Mott-insulator phase of coupled 1D atomic gases in a 2D optical lattice

D.M. Gangardt[1], P. Pedri[2,3,4], L. Santos[2,3], and G.V. Shlyapnikov[1,5]

[1]*Laboratoire Physique Théorique et Modèles Statistiques, Université Paris Sud, Bât. 100 91405 Orsay Cedex, France*
[2]*Institut für Theoretische Physik III, Universität Stuttgart, Pfaffenwaldring 57, D-70550, Stuttgart, Germany*
[3]*Institut für Theoretische Physik, Universität Hannover, D-30167 Hannover, Germany*
[4]*Dipartimento di Fisica, Università di Trento and BEC-INFM, I-38050 Povo, Italy*
[5]*Van der Waals - Zeeman Institute, University of Amsterdam, Valckenierstraat 65/67, 1018 XE Amsterdam, The Netherlands*

We discuss the 2D Mott insulator (MI) state of a 2D array of coupled finite size 1D Bose gases. It is shown that the momentum distribution in the lattice plane is very sensitive to the interaction regime in the 1D tubes. In particular, we find that the disappearance of the interference pattern in time of flight experiments will not be a signature of the MI phase, but a clear consequence of the strongly interacting Tonks-Girardeau regime along the tubes.

Remarkable developments in atomic cooling and trapping have triggered the interest in strongly correlated atomic systems [1, 2, 3, 4, 5]. In particular, the physics of cold atoms in periodic potentials induced by laser standing waves (optical lattices) has attracted a major attention, mostly due to its links to solid state physics [6], and due to the observation of the superfluid (SF) to Mott-insulator (MI) transition [7] in Munich experiments [8].

The reduction of spatial dimensionality in these systems is now a "hot topic", in particular with regard to the creation of 1D gases, where the interaction between particles becomes more important with decreasing the gas density. For low densities or large repulsive interactions the system enters the strongly-interacting Tonks-Girardeau (TG) regime, in which the bosons acquire fermionic characteristics [9] and dynamical and correlation properties drastically change [10, 11, 12, 13]. This regime requires tight transverse trapping, low atom numbers, and possibly the enhancement of interactions via Feshbach resonances [3, 10, 14]. In this sense, 2D optical lattices are favorable, since the on-site transverse confinement can be made very strong and for sufficiently small tunneling rate each lattice site behaves as an independent 1D system. Recent experiments on strongly correlated 1D gases have been performed along these lines [15, 16, 17, 18].

These studies motivate the analysis of an interesting physics in a (2D) array of coupled 1D Bose gases. In a 2D lattice the coupling is provided by the inter-site tunneling, and each lattice site is a 1D tube filled with bosonic atoms. This regime is easily achievable experimentally by lowering the lattice potential, and it represents the bosonic analog of 1D coupled nanostructures [19]. As was first shown by Efetov and Larkin [20], for infinitely long 1D tubes at zero temperature any infinitesimally small tunneling drives the system into the superfluid phase. The gas then enters an interesting cross-dimensional regime, in which it presents 1D properties in a 3D environment [21, 22]. For 1D tubes of finite length L, at sufficiently small tunneling rate the system can undergo a cross-over from such anisotropic 3D superfluid state to the 2D Mott insulator state [22]. Strictly speaking, this 2D MI phase requires a commensurable filling of the tubes, i.e. an integer average number of particles N per tube. Then the system of finite-length tubes at zero temperature is analogous to that of infinite tubes at a finite temperature T, and the critical tunneling t_c for the $T = 0$ cross-over to the MI phase can be obtained from the finite-temperature results of Ref. [20] by making a substitution $1/T \to L$ [23].

This Letter is dedicated to the analysis of correlation properties of this 2D Mott insulator. We show that the momentum distribution is crucially modified by a combined effect of correlations along the 1D tubes and inter-tube hopping. For the case of a weakly interacting gas in the tubes, the phase coherence is maintained well inside the MI phase. This is similar to the situation in 2D and 3D lattices, studied by means of Quantum Monte Carlo calculations [24] and investigated experimentally through the observation of an interference pattern after switching off the confining potential [8]. However, an increase of the interaction between particles in 1D tubes reduces the inter-tube phase coherence and flattens the momentum distribution in the transverse direction(s). In particular, the interference pattern observed in Ref. [8] should be largely blurred if the 1D tubes are in the TG regime. This effect can be revealed in current experiments. Remarkably, the disappearance of the interference pattern will not be a signature of the MI phase, but a clear consequence of the strongly interacting regime for 1D tubes.

In the following we consider a Bose gas at zero temperature in a 2D optical lattice, such that every lattice site can be considered as an axially homogeneous 1D tube of finite size L, with $N = nL$ being the number of particles per tube, and n the 1D density. The tunneling between neighboring tubes is characterized by the hopping t, which depends on a particular lattice potential and atomic species employed. We label tubes by the index j and denote by x the coordinate along the tubes.

The action describing the coupled tubes has the form:

$$S = \sum_j S_j - t \sum_{<ij>} \int_{-\infty}^{\infty} d\tau \int_{-L/2}^{L/2} dx \ (\bar{\psi}_i \psi_j + \bar{\psi}_j \psi_i), \quad (1)$$

where $\psi_j(x,\tau), \bar{\psi}_j(x,\tau)$ are complex bosonic fields associated with the j-th tube, the symbol $<ij>$ denotes nearest neighbors, and S_j is the action describing the physics along the j-th tube.

In the absence of tunneling, there are no correlations between different tubes, and the one-body Green function is diagonal:

$$
\begin{aligned}
G_{ij}(x_1-x_2,\tau_1-\tau_2) &= \langle \psi_i(x_1,\tau_1)\bar{\psi}_j(x_2,\tau_2)\rangle \\
&= \delta_{ij} G_0(x_1-x_2,\tau_1-\tau_2). \quad (2)
\end{aligned}
$$

The presence of tunneling between neighboring tubes, provided by the second term on the rhs of Eq. (1), modifies the momentum distribution. Above a critical tunneling amplitude t_c the system undergoes a cross-over from the MI to an anisotropic 3D SF phase [22]. This crossover and the MI phase can be analyzed within the random phase approximation (RPA) [25], successfully used in the studies of coupled spin chains [26]. Decoupling the tunneling term in the action (1) by using the Hubbard-Stratonovich transformation and keeping only the leading quadratic terms, yields the RPA Green function in the momentum-frequency representation:

$$G(\vec{q},k,\omega) = \frac{G_0(k,\omega)}{1 - T(\vec{q})G_0(k,\omega)}, \quad (3)$$

with $\vec{q} = (q_y, q_z)$ being the quasimomentum in the lattice plane, $T(\vec{q}) = 2t(\cos q_y a + \cos q_z a)$, a the lattice constant, and $G_0(k,\omega)$ the Fourier transform of the Green function (2) (hereinafter we put $\hbar = 1$):

$$G_0(k,\omega) = \int_{-\infty}^{\infty} d\tau \int_{-L/2}^{L/2} dx \, e^{-ikx+i\omega\tau} G_0(x,\tau). \quad (4)$$

The long-wavelength behavior of the Green function $G_0(x,\tau)$ can be found using Luttinger liquid theory [27]. At zero temperature, employing a conformal transformation in order to take into account the finite size L of the tubes [25], we obtain:

$$G_0(x,\tau) = n \left(\frac{\pi^2/N^2}{\sinh\left(\pi\zeta/L\right)\sinh\left(\pi\bar{\zeta}/L\right)} \right)^d, \quad (5)$$

where $\zeta = v_s\tau + ix$, and v_s is the sound velocity. The interactions enter Eq.(5) through the factor $d = 1/4K$ related to the interaction-dependent Luttinger parameter K. The Fourier transform of Eq. (5) yields

$$G_0(k,\omega) = \frac{1}{nv_s}\left(\frac{N}{2\pi}\right)^{2-2d} I\left(\frac{kL}{2\pi}, \frac{\omega L}{2\pi v_s}\right), \quad (6)$$

where the quantity $I(p,\Omega)$ is expressed through the hypergeometric function $_3F_2$:

$$
\begin{aligned}
I(p,\Omega) = \frac{4\pi}{p!}\frac{\Gamma(d+p)}{\Gamma(d)} \times \\
\mathrm{Re}\left[\frac{_3F_2\left(d, d+p, \frac{d+p-i\Omega}{2}; 1+p, 1+\frac{d+p-i\Omega}{2}; 1\right)}{d+p-i\Omega} \right], \quad (7)
\end{aligned}
$$

with $p = kL/2\pi$ and $\Omega = \omega L/2\pi v_s$ being the dimensionless momentum and frequency. Integrating Eq. (6) over ω one obtains the momentum distribution $N_0(kL/2\pi) = \int d\omega G_0(k,\omega)/2\pi$ in the absence of tunneling:

$$\frac{N_0(p)}{N} = \left(\frac{N}{2\pi}\right)^{-2d}\frac{\Gamma(d+p)}{p!\Gamma(d)} {}_2F_1(d, d+p; 1+p; 1), \quad (8)$$

which behaves as p^{2d-1} for $p \gtrsim 1$. The Luttinger liquid description employed here is valid for low momenta $k \ll \pi n$. Accordingly, the dimensionless axial momentum $p = kL/2\pi$, which is an integer number, should satisfy the inequality $p \ll N$. The momentum distribution (8) represents the fraction of particles in the state with momentum p and is normalized as $\sum_p N_0(p) = N$.

The critical tunneling t_c for the MI to SF cross-over is obtained as the value of t for which the denominator of Eq. (3) vanishes for zero momenta k and $\vec{q}$ and zero frequency ω. We thus have

$$\frac{t_c}{\mu} = \frac{nv_s}{4\mu}\left(\frac{N}{2\pi}\right)^{2d-2}\frac{1}{I(0,0)}. \quad (9)$$

Note that with t_c from Eq. (9), the Green function G in Eq. (3) becomes a universal function of the dimensionless quantities t/t_c, p, qa and Ω. For the TG regime of 1D bosons in the tubes, the Luttinger parameter is $K = 1$ and $d = 1/4$. Then, as the chemical potential is $\mu = mv_s^2 = \pi^2 n^2/2m$, from Eq.(9) we obtain $t_c/\mu \simeq 0.05N^{-3/2}$. For the weakly interacting regime, the Luttinger parameter in the 1D tubes is $K = \pi(n/mg)^{1/2} \gg 1$ and Eq.(7) gives $I(0,0) = 16\pi K \gg 1$. In this regime the chemical potential is $\mu = mv_s^2 = ng$, and Eq.(9) then yields $t_c/\mu \simeq (1/16)N^{-2}$ (as expected from the mean-field calculations for a 2D lattice of zero-dimensional sites [28]). These results are in qualitative agreement with the recent calculations of Ho et al. [22]. One clearly sees that strong correlations along the tubes drastically shift the boundaries of the MI phase.

The momentum distribution for the coupled 1D tubes in the MI phase, $N(\vec{q},k)$, is obtained by integrating the Green function (3) over the frequency. Our calculations show that only the lowest axial mode for which the momentum $k = 0$, is significantly affected by the tunneling. The physical reason is that the $k = 0$ mode is approaching the instability on approach to the critical tunneling t_c, whereas $k \neq 0$ modes are still far from instability. This is
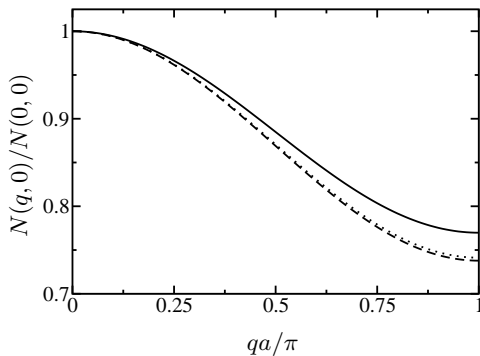
Figure 1: Transverse momentum distribution for $k = 0$ at $t/t_c = 0.3$ for $K = 1$ (solid), $K = 4$ (dotted), and $K = 25$ (dashed). In the figure we have chosen $q_y = q_z = q$.
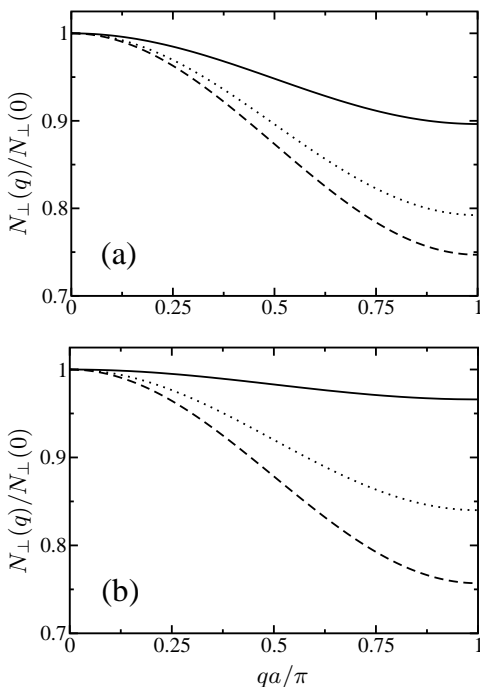

Figure 2: Transverse momentum distribution for $t/t_c = 0.3$, at $K = 1$ (solid), $K = 4$ (dotted), and $K = 25$ (dashed), for $N = 50$ (a) and $N = 500$ (b). In the figures we have chosen $q_y = q_z = q$.

reflected in the resonance character of the Green function (3) for $k = 0$ and $t \to t_c$. Our results in Fig. 1 show that the transverse distribution $N(\vec{q}, 0)$ corresponding to the $k = 0$ axial mode is non-flat for any interaction regime along the tubes. In contrast, for $k \neq 0$ the quantity $T(\vec{q})G_0(k, \omega)$ is always small. Therefore, expanding the rhs of Eq. (3) in powers of $T(\vec{q})$ up to linear order and integrating over ω we obtain an almost flat transverse momentum distribution for $k \neq 0$ modes: $N(\vec{q}, p)/N(0, p) = 1 - (Ad^2/4p^{2-d})(t/t_c)(2 - \sum_{i=y,z} \cos q_i a)$, where the coefficient A is of order unity and the second (q-dependent)

term is always very small.

We now turn to the discussion of the transverse quasi-momentum distribution $N_\perp(\vec{q}) = \sum_k N(\vec{q}, k)$. The summation over the axial modes changes the picture drastically compared to the distribution for a given k. As only the $k = 0$ component is significantly affected by the tunneling, one can rewrite Eq. (3) in the form:

$$ G(\vec{q}, k, \omega) \simeq G_0(k, \omega) + \frac{T(\vec{q})G_0^2(0, \omega)}{1 - T(\vec{q})G_0(0, \omega)} \delta_{k,0}. \quad (10) $$

In the second term on the rhs of Eq.(10) we may use the Green function $G_0(0, \omega)$ following from Eqs. (6) and (7). For $k = 0$ ($p = 0$), one can put the hypergeometric function ${}_3F_2 = 1$ in Eq.(7), which gives $I(0, \Omega) \simeq 4\pi d/(d^2 + \Omega^2)$. Omitted terms give a very small relative correction of the order of $d^3 < 1/4^3$. Hence, using Eq.(9), for the Green function at $k = 0$ in the absence of tunneling we have $G_0(0, \omega) = d^2/4t_c(d^2 + \Omega^2)$. Then, integrating Eq.(10) over Ω, summing over the axial modes k, and imposing the normalization condition $N = \sum_k \int d\omega G_0(k, \omega)/2\pi$ for the first term on the rhs, we obtain the transverse momentum distribution

$$ \frac{N_\perp(\vec{q})}{N} = 1 + \left(\frac{2\pi}{N}\right)^{2d} \left[\left(1 - \frac{t}{2t_c} \sum_{i=y,z} \cos q_i a\right)^{-1/2} - 1\right], \quad (11) $$

normalized by the condition $(a/2\pi)^2 \int d^2q N_\perp(\vec{q}) = N$.

In Fig. 2 we depict the results of Eq. (11) for different values of N and the Luttinger parameter K. Due to the prefactor in the second term on the rhs of Eq. (11) the transverse momentum distribution strongly depends on the interaction regime along the tubes.

For the weakly interacting regime ($d \ll 1$), the distribution $N_\perp(\vec{q})$ is not flat even deeply inside the MI phase. Similar results have been obtained by means of Quantum Monte Carlo calculations [24] for the case of lattices of zero-dimensional sites. In our case, only for rather low tunneling ($t/t_c \lesssim 0.1$) the quasimomentum distribution becomes flat, and switching off the lattice potential should lead to a blurred picture as that observed by Greiner et al. [8]. Non-flat distributions in the MI phase as those of Fig. 2 will manifest themselves through the appearance of interference peaks in the same type of experiment.

On approach to the TG regime, the quasimomentum distribution becomes progressively flatter. The main reason for this behavior is that when the system becomes more interacting, the $k = 0$ component is more depleted, contributing less to the total quasimomentum distribution. Therefore, if the 1D tubes approach the strongly interacting TG regime, in experiments as those of Ref. [8] the interference pattern will be essentially smeared out. One may expect a partial destruction of the interference pattern even for moderate values of the Luttinger parameter (see, e.g., the case $K = 4$ in Fig. 2).

The random phase approximation used in our calculations, was shown to be a good approximation for a wide range of parameters of coupled one-dimensional Heisenberg spin chains [26]. Here we give yet another estimate for the applicability of RPA, relying on the Ginzburg criterion adapted to a quantum phase transition at zero temperature. We compare fluctuations of the order parameter in a volume determined by the correlation radius extracted from the Green function (3), with the scale on which the non-linear effects become important. The latter is obtained from the four-point correlation function of each tube. We have found that RPA is adequate for $(t_c-t)/t_c \gg B(d)$, where $B(d)$ has been obtained numerically from the four-point correlation function. In the case of the Tonks-Girardeau regime along the tubes, we have $B \approx 0.1$, and it decreases significantly with decreasing d and entering the Gross-Pitaevskii regime.

In conclusion, we have considered a bosonic gas in a 2D optical lattice of finite 1D tubes at zero temperature, focusing our attention on the momentum distribution in the MI phase. We have shown that the strong correlations along the 1D tubes significantly modify the quasi-momentum distribution in the lattice plane. We have found that in the MI regime only the lowest momentum along the tubes is affected by the inter-site hopping, and hence only this component contributes to the formation of interference fringes. Consequently, the larger the interactions are (larger depletion) the less pronounced is the visibility of the interference fringes. In particular, for the TG regime in the tubes, the quasimomentum distribution becomes progressively flatter, leading to an observable blurring of the interference pattern after expansion. This effect can be observed in current time of flight experiments, and can be used to reveal a clear signature of the strong correlations along the sites.

[1] S. Cowell *et al.*, Phys. Rev. Lett. **88**, 210403 (2002).

[2] N. K. Wilkin and J. M. F. Gunn, Phys. Rev. Lett. **84**, 6 (2000).

[3] M. Olshanii, Phys. Rev. Lett. **81**, 938 (1998).

[4] A. Recati, P. O. Fedichev, W. Zwerger, and P. Zoller Phys. Rev. Lett. **90**, 020401 (2003).

[5] D. Jaksch *et al*, Phys. Rev. Lett. **81**, 3108 (1998).

[6] B. P. Anderson and M. Kasevich, Science **282**, 1686 (1998); O. Mörsch *et al.*, Phys. Rev. Lett. **87**, 140402 (2001); W. K. Hensinger *et al.*, Nature **412**, 52 (2001); F. S. Cataliotti et al., Science, 293 843 (2001); C. Orzel et al., Science 291, 2386 (2001).

[7] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher Phys. Rev. B **40**, 546 (1989).

[8] M. Greiner *et al.*, Nature **415**, 39 (2002).

[9] M. Girardeau, J. Math. Phys. **1**, 516 (1960); M. D. Girardeau, E. M. Wright, and J. M. Triscari, Phys. Rev. A **63**, 033601 (2001).

[10] V. Dunjko, V. Lorent, and M. Olshanii, Phys. Rev. Lett. **86**, 5413 (2001).

[11] C. Menotti and S. Stringari, Phys. Rev. A **66**, 043610 (2002).

[12] P. Öhberg and L. Santos, Phys. Rev. Lett. **89**, 240402 (2002); P. Pedri, L. Santos, P. Öhberg, and S. Stringari, Phys. Rev. A. **68**, 043601 (2003).

[13] D. M. Gangardt and G. V. Shlyapnikov, Phys. Rev. Lett. **90**, 010401 (2003); D. M. Gangardt and G. V. Shlyapnikov, New J. Phys. **5**, 79 (2003); K. V. Kheruntsyan, D. M. Gangardt, P. D. Drummond, and G. V. Shlyapnikov, Phys. Rev. Lett. **91**, 040403 (2003); G.E. Astrakharchik, and S. Giorgini, Phys. Rev. A **68**, 031602 (2003); M. Olshanii and V. Dunjko, Phys. Rev. Lett. **91**, 090401 (2003).

[14] D. S. Petrov, G. V. Shlyapnikov, and J. T. M. Walraven, Phys. Rev. Lett. **85**, 3745 (2000).

[15] H. Moritz, T. Stöferle, M. Köhl, and T. Esslinger, Phys. Rev. Lett. **91**, 250402 (2003).

[16] T. Stöferle *et al.*, Phys. Rev. Lett. **92**, 130403 (2004).

[17] B. Laburthe Tolra *et al.*, Phys. Rev. Lett. **92**, 190401 (2004).

[18] B. Paredes *et al.*, Nature **429**, 277 (2004).

[19] S. Biermann, A. Georges, A. Lichtenstein, and T. Giamarchi, Phys. Rev. Lett. **87**, 276405 (2001).

[20] K. B. Efetov and A. I. Larkin, Sov. Phys. JETP **42**, 390 (1975).

[21] P. Pedri and L. Santos, Phys. Rev. Lett. **91**, 110401 (2003).

[22] A. F. Ho, M. A. Cazalilla, and T. Giamarchi, Phys. Rev. Lett. **92**, 130405 (2004).

[23] We assume that the commensurability condition is satisfied. Note, however, that for a large non-integer N one has only a tiny superfluid fraction ($\sim 1/2N$ or less), and below t_c the system behaves in almost all aspects as the MI phase.

[24] V. A. Kashurnikov, N. V. Prokof'ev, and B. V. Svistunov Phys. Rev. A **66**, 031601 (2002); S. Wessel, F. Alet, M. Troyer, and G. G. Batrouni, cond-mat/0404552.

[25] See e.g. A. M. Tsvelik, *"Quantum field theory in condensed matter physics"*, Cambridge University Press, 1995.

[26] H.J. Schulz, Phys. Rev. Lett. **77**, 2790 (1996); V.Yu. Irkhin and A.A. Katanin, Phys. Rev. B **61**, 6757 (1999); M. Bocquet, Phys. Rev. B **65**, 184415 (2002).

[27] F. D. M. Haldane, Phys. Rev. Lett. **47**, 1840 (1981).

[28] D. van Oosten, P. van der Straten, and H. T. C. Stoof, Phys. Rev. A **63**, 053601 (2001).