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.

Atomic gases are developing into the ultimately tunable laboratory system allowing 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. This 3D bulk transition involves weakly interacting bosons and is well understood within the Bose-Hubbard description [3, 4]: 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 strong lattice potential. Amazingly, by confining the atomic gas to one dimension, the strong coupling limit can be reached without the optical lattice: in 1D, the ratio $\gamma$ 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) [5]. A new instability then appears in the strongly interacting 1D quantum gas: the superfluid groundstate in the homogeneous system turns insulating in the presence of an arbitrarily weak commensurate optical lattice and the S–MI transition changes to a transition of the incommensurate–commensurate type.

In this letter, we analyze this new instability and derive the complete 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 in Ref. 4) and the sine-Gordon problem describing the incommensurate–commensurate transition), $V$ (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 dashed-dotted line derives from the Bose-Hubbard criterion $U/J|_{\gamma=\infty} \approx 3.84$. A weakly interacting atomic gas subject to an optical lattice is well described by the Bose-Hubbard model, which starts from a tight-binding model and takes the interaction between bosons into account perturbatively; the hopping amplitude $J(V)$ and the on-site interaction energy $U(V, \gamma)$ follow from the underlying parameters of the atomic gas, the dimensionless interaction parameter $\gamma$ and the amplitude $V$ of the optical lattice. The phase diagram of the Bose-Hubbard model is well known [6] and involves insulating Mott-lobes embedded in a superfluid phase. In 3D, the mean-field analysis for densities commensurate with the lattice provides the critical parameter $U/J|_{\gamma=\infty} \approx 5.8$, in good agreement with the experimental findings of Greiner et al. [2] (here, $z$ denotes the number of nearest neighbors). Going to 1D, fluctuations become important and appreciably modify the mean-field result: numerical simulations [6, 7] place the transition at the critical value $U/J|_{\gamma=\infty} = 2C \approx 3.84$. This result is easily transformed into the $\gamma-V$ phase diagram of the weakly interacting atomic gas, once the relations $J(V)$ and $U(V, \gamma)$ to the Mott-Hubbard parameters are known; combining $J \propto \exp[-2(V/E_r)^{1/2}]$ as derived from a WKB-calculation, with the on-site repulsion $U \propto \gamma$, the transition line $V_c(\gamma)$ (see Fig. 1) then derives from the implicit equation

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

Here, $E_r = \hbar^2k^2/2m$ is the recoil energy with $m$ the boson mass and $k = 2\pi/\lambda$ the wave vector of the light generating the optical lattice $V(x) = V \sin^2(kx)$. The dimen-
tionless interaction strength $\gamma$ is defined via $\gamma = mg/h^2 n$, with $n$ the density and $g$ the strength of the $\delta$-function interaction potential; $g$ is related to the 3D scattering length $a_s$ and the transverse confining frequency $\omega_\perp$ via $g = 2h\omega_\perp a_s$.

Increasing the interaction strength $\gamma$, the critical amplitude $V_c$ of the optical lattice triggering the S-MI transition decreases, see Fig. 1; the description of the atom gas in terms of the Bose-Hubbard model breaks down and we have to look for a new starting point. For a weak optical potential, a natural choice is the 1D Bose gas with $\delta$-function interaction, which resides in the strong coupling regime at small densities $n$ [5]; the presence of the optical lattice is taken into account perturbatively. The homogeneous 1D Bose gas with $\delta$-function interaction has been solved exactly by Lieb and Liniger [1]; the corresponding physics is similar to that of the commensurate-incommensurate transition near integer filling $i = 1$, where the incommensurate phase has maximal stability.

For a quantitative theoretical analysis, it is convenient to use Haldane’s description of the interacting 1D Bose gas in terms of its long wave length density oscillations [12]. Introducing the two fields $\phi(x)$ and $\theta(x)$ describing phase and density fluctuations, the Hamiltonian of the homogeneous gas (without longitudinal confining trap and periodic potential) is a quadratic form involving kinetic and interaction energies,

$$H_0 = \frac{\hbar}{2\pi} \int dx \left[ v_J (\partial_x \phi)^2 + v_N (\partial_x \theta - \pi n)^2 \right].$$

(2)

Here, $v_J = \pi \hbar n/m$ is the analog of thebare ‘Fermi’ velocity at given average density $n$ while $v_N = \partial_n \mu/\pi \hbar$ is determined by the inverse compressibility, giving a sound velocity $v_s = \sqrt{v_J v_N}$ consistent with the standard thermodynamic relation $mv_s^2 = n\hbar^2 \mu$. For short-range repulsive interactions, the dimensionless ratio $K = \beta^2/4\pi = v_J/v_s$ is larger than one, approaching $\infty$ in the noninteracting case and unity in the hard core limit [12]. In the idealized model with $\delta$-function interactions, the exact solution by Lieb and Liniger shows that $K$ is monotonically decreasing function of the ratio $\gamma = mg/h^2 n$ between the interaction and kinetic energies; the limiting behavior for small values of $\gamma$

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

(3)

follows from the Bogoliubov approximation in 1D. Surprisingly, this result remains quantitatively correct for $\gamma$ values up to 10 [4]. At large $\gamma > 10$, the asymptotic behavior is $K(\gamma \to \infty) = (1 + 2\gamma/\pi)^2$.

For our subsequent analysis, it is convenient to introduce the conjugate fields $\Theta(x) = (2/\beta) [\theta(x) - \pi n x]$ and $\Pi(x) = -\hbar (\beta/2\pi) \partial_x \phi(x)$ obeying the commutation relation $[\Theta(x), \Pi(x')] = i\hbar \delta(x - x')$. Using these fields,

$$H_0 = \frac{\hbar v_s}{2} \int dx \left[ (\Pi/h)^2 + (\partial_x \Theta)^2 \right]$$

(4)

takes the form of the Hamiltonian for a 1D harmonic string with a linear spectrum $\omega = v_s q$ describing the long wave length density modulations of the interacting Bose gas. The assumption of a linear spectrum inherent in the simple form [4] is valid only below a momentum cutoff $1/\alpha \approx \pi n$ [4]; the choice of the length scale $\alpha$ fixes the energy scale of $H_0$. The Boson density operator $n(x)$ is related to the field $\Theta(x)$ by [12]

$$n(x) = \left[ n + \frac{\beta}{2\pi} \partial_x \Theta \right] \left( 1 + 2 \sum_{l=1}^\infty \cos \left( \frac{l\beta \Theta}{2} + l\pi n x \right) \right);$$

(5)

the last factor accounts for the discrete nature of the particles. Adding an external periodic potential with amplitude $V/2$ and period $\lambda$ gives rise to the perturbation

$$H_V = \frac{V}{2} \int dx \ n(x) \cos \frac{4\pi x}{\lambda}$$

(6)

thus confine ourselves to studying the commensurate-incommensurate transition near integer filling $i = 1$, where the incommensurate phase has maximal stability.
As noted already by Haldane, insertion of the Fourier expansion \( \tilde{x} \) generates terms of the type appearing in the quantum \((1+1)\)-dimensional sine-Gordon theory \([3, 4]\). Close to commensurability the dominant term arising from the lowest harmonic in \( \tilde{x} \) has the conventional sine-Gordon form \([3]\)

\[
H_c = \frac{V}{2} \int dx \cos [\beta \Theta + Qx] 
\]

(7)

with coupling parameter \( \beta = 2(\pi K)^{1/2} \) and a twist \( Q = 2\pi \eta (n - 2/\lambda) \). The strength of the nonlinear \( \cos \Theta \)-perturbation is conveniently expressed through the dimensionless parameter \( u = \pi \omega/2\hbar v_o \) which naturally involves the cutoff parameter \( u \) \([15]\). The twist \( Q \) vanishes at commensurability; away from commensurability the finite twist \( Q \) acts as a chemical potential for excitations and is preferably incorporated into the free Hamiltonian \([3]\) via the replacement \( \partial_x \Theta \rightarrow \partial_x \Theta - Q / \beta \).

At fixed potential \( V \), the quantum sine-Gordon model describes the competition between the preferred average inter-particle distance at given density due to the repulsive interaction and the period imposed by the external potential. A perturbative calculation (see Ref. \([1]\) for a review) tells that for \( \beta^2 / 4\pi \) \( = 2 \) a weak periodic potential is unable to pin the density; hence for \( K > K_c \) \((\gamma \leq \gamma_c \approx 3.5)\) the ground state remains gapless and superfluid in the presence of a small-amplitude lattice potential. In the strong coupling regime \( K < 2 \), however, the atoms are locked even to a weak lattice, as long as the twist \( Q \) is less than a critical value \( Q_c \). Beyond that, there is a finite density of ‘solitons’ (or domain walls for adsorbates on a periodic substrate, see Ref. \([1]\)), which interpolate between minima of the external potential, relieving the frustration present in incommensurate densities \( Q \neq 0 \). The ‘solitons’ behave like relativistic particles with energy \( E_q = \hbar v_o \sqrt{q^2 + M^2} \) and reestablish the superfluid response. The ‘mass’ \( M \) determines the excitation gap in the Mott insulating state, which translates into a jump \( \Delta \mu \) in the chemical potential at the commensurate density: given that an additional/missing atom involves \( K \) solitonic excitations with energy \( E_q = 0 = \hbar v_o M \) \([16]\) one obtains

\[
\Delta \mu = \frac{2\pi \hbar^2 n}{m} M; 
\]

(8)

furthermore, this mass is also simply related to the critical twist via \( Q_c = 2K^2M \). The precise numerical value of \( M \) depends on the high momentum cutoff \( 1/a \) via the dimensionless amplitude \( u \) of the lattice potential. The free-fermion limit \( K = 1 \) fixes this cutoff at \( 1/a \approx \pi n \), resulting in the simple form \( u = V/4E_r \); we ignore small corrections arising due to a possible modification in the cutoff away from \( K = 1 \). The dependence of the mass \( M \) on \( u \) can be obtained from a recent nonperturbative renormalization group analysis of the quantum sine-Gordon model by Kel’rein \([3]\); for small values \( V \ll E_r \) and \( K \) away from \( K_c \), the gap in the chemical potential takes the form

\[
\Delta \mu = 2E_r \left[ \frac{V}{(2 - K)4E_r} \right]^{1/(2 - K)}. 
\]

(9)

In the limit \( K \rightarrow 1 \), the size of the gap approaches \( V/2 \), in agreement with the above fermionic picture of the Tonks gas limit, where the appearance of an insulating ground state, even for a weak periodic potential, is due to the opening of a single-particle band gap at the Fermi energy. In the practically accessible regime of large but finite \( \gamma \) \( > \gamma_c \) the gap depends on \( V \) in the more complicated manner as given by \( \tilde{\mu} \) and vanishes exponentially as \( K \) approaches \( K_c = 2 \) \([15]\), see Fig. 2(a). Similarly, the density range \( n - 2/\lambda = \pm Q_c / 2\pi \) over which the ground state remains locked approaches zero as \( K \rightarrow K_c \). Finally, for \( K > 2 \), the dependence of the critical interaction parameter \( K_c \) \((\gamma_c) \) on the lattice amplitude \( V \) follows easily 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 \( \tilde{\mu} \) it is straightforward to determine the line \( \tilde{V}(\gamma) \) separating the gapped insulating regime from the superfluid at small but finite values of \( u \), see Fig. 1.

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

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 inter-particle distance, the density profile in this inhomogeneous situation may be obtained from the Thomas-Fermi approximation \([17]\)

\[
\mu[n(x)] + V(x) = \mu[n(0)] 
\]

(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 is obtained from the normalization condition

\[
N = \int_{-R}^{+R} dx \, n(x) = 2R \int_{0}^{n(0)} dn \sqrt{1 - \frac{\mu[n]}{\mu[n(0)]}}. 
\]

(11)
with $N$ the particle number, provided the relation $\mu[n]$ is known explicitly.

In the absence of an optical lattice the density profiles are smooth functions of the coupling $\gamma$ \cite{17}. In the limit $\gamma \gg 1$, $\mu[n] \to \nu_\nu[n] = (\hbar \pi n)^2 / 2m$ approaches the Fermi energy of an ideal Fermi gas with density $n$, resulting in a profile $\rho(x) = (2N/\pi R)^2 \sqrt{1 - (x/R)^2}$ with radius $R = (2N)^{1/2} / 2$. Adding now a periodic potential which is nearly commensurate with the density in the trap center opens a gap $\Delta \mu$ in the chemical potential. The density profile will then exhibit a flat, incompressible regime in the trap center. In order to find the detailed shape of the density profile, we approximate the size-Gordon model in its strong coupling, gapped phase by a gas of noninteracting relativistic Fermions of mass $M$; in the relevant regime $1 < K < 2$, this approximation is known to work extremely well \cite{15}. The chemical potential as a function of density can then be calculated explicitly,

$$\mu[n] \approx \nu_\nu[n] + \frac{\Delta \mu}{2} f \left( \frac{4KE_\nu \delta n}{\Delta \mu \nu_\nu[n]} \right)$$

(12)

with $\delta n = n - n_c$ ($n_c = 2/\lambda$). The dimensionless function

$$f(z) = \pm \left( 1 + z^2 \right)^{1/2} - z$$

(13)

is discontinous at $z = 0$ and incorporates, via (12), the jump $\Delta \mu$ in the chemical potential at $n_c$ associated with the incompressible commensurate state. Using this approximation, the density profile and the fraction of particles participating in the commensurate phase derive 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 \cite{3}. Alternatively, it should be possible to directly observe the increase in the long-range translational order in the Mott phase via Bragg diffraction \cite{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 \textit{et al.} \cite{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 $n(0) = 2 \mu m^{-1}$ for $\gamma \gg 1$, commensurate with the lattice constant $\lambda/2 \approx 0.5 \mu m$ of a typical optical lattice \cite{2}. A weak periodic potential will then lead to an incompressible Mott state in the center of the cloud, provided the parameter $\gamma = 2a_s / n(0)f_\perp^2$ is larger than the critical value $\gamma_c \approx 3.5$. For $^{87}$Rb with a scattering length $a_s \approx 5 \mu m$, the resulting $\gamma$ is equal to one, i.e., not quite in the required range. As noted already by Petrov \textit{et al.} \cite{5}, however, larger and in particular tunable values of $\gamma$ may be realized by changing $a_s$ via a Feshbach resonance as present, e.g., in $^{85}$Rb.

In conclusion we have shown that a commensurate Mott state can be realized in dilute 1D BEC’s already with an arbitrary weak lattice potential, provided that the ratio $\gamma$ 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.

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