Mott-Hubbard transition of cold atoms in optical lattices

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Abstract. We discuss the superfluid to Mott-insulator transition of cold atoms in optical lattices recently observed by Greiner et.al. (Nature 415, 39 (2002)). The fundamental properties of both phases and their experimental signatures are discussed carefully, including the limitations of the standard Gutzwiller-approximation. It is shown that in a one-dimensional dilute Bose-gas with a strong transverse confinement (Tonks-gas), even an arbitrary weak optical lattice is able to induce a Mott like state with crystalline order, provided the dimensionless interaction parameter is larger than a critical value of order one. The superfluid-insulator transition of the Bose-Hubbard model in this case continuously evolves into a transition of the commensurate-incommensurate type with decreasing strength of the external optical lattice.
1. Introduction

The realization of BEC in ultracold atomic gases [1-3] has opened a wide area of research in atomic physics, where quantum-statistical effects are of crucial importance: upon cooling, bosonic atoms in a trap condense into a superfluid state at a rather sharply defined critical temperature $T_c$ while fermionic atoms continuously evolve into a degenerate noninteracting gas, resisting spatial compression due to their Fermi pressure [4]. Both features are a consequence of the purely statistical interaction between the atoms. By contrast, the actual interparticle potential plays only a comparatively minor role. To see this, we start from the standard pseudopotential description, which replaces the complicated interatomic potential by an effective contact interaction of the form

$$U(\vec{x}) = \frac{4\pi \hbar^2 a_s}{m} \cdot \delta(\vec{x}) = g \cdot \delta(\vec{x})$$

containing the exact s-wave scattering length $a_s$ as the only parameter. For identical fermions, there is no s-wave scattering due to the Pauli-principle and thus we obtain an ideal Fermi gas to lowest order. For bosons, in turn, $a_s$ is finite, however at a given density $n$ the importance of direct interaction effects can be estimated from the ratio

$$\gamma = \frac{\epsilon_{\text{int}}}{\epsilon_{\text{kin}}} = \frac{gn}{\hbar^2 n^{2/3}/m} \approx n^{1/3} a_s$$

between the interaction and the kinetic energy per particle. Now the average interparticle spacing $n^{-1/3}$ is usually much larger than the scattering length and thus $\gamma$ is very small, with typical values around 0.02. This puts us into the weak coupling limit where the many body ground state of $N$ bosons is well approximated by a simple product [5]

$$\Psi_{\text{GP}}(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N) = \prod_{i=1}^N \phi(\vec{x}_i)$$

in which all atoms are in the identical single particle state $\phi(\vec{x})$. Taking (3) as a variational ansatz, the optimal 'macroscopic wave function' $\phi(\vec{x})$ is found to obey the well known Gross-Pitaevski equation. It describes - even on a quantitative level - a wealth of remarkable and nontrivial properties of trapped condensates from interference between different condensates [6] to collective modes [7] or vortices [8]. From a many body point of view, the effective single particle or Hartree-description (3) is of course the simplest of all possible cases, containing no interaction induced correlations between different atoms at all. A first step to go beyond this mean field description is the well known Bogoliubov theory. This is usually introduced by considering small fluctuations around the Gross-Pitaevski equation in a systematic expansion in the number of noncondensed particles [9]. As emphasized, for example, by Leggett [5], it is more instructive from a many body point of view to formulate Bogoliubov theory in such a way that the many body boson ground state is approximated by an optimized product.
\[ \Psi_{Bog.}(\vec{x}_1, \vec{x}_2, \ldots \vec{x}_N) = \prod_{i<j} \phi_2(\vec{x}_i, \vec{x}_j) \]  

of identical, symmetric two particle wave functions \( \phi_2 \). This allows us to build in the interaction beyond the mean field potential by suppressing configurations in which particles \( i \) and \( j \) are close together. The many body state thus incorporates two-particle correlations which are important e.g. to obtain the standard sound modes and the related coherent superposition of 'particle' and 'hole' excitations [10]. However, even the Bogoliubov description is restricted to the regime \( \gamma \ll 1 \), where interactions lead only to a small depletion of the condensate at zero temperature. The associated ground state is again characterized by a macroscopic matter wave field and continuously evolves from that of a noninteracting gas.

An obvious way to go beyond the weak coupling regime is to increase the dimensionless interaction strength parameter \( \gamma \) by increasing the scattering length via a Feshbach resonance. Of course, this method is limited by the fact that the associated condensate lifetime strongly decreases due to three-body losses which occur at a rate [11]

\[ \dot{n}/n = -\text{const.} \frac{\hbar}{m} (na_s^2)^2 \]  

In spite of this problem, this method of reaching the strong coupling regime has been followed quite successfully recently, see e.g. [12] and [13]. In the following, we will discuss an alternative route to reach strong coupling even at small values of \( n^{1/3}a_s \). It is based on confining cold atoms in the periodic potential of an optical lattice generated via the dipole force which atoms experience in a standing, off-resonant light field. Depending on the sign of the polarizability, the atoms are attracted either to the nodes or the antinodes of the laser intensity. In this manner, one-, two-, or three-dimensional lattices can be created with a lattice constant \( a = \lambda/2 \) which is half the laser wavelength (typically \( a \) is in the range between 0.5 \( \mu \)m and 5 \( \mu \)m). In the simplest case, three orthogonal, independent standing laser fields with wave vector \( k \) produce a separable 3d lattice potential

\[ V(x, y, z) = V_0 \left( \sin^2 kx + \sin^2 ky + \sin^2 kz \right) \]  

with a tunable amplitude \( V_0 \). A convenient measure for the strength \( V_0 \) of the lattice potential is the recoil energy \( E_r = \hbar k^2/2m \) which is typically in the few kHz range. In a deep optical lattice with \( V_0 \gg E_r \), the energy \( \hbar \omega_0 = 2E_r \left( V_0/E_r \right)^{1/2} \) of local oscillations in the well is much larger than the recoil energy and each well supports many quasi-bound states. For instance in the deepest lattices generated in the recent experiments by Greiner et.al [14] with \( V_0 = 22E_r \) this number is around four while the local oscillation frequency has reached 30kHz. Provided all the atoms are in the lowest vibrational level at each site, their motion is frozen except for the small tunneling amplitude to neighbouring sites. The atoms are then effectively confined to move in the lowest band
of the lattice. With $|\vec{I}\rangle$ as the states localized at site $\vec{I}$, the appropriate single particle eigenstates are Bloch-waves $|\vec{q}\rangle = \sum_l \exp i\vec{q} \cdot \vec{l} |\vec{l}\rangle$ with quasimomentum $\vec{q}$ and energy

$$\epsilon(\vec{q}) = \frac{3}{2} \hbar \omega_0 - 2J (\cos q_x a + \cos q_y a + \cos q_z a)$$

(7)

The bandwidth parameter $J$ is essentially the gain in kinetic energy due to nearest neighbour tunneling. In the limit $V_0 \gg E_r$ it can be obtained from the exact result for the width of the lowest band in the 1d Mathieu-equation

$$J = \frac{4}{\sqrt{\pi}} E_r \left( \frac{V_0}{E_r} \right)^{3/4} \exp -2 \left( \frac{V_0}{E_r} \right)^{1/2}$$

(8)

Obviously, in a lattice, it is $J$ which plays the role of the kinetic energy per particle in the homogeneous case. The effective value of $\gamma = \epsilon_{int}/\epsilon_{kin}$ is therefore very large in optical lattices, increasing exponentially with $V_0/E_r$. Thus it is the quenching of the kinetic energy for motion in the lowest band which drives cold atoms into the strong coupling regime, even though $n^{1/3}a_s$ may still be much smaller than one. Alternatively, one may argue that $\epsilon_{kin}$ becomes small because atoms in a deep optical lattice have an exponentially large effective mass $m^* = \hbar^2 / 2a^2 J$. To really obtain interesting many body effects it is of course necessary to have the interaction and the kinetic energy of the same order. This requires optical lattices in which the number of atoms per site is of order one or larger, a regime which has been possible to reach only recently with Bose-Einstein-condensates.

2. The superfluid- to Mott-insulator transition

In the following, I will discuss the Mott-Hubbard transition for bosonic atoms, as a generic example illustrating how cold atoms in optical lattices can be used to study genuine many body phenomena in dilute gases. The original idea suggesting the possibility of nontrivial many body states using cold atoms in optical lattices is due to Jaksch et.al. [15]. Their starting point is the so called Bose-Hubbard model, originally introduced by Fisher et.al. in a rather different context [16]. It describes bosons hopping with amplitude $J$ to nearest neighbors on a regular lattice of sites $l$. The particles interact with a zero-range, on-site repulsion $U$, disfavouring configurations with more than one atom at a given site. With $\hat{b}_l^\dagger$ as the creation operator of a boson at site $l$ and $\hat{n}_l = \hat{b}_l^\dagger \hat{b}_l$ the associated number operator, the Hamiltonian reads

$$\hat{H} = -J \sum_{<ll'>} \hat{b}_l^\dagger \hat{b}_{l'} + \frac{U}{2} \sum_l \hat{n}_l(\hat{n}_l - 1) + \sum_l \epsilon_l \hat{n}_l$$

(9)

Here $<ll'>$ denotes a sum over nearest neighbour pairs, including double counting. The last term with a variable on-site energy $\epsilon_l$ is introduced to describe the effect of the trapping potential and acts like a spatially varying chemical potential. The form of the interaction term is precisely that obtained by viewing each site as a local condensate
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with a Gross-Pitaevski mean field potential. The relevant interaction parameter $U$ is thus given by an integral over the on-site wave function $w(\vec{x})$ via

$$U = g \int |w(\vec{x})|^4 = \sqrt{\frac{8}{\pi}} k a_s E_r \left( \frac{V_0}{E_r} \right)^{3/4}$$

(10)

The explicit result is obtained by taking $w(\vec{x})$ as the Gaussian ground state in the local oscillator potential around any of the sites. More precisely, $w(\vec{x})$ is the exact Wannier wave function of the lowest band. In a separable periodic potential like that in (6), $w(\vec{x})$ decays exponentially in all directions rather than in a Gaussian manner [17], however this does not seriously affect the calculation of $U$ in the deep lattice limit $V_0 \gg E_r$. From eqn.(10), it is obvious that the strength of the repulsion increases with $V_0$ due to the tighter squeezing of the on-site wave function $w(\vec{x})$. With increasing $V_0/E_r$, therefore, not only does the kinetic energy drop exponentially, but at the same time the interaction energy increases. As a result, it is possible to reach the strong coupling regime $U \approx J$ simply by increasing the depth of the optical lattice potential. Regarding the requirements necessary for the validity of the discrete lattice model (9), it is obvious that the atoms have to remain in the lowest vibrational state at each site even in the presence of strong interactions. We thus require that $U \ll \hbar \omega_0$ which is well obeyed even in deep optical lattices as long as $k a_s \ll 1$.

The zero temperature phase diagram of the homogeneous Bose-Hubbard model was first discussed by Fisher et.al. [16]. Although there are considerable quantitative differences between the case of one-, two- or three-dimensional lattices, the qualitative structure is similar in all cases and is shown schematically in Figure 1. At large $J/U$ the kinetic energy dominates and the ground state is a delocalized superfluid (SF). At small values of $J/U$, interactions dominate and one obtains a series of so called Mott-insulating (MI) phases with fixed integer filling $\bar{n} = 1, 2, \ldots$ depending on the value of the chemical potential $\mu$. To understand the peculiar structure of these 'Mott-lobes', consider first the case of unit filling, i.e. the number $N$ of atoms is precisely equal to the number $M$ of lattice sites. In the limit where $V_0$ is very large compared to $E_r$, there is no hopping ($J = 0$) and the obvious ground state

$$|\Psi_{MI} > (J = 0, \bar{n}) = \prod_l (|\bar{n} >_l)$$

(11)

is a simple product of local Fock-states with precisely one atom ($\bar{n} = 1$) per site. Upon lowering $V_0$, the atoms start to hop around, which necessarily involves double occupancy, increasing the energy by $U$. Now as long as the gain $J$ in kinetic energy due to hopping is smaller than $U$, the atoms remain localized although the ground state is no longer a simple product state as in (11). Once $J$ becomes of order or larger than $U$, the gain in kinetic energy outweighs the repulsion due to double occupancies and the atoms will be delocalized over the whole lattice. In the limit $J \gg U$ the many body ground state becomes simply an ideal Bose-Einstein-condensate where all $N$ atoms are in the $\vec{q} = 0$ Bloch-state of the lowest band. Including the normalization factor in a lattice with a total number of $M$ sites, this state can be written in the form
Figure 1. Schematic zero temperature phase diagram of the Bose-Hubbard model. The dashed lines of constant integer density $<\hat{n}> = 1, 2, 3$ in the superfluid phase (SF) hit the corresponding Mott-insulating (MI) phases at the tips of the lobes at a critical value of $J/U$, which decreases with density $\bar{n}$. For $<\hat{n}> = 1 + \varepsilon$ the line of constant density stays outside the $\bar{n} = 1$ MI because a fraction $\varepsilon$ of the particles remains superfluid down to the lowest values of $J$. In an external trap with a $\bar{n} = 3$ MI phase in the center, a series of MI and SF regions appear by going towards the edge of the cloud, where the local chemical potential has dropped to zero.

$$|\Psi_{SF,N} > (U = 0) = \left( \frac{1}{\sqrt{M}} \sum_{i=1}^{M} \hat{b}_{i}^{\dagger} \right)^{N} |0 >. \quad (12)$$

For large enough $J$ therefore, we recover a Gross-Pitaevski like description in terms of one, macroscopically occupied state. In two- and three-dimensional lattices, the critical value for the transition from a MI to a SF is reasonably well described by a mean-field approximation, giving $(U/J)_c = 5.8z$ for $\bar{n} = 1$ and $(U/J)_c = 4\bar{n}z$ for $\bar{n} \gg 1$. Here $z$ is the number of nearest neighbours. In one dimension there are strong deviations from a mean-field approximation and the corresponding values are $(U/J)_c = 3.84$ for $\bar{n} = 1 [18,19] \text{ and } (U/J)_c = 2.2\bar{n}$ for $\bar{n} \gg 1$. The latter result follows from mapping the Bose-Hubbard model to a chain of Josephson junctions, for which the critical value of the transition to a MI phase is known precisely.

Consider now a filling with $<\hat{n}> = 1 + \varepsilon$ which is slightly larger than one. For large $J/U$ the ground state has all the atoms delocalized over the whole lattice and the situation is hardly different from the case of unit filling. Upon lowering $J/U$, however, the line of constant density remains slightly above the $\bar{n} = 1$ 'Mott-lobe', and stays in the SF regime down to the lowest $J/U$ (see Fig.1). For any noninteger filling, therefore,
the ground state remains SF as long as the atoms can hop at all. This is a consequence of the fact, that even for \( J \ll U \) there is a small fraction \( \varepsilon \) of atoms which remain SF on top of a frozen MI-phase with \( \bar{n} = 1 \). Indeed this fraction can still gain kinetic energy by delocalizing over the whole lattice without being blocked by the repulsive interaction \( U \) because two of those particles will never be at the same place. The same argument applies to holes when \( \varepsilon \) is negative.

In order to describe the situation in a weak harmonic trap, we use the standard approximation that a slowly varying external potential may be accounted for by a spatially varying chemical potential \( \mu_l = \mu(0) - \epsilon_l \) (we choose \( \epsilon_l = 0 \) at the trap center). Assuming that the chemical potential \( \mu(0) \) at trap center falls into the \( \bar{n} = 3 \) 'Mott-lobe', one obtains a series of MI domains separated by a SF by moving to the boundary of the trap where \( \mu_l \) vanishes (see Fig.1) [15]. In this manner, all the different phases which exist for given \( J/U \) below \( \mu(0) \) are present simultaneously. Since the defining property of a MI-phase is its incompressibility \( \partial n/\partial \mu = 0 \), the atomic density stays constant in the Mott-phases, even though the external trapping potential is rising. An estimate for the width of the incompressible domains is obtained by noting that for \( J \ll U \) the range in chemical potential over which the density remains constant is close to \( U \). In a quadratic confining potential with axial frequency \( \nu_z \approx 40\text{Hz} \) and with typical values \( U/h = 1\text{kHz} \), the width of the incompressible MI-states is around 10\( \mu\text{m} \). It remains an experimental challenge to spatially resolve the SF and MI phases in a trap, thus verifying the crucial property of incompressibility.

In practice, the observation of the SF to MI transition is done in the usual manner by absorption imaging the atomic cloud after a given expansion time. The corresponding series of images is shown in Fig.2 for different values of \( V_0 \), ranging between \( V_0 = 0 \) (a) and \( V_0 = 20E_r \) (h). One observes a series of 'Bragg-peaks' around the characteristic 'zero-momentum' peak of a condensate in the absence of an optical lattice. With increasing \( V_0 \) these peaks become more pronounced. Beyond a critical lattice depth around \( V_0 = 13E_r \) (e), this trend is suddenly reversed, however, and the 'Bragg peaks' eventually disappear completely. In order to understand, to which extent these pictures actually provide a direct evidence for the existence of a SF to MI transition predicted by the Bose-Hubbard model, we neglect the inhomogeneous nature of the atomic cloud and assume that the absorption images simply reflect the momentum distribution. For atoms which are confined to move in the lowest band of the lattice, it is straightforward to show that the momentum (not quasi-momentum [20]) distribution

\[
n(\vec{k}) = n|w(\vec{k})|^2 \sum_{\vec{R}} e^{i\vec{k} \cdot \vec{R}} \rho_1(\vec{R})
\]

(13)

can be expressed in terms of the exact one-particle density matrix \( \rho_1(\vec{R}) = < \hat{b}^\dagger_{\vec{R}} \hat{b}_{\vec{R}} > \) at separation \( \vec{R} \) and the Fourier transform \( w(\vec{k}) \) of the associated Wannier wave-function. The summation in (13) is over all lattice vectors \( \vec{R} \), which are integer multiples of the three primitive vectors of the given lattice. Now the SF and MI phases are distinguished quite generally by the behaviour of the one particle density matrix (or first order
coherence function in quantum optics terminology) at large separation. In the SF, $\rho_1(\vec{R})$ approaches a finite value $\lim_{|\vec{R}| \to \infty} \langle \hat{b}_\vec{R}^\dagger \hat{b}_0 \rangle = n_0/n$ which defines the condensate density $n_0$ [21]. For the MI phase, in turn, $\rho_1(\vec{R})$ decays to zero exponentially. Using (13), the SF phase of cold atoms in an optical lattice can thus quite generally be characterized by the fact that at reciprocal lattice vectors $\vec{k} = \vec{G}$ defined by $\vec{G} \cdot \vec{R} = 2\pi$ times an integer, the momentum distribution $n(\vec{k} = \vec{G})$ has a peak

$$n(\vec{k} = \vec{G}) = N \cdot n_0 |w(\vec{G})|^2$$

which scales with the total number $N$ of particles. This is the expected behaviour for the interference pattern from a periodic array of phase coherent sources of matter waves and is precisely analogous to the more standard Bragg-peaks in the static structure factor of a solid, with the condensate fraction playing the role of the Debye-Waller factor [22]. The fact that the peaks in the momentum distribution at $\vec{k} = \vec{G}$ initially grow with increasing depth of the lattice potential is a result of the strong decrease in spatial extent of the Wannier function $w(\vec{x})$, which entails a corresponding increase in its Fourier transform $w(\vec{k})$ at higher momenta. It is important to realize that there is no broadening of the peaks as long as $\rho_1(\vec{R} \to \infty)$ is finite, in agreement with the experimental observations [14]. In the MI regime, where $\rho_1(\vec{R})$ decays to zero, remnants of the 'Bragg-peaks' still remain (see e.g. (f) in Fig.2) as long as $\rho_1(\vec{R})$ extends over several lattice spacings, because the series in (13) adds up constructively at $\vec{k} = \vec{G}$. Physically this reflects the fact that phase coherence is still present over distances much larger than one lattice spacing provided one is close to the transition to superfluidity. In contrast to the SF regime, however, these peaks are now broadened and do not scale with the total number $N$ of particles. In the extreme MI limit $J \ll U$, hopping of atoms completely vanishes and $\rho_1(\vec{R})$ is zero beyond $\vec{R} = 0$. Coherence is then completely lost and the momentum distribution is a structureless Gaussian, reflecting the Fourier transform of the Wannier wave function (see (h) in Fig.2). These arguments show that
for a large and homogeneous system there is indeed a sharp signature of the SF to MI transition in the interference pattern. It is connected with the existence or not of (off-diagonal) long range order in the one particle density matrix, which effectively measures the range of phase coherence and the condensate fraction. Of course the actual system is not homogeneous and a numerical computation of the interference pattern is necessary for a quantitative comparison with experiment [23]. Due to the finite size and the fact that different MI phases are involved, the pattern evolves continuously from the SF to the MI regime. Indeed, as is evident from the phase diagram in Fig.1, the critical value of $J/U$ is different for the two different MI phases $\tilde{n} = 1$ and $\tilde{n} = 2$ which are present in the trap. Nevertheless, a rather sharp transition is observed experimentally, because $J/U$ depends exponentially on the control parameter $V_0/E_r$. The small change from $V_0 = 13E_r$ in (e) to $V_0 = 14E_r$ in (f) thus covers a range in $J/U$ wider than that which would be required to distinguish the $\tilde{n} = 1$ from the $\tilde{n} = 2$ transition.

A second signature of the SF to MI transition is the appearance of a finite excitation gap $\Delta \neq 0$ in the MI. Deep in the MI phase, this gap has size $U$, which is just the increase in energy if an atom tunnels to an already occupied adjacent site (note that this is much smaller than the gap $\hbar\omega_0$ for the excitation of the next vibrational state). The existence of this gap has been verified experimentally by applying a phase gradient in the MI and measuring the resulting excitations produced in the SF at smaller $V_0/E_r$ [14]. In this manner the fact that $\Delta(J \ll U) = U$ was verified for a range of $V_0$, all reasonably deep in the MI phase. For reasons discussed above, however, it has not been possible to see the vanishing of the gap near the transition, which should scale like $\Delta \sim (J_c - J)^{1/2}$ in the three-dimensional case [16]. In the SF regime, there is no excitation gap and instead the homogeneous system exhibits a sound like mode with frequency $\omega(q) = cq$. The associated sound velocity follows from the thermodynamic relation $mc^2 = n_s \partial\mu/\partial n$ and thus gives information about the superfluid density $n_s$. The existence of a sound like excitation even in the presence of an underlying lattice which explicitly breaks translation invariance is a consequence of long range phase coherence in the SF. Its observation would thus constitute an independent proof that the atoms move coherently over the whole lattice and thus phase gradients give rise to dissipationless currents.

Finally we discuss the change in the atom number statistics at individual sites between the SF and the MI regime. This issue has been investigated in a very recent beautiful experiment, observing collapse and revival of the matter wave due to the coherent superposition of states with different atom numbers in the SF [24]. As noted above, the ground state (11) in the extreme MI limit is a product of Fock states with a definite number $\tilde{n}$ of particles at each site. At finite hopping $J \neq 0$, this simple picture breaks down because the atoms have a finite amplitude to be at different sites. The many body ground state can then no longer be written as a simple product state as in (11). In the opposite limit $U \to 0$, the ground state is a condensate of zero quasimomentum Bloch states. It turns out, that the probability of finding precisely $n$ atoms at any given site in the associated state (12) is close to a Poissonian distribution. More precisely, in
the limit $N, M \to \infty$ at fixed 'density' $N/M$, the state (12) becomes indistinguishable in a local measurement from a coherent state

$$|\Psi_{SF} > (U = 0) = \exp \sqrt{N} b_q^\dagger 0 > \prod_{l=1}^{M} \left( \exp \sqrt{\frac{N}{M}} b_l^\dagger 0 >_l \right)$$

(15)

which factorizes into a product of local Poissonian states with average $< \hat{n}_l > = N/M$ because boson operators at different sites commute. We have thus come to the remarkable conclusion that for integer densities $N/M = \bar{n} = 1, 2, \ldots$ the many body ground state may be written in a local product form

$$|\Psi_{GW} > = \prod_{l} \left( \sum_{n=0}^{\infty} c_n | n >_l \right)$$

(16)

in both limits $J \to 0$ and $U \to 0$. The associated atom number probability distribution $p_n = |c_n|^2$ is either a pure Fock or a full Poissonian distribution. It is now very plausible to use the factorized form (16) as an approximation for arbitrary $J/U$, taking the coefficients $c_n$ as variational parameters which are determined by minimizing the ground state energy [25]. As first pointed out by Rokhsar and Kotliar [26], this is effectively a Gutzwiller ansatz for bosons. Beyond being very simple computationally, this ansatz describes the SF to MI transition in a mean-field sense, becoming exact in infinite dimensions. In addition, it provides one with a very intuitive picture of the transition to a MI state, which occurs precisely at the point where the local number distribution becomes a pure Fock distribution. This is consistent with a vanishing expectation value of the local matter wave field

$$< \Psi_{GW} | \hat{b}_l | \Psi_{GW} > = \sum_{n=1}^{\infty} \sqrt{n} c_{n-1}^* c_n$$

(17)

in the Gutzwiller approximation. It is important, however, to emphasize that the ansatz (16) fails to account for the nontrivial correlations between different sites present at any finite $J$. These correlations imply that the one particle density matrix $\rho_1(\vec{R})$ is different from zero at finite distance $|\vec{R}| \neq 0$, becoming long ranged at the transition to a SF. By contrast, in the Gutzwiller approximation, the one particle density matrix has no spatial dependence at all: it is zero at any $|\vec{R}| \neq 0$ in the MI and is completely independent of $\vec{R}$ in the SF. Moreover, in the Gutzwiller approximation the phase transition is directly reflected in the local number fluctuations, with the variance of $n_l$ vanishing throughout the MI phase. By contrast, in an exact theory local variables like the on-site number distribution will change in a smooth manner near the transition and the variance of the local particle number will only vanish in the limit $J \to 0$. Concerning the dynamics, one expects that the Gutzwiller approximation qualitatively captures the time scales for local changes of the configuration, however it fails to correctly describe long wavelength excitations [26].

The realization of a SF to MI transition with cold atoms in optical lattices provides an essentially perfect realization of one of the most prominent models in many body...
physics. It allows to study a quantum phase transition by simply tuning the depth of the optical lattice. There remain, however, a number of open questions in particular concerning the detailed spatial structure in the trap and the dynamical behaviour [27].

3. Crystallization in weak optical lattices

As we have discussed above, superfluidity of cold atoms is destroyed in a deep optical lattice where the ground state looses phase coherence and - essentially - has a fixed number of atoms per site. The associated Mott-Hubbard transition occurs when the ratio $U/J$ is of order one. Using the expressions (8) and (10) for $J$ and $U$ in terms of the optical lattice parameters, this translates into a condition of the form

$$\frac{a_s}{a} \cdot \exp 2 \left( \frac{V_0}{E_r} \right)^{1/2} = \frac{\sqrt{2}}{\pi} \cdot (U/J)_c$$

for the critical value of the dimensionless lattice depth $V_0/E_r|_c$. In the interesting regime with one or two atoms per site, the lattice constant $a$ is roughly equal to the the mean interparticle spacing $n^{-1/3}$. The prefactor $a_s/a$ in (18) thus coincides with the dimensionless interaction parameter $\gamma$ introduced in (2). For weak interactions $\gamma \ll 1$ therefore, the SF to MI transition requires deep optical lattices, for instance $V_0|_c \approx 13E_r$ in the experiments by Greiner et.al.[14], where $a_s/a \approx 0.01$. In the following we want to adress the question what happens in a situation where the effective gas parameter $\gamma$ becomes of order one or larger. The superfluid ground state is then expected to be destroyed already in a weak optical lattice, where the description in terms of a Bose-Hubbard model is no longer applicable. It turns out that this problem can be solved completely in the special case of one-dimensional Bose gases in which the transverse motion is frozen into the lowest eigenstate of a strong confining potential [28]. As pointed out by Petrov et.al. [29], the ratio between the interaction and kinetic energy per particle in one dimension

$$\gamma_1 = \frac{g_1 n_1}{\hbar^2 n_1^2 / m} = \frac{2a_s}{n_1 l_1^2}$$

scales inversely with the 1d density $n_1$. Here $g_1$ is the strength of the effective delta-function interaction in 1d and $l_1$ the oscillator length for the transverse confinement [29]. In one dimension, it is thus the low density limit where interactions dominate. This somewhat counterintuitive result can be understood physically by noting that at low 1d densities, the average kinetic energy per particle $\epsilon_{kin} \sim n_1^2$ vanishes so quickly that the atoms are perfectly reflected by the repulsive potential of the surrounding particles. For $\gamma_1 \gg 1$, therefore, the system aproaches a gas of impenetrable bosons which is called the Tonks-limit [29]. In particular at $\gamma_1 = \infty$ the exact many body wave function is just the absolute value of that of a free Fermi gas, as was shown a long time ago by Girardeau [30]. This equivalence remains valid in the presence of an arbitrary additional one-particle potential like that of an optical lattice. For a qualitative understanding of what happens in the strongly interacting regime it is therefore useful to consider a free Fermi
gas in a weak periodic potential \( V(x) = V_0 \sin^2 kx \) with \( V_0 \) of order \( E_r \) or smaller. This is an elementary problem in solid state physics, equivalent to the nearly free electron limit of a one-dimensional bandstructure. The single particle spectrum consists of a series of free particle like bands separated by energy gaps \( \Delta_l \) for \( l = 1, 2, \ldots \). The gaps become exponentially small with increasing energy, scaling like \( \Delta_l \sim |V_0|^l \) in the limit \( V_0 \ll E_r \). For a commensurate density, where an integer number \( \ell \) of particles fit into one unit cell, the \( \ell \) lowest bands are completely filled. The groundstate of noninteracting fermions is thus a trivial band insulator. Similar to the incompressible Mott-insulating phase of the Bose-Hubbard model, the state with a fixed integer density remains locked over a finite range \( \Delta_l \) of the chemical potential. For weak optical lattices \( V_0 \ll E_r \) the lowest gap \( \Delta_{l=1} = |V_0|/2 \) is much larger than the higher order ones. As a result, it is the commensurate phase with unit filling \( N = M \) which has maximal stability.

In the Tonks limit \( \gamma_1 \rightarrow \infty \) we have thus found that an arbitrary weak optical lattice which is commensurate with the average density will pin the atoms into an incompressible optical crystal. The crucial question is obviously whether this peculiar feature of hard core bosons in one dimension is still present at finite and experimentally realizable values of \( \gamma_1 \). To answer that, it is convenient to use Haldane’s description of Bose gases with arbitrary repulsive, short range interactions in terms of their long wavelength density oscillations [31]. Introducing a field \( \phi(x) \) which is related to the fluctuations \( \delta n(x) \) around the average density via \( \delta n(x) = \beta \partial_x \phi/2\pi \), the Hamiltonian in the presence of a weak, commensurate optical lattice can be shown [28] to be that of a quantum \((1 + 1)\) -dimensional sine-Gordon model

\[
\hat{H} = \frac{\hbar v_s}{2} \int dx \left[ \hat{\Pi}^2(x) + (\partial_x \hat{\phi})^2 + \frac{2V_0n_1}{\hbar v_s} \cos \beta \hat{\phi} \right] \tag{20}
\]

Here \( v_s \) is the actual sound velocity and \( \hat{\Pi}(x) \) is canonically conjugate to \( \hat{\phi}(x) \) such that \( [\hat{\phi}(x), \hat{\Pi}(x')] = i\hbar \delta(x-x') \). The coupling parameter \( \beta \) is related to the dimensionless ratio \( \bar{K} = \pi \hbar n_1 / m v_s = \beta^2 / 4\pi \) which characterizes the power in the characteristic decay

\[
\rho_1(x, T) \sim \left( \frac{\hbar v_s}{k_B T} \sinh \frac{\pi |x| k_B T}{\hbar v_s} \right)^{-1/2} \tag{21}
\]

of the one particle density matrix in the absence of the optical lattice, typical for one-dimensional quantum liquids [31]. In Haldane’s description, the correlation exponent \( \bar{K} \) is a phenomenological parameter which approaches \( \bar{K} \rightarrow 1 \) for hard core Bosons and \( \bar{K} \rightarrow \infty \) in the ideal gas limit. For given \( \bar{K}, n_1 \) and strength \( V_0 \) of the optical lattice, the sine-Gordon model (20) is an exactly soluble field theory [32]. It exhibits a transition at a critical value \( \beta_1^2 = 8\pi (K_c = 2) \) such that for \( \bar{K} > 2 \) the Bose gas ground state remains gapless and superfluid in a weak optical lattice while for \( (1 <) \bar{K} < 2 \) the atoms are locked even in an arbitrary weak periodic lattice as long as the deviation \( Q = 2\pi (n_1 - 1/a) \) between the period \( a \) and the average interparticle spacing \( n_1^{-1} \) is less than a critical value \( Q_c \). The commensurate phase is characterized by a finite excitation gap [28].
\[ \Delta = \frac{2E_r}{K} \left( \frac{K|V_0|}{(2 - K)4E_r} \right)^{1/(2-K)} \]  

which is nonanalytic in \( V_0 \). It approaches \( |V_0|/2 \) in the Tonks gas limit \( K \to 1 \) in agreement with the ideal Fermi gas picture discussed above. The size of the gap also determines the critical value \( Q_c = K^2 \pi n_1 \Delta / 2E_r \) of the deviation from exact commensurability which can still be accomodated into a locked groundstate. In order to relate \( K \) to the microscopic and experimentally tunable parameter \( \gamma_1 \) introduced in (19), we use the exact solution by Lieb and Liniger [33] of the 1d Bose gas with a delta-function interaction of strength \( g_1 \). It turns out that \( K(\gamma_1) \) is a monotonically decreasing function which reaches the critical value \( K_c = 2 \) at \( \gamma_{1,c} \approx 3.5 \). The transition to a commensurate, incompressible state in a weak optical lattice thus occurs long before the Tonks limit is reached. As is evident from eqn. (22), however, the gap is exponentially small in the vicinity of the critical value \( K_c = 2 \). In order to reach appreciable values of the gap, one thus needs \( \gamma \approx 10 \) where \( K \approx 1.4 \).

In a one-dimensional Bose gas we have thus found that a transition from a SF to a MI state at weak coupling \( \gamma \ll 1 \) requires a deep optical lattice, while at strong coupling \( \gamma \gg 1 \) an arbitrary weak lattice is sufficient to destroy phase coherence (similar to the MI phase of the Bose-Hubbard model, the one particle density matrix \( \rho_1(x) \) will decay exponentially in the phase where the atoms are locked to the external lattice potential). For weak coupling, the criterion \( U/J|_{c} = 2C \approx 3.84 \) for the transition in the anisotropic, one-dimensional Bose-Hubbard model can be written in a form similar to eqn. (18)

\[ \frac{4V_0}{E_r} = \ln^2 \left[ 4\sqrt{2} \pi C (V_0/E_r)^{1/2}/\gamma \right]. \]  

The solution of this transcendental equation gives a critical value \( V_0/E_r|_{c} \) which increases rather slowly as a function of the inverse interaction parameter \( 1/\gamma \). From the exact solution of the sine-Gordon model, in turn, we know that - at least in one dimension - this critical amplitude of the optical lattice vanishes at the finite value \( 1/\gamma|_{c} \approx 0.29 \). More precisely, the Kosterlitz-Thouless nature of the transition near \( K_c = 2 \) determines the critical value of \( K \) for small \( u = KV_0/4E_r \) to behave like \( K_c(u) = 2(1 + u) \) to linear order in \( u \) [28]. The complete phase diagram for unit filling at arbitrary values of \( V_0/E_r \) can then be obtained by combining these two asymptotic results in a smooth interpolation, as shown in Fig.3. The Bose-Hubbard transition (BH) for weakly interacting gases in a deep optical lattice thus continuously evolves into one of the commensurate-incommensurate (C-IC) type for strongly interacting gases in a weak lattice. It remains a challenge to extend these results to situations with two or more particles per lattice period and - in particular - to the case of two- or three-dimensional lattices.

Regarding the prospects for an experimental observation of the C-IC transition discussed above, we have seen that realistic values of the excitation gap \( \Delta \) require \( \gamma_1 \) to be of order 10. One-dimensional Bose gases with parameters in this range may
be realized with a strong optical lattice in only two directions $x, y$ which confine the atoms transversely but leave the motion along $z$ essentially free, except for a rather weak axial trap with frequency $\nu_z$. As an example, using numbers close to those in the experiments by Greiner et.al. [14] on the SF to MI transition, it is possible to generate a few thousand parallel one-dimensional gases with about $N = 50$ atoms per wire. Taking realistic values $\nu_\perp = 20$ kHz and $\nu_z = 40$ Hz, the central density for large $\gamma$ is close to $n_1(0) = 2 \mu$m$^{-1}$ [34]. This is precisely commensurate with the lattice constant $a \approx 0.5 \mu$m of the optical lattice used in these experiments. Adding a weak optical lattice in $z$–direction, will thus lead to an incompressible state in the center of the trap provided $\gamma_1$ is larger than the critical value $\gamma_{1,c} \approx 3.5$. For $^{87}$Rb with a scattering length $a_s \approx 5$ nm, the resulting $\gamma_1$ is close to one and thus not in the required range. With a tunable scattering length as in $^{85}$Rb, however, it is perfectly feasible to increase $a_s$ by one order of magnitude and thus a Mott-insulating state could be realized with a very weak optical lattice. Since three-body losses are very strongly reduced in one dimension at large $\gamma$ [35], there is no problem with the condensate lifetime here. The transition may be observed in a similar manner than in the Bose-Hubbard case. More interesting however would be to measure the long range translational order present in the locked phase by Bragg diffraction, as was done for cold atoms in deep optical lattices even at very low densities [22]. This method has the advantage that the signal from many parallel wires adds up constructively because they all experience the same modulation in $z$–direction.
4. Conclusion and Outlook

With the recent realization of a quantum phase transition between a superfluid and a Mott-insulating state by Greiner et al. [14], the field of cold atoms has entered a regime, where strong correlation effects may be studied in an unprecedentedly clean manner. Indeed, basic models in many body theory like the Hubbard-model for bosons or fermions with on-site interaction, which were originally introduced in a condensed matter context as a rather schematic description of say superfluid Helium in Vycor or electrons in high-temperature superconductors can now be applied even on a quantitative level. Moreover the crucial parameters $J, U$ and density can easily be tuned in a controlled fashion. This opens a wide area of possibilities for strong correlation physics with cold atoms, in particular if degenerate fermions may be loaded into an optical lattice. With two equivalent species of fermions the resulting version of the Hubbard model displays a wealth of different phases: in the attractive case it describes the BCS- to Bose-crossover for Cooper-pairing, in the repulsive case antiferromagnetic or unconventional superconducting phases appear, as recently discussed by Hofstetter et al. [36]. From the perspective of atomic and molecular physics, a Mott-insulating state with precisely two atoms per site is an ideal starting point for the formation of molecular condensates via local photoassociation and subsequent melting of the Mott-phase as suggested by Jaksch et al. [37]. Finally, controlled interactions (‘collisions’) between atoms in different internal states in an optical lattice may be used to generate highly entangled states useful for quantum computation schemes [38,39]. Cold atoms in optical lattices have therefore started to fascinate people not only in the field of atomic physics and quantum optics but far beyond that and it seems that the field is at the beginning of a promising area in research.

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By removing the lattice potential in an adiabatic manner, it is possible also to map out the quasi-momentum distribution and thus directly visualize the occupation within the Brillouin zone, see Greiner M et al 2001 Phys. Rev. Lett. 87 160405

This property only holds in the two- or three-dimensional case, while in 1d, the behaviour is algebraic even in the ground state, as shown by eqn. (21) below. Experimentally the existence of ‘off-diagonal long range order’ in dilute gases was verified by I. Bloch et al 2000 Nature 403 166

Note that the static structure factor $S(\vec{k})$ which is the Fourier transform of the diagonal two-particle density matrix, exhibits Bragg peaks even if the atoms are localized at random sites of the optical lattice without phase coherence between them. These peaks simply reflect the externally imposed periodicity and were observed e.g. by Weidemüller M. et al 1995 Phys. Rev. Lett. 75 4583

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