \pm(1+z^2)^{1/2} - z. \quad (13)$$

The expression (13) for $f(z)$ has been derived exploiting again the equivalence between strongly interacting bosons and free fermions valid at $K = 1$ [16]. Ignoring the residual interaction between the solitons appearing for $K > 1$, the expression (13) remains a valid approximation in the relevant regime $1 < K < 2$ [13]. As a consequence, an incompressible region with a flat density profile appears in the center as the trap is filled up to the commensurate density $n = 2/\lambda$. Using the approximation (13), the density profile and the fraction $\Delta N/N$ of particles in the commensurate phase are obtained from an integration of (11) with (12); see Fig. 2(b).

Knowledge of the locked fraction $\Delta N/N$ plays an important role in the experimental detection of a commensurate Mott phase. This can be achieved by measuring the excitation gap through a phase gradient method as done previously for the Bose-Hubbard transition [2]. A more interesting alternative, however, would be to directly observe the increase in the long-range translational order in the Mott phase via Bragg diffraction [18,19]; in either case the fraction $\Delta N/N$ determines the experimentally available signal. The latter can be further enhanced by generating an array of parallel "atom wires" with the help of a strong 2D optical transverse lattice. Using numbers similar to those in the recent experiment by Greiner *et al.* [2], it is possible to generate several thousand parallel 1D wires with a transverse confining frequency $\nu_\perp = 20$ kHz. A longitudinal harmonic trap with frequency $\nu = 40$ Hz then encloses $N \approx 50$ atoms in each 1D wire; the associated central density in the absence of a longitudinal periodic potential is $n(0) = 2\ \mu\mathrm{m}^{-1}$ for $\gamma \gg 1$, commensurate with the lattice constant $\lambda/2 \approx 0.5\ \mu$m of a typical optical lattice [2]. A weak periodic potential will then lead to an incompressible Mott state in the center of the cloud, provided the parameter $\gamma = 2a_s/n(0)l_\perp^2$ is larger than the critical value $\gamma_c \approx 3.5$. For ^{87}Rb with a scattering length $a_s \approx 5$ nm, the resulting γ is equal to 1, i.e., not quite in the required range. As noted already by Petrov *et al.* [6], however, tunable and, in particular, larger values of γ may be realized either by changing a_s via a Feshbach resonance as present, e.g., in ^{85}Rb, or simply by increasing the transverse confinement frequency.

In conclusion we have shown that a commensurate Mott state can be realized in dilute 1D Bose-Einstein condensates already with an arbitrary weak lattice potential, provided that the ratio γ between the interaction and kinetic energies is larger than a critical value $\gamma_c \approx 3.5$. This instability provides a new and experimentally accessible tool for the quantitative characterization of 1D atomic gases in the strongly correlated "Tonks gas" limit. Also, the observation of a Mott state in a regime where the atoms are not confined to discrete lattice sites would give direct evidence for the granularity of matter in strongly interacting dilute gases [3].

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