Deconfinement in a 2D optical lattice of coupled 1D boson systems

A. F. Ho,1 M. A. Cazalilla,2 and T. Giamarchi3

1School of Physics and Astronomy, The University of Birmingham, Edgbaston, Birmingham B15 2TT, UK.
2Donostia International Physics Center (DIPC), Manuel de Lardizabal 4, 20018-Donostia, Spain.
3University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Geneva 4, Switzerland.

We show that a two-dimensional (2D) array of 1D interacting boson tubes has a deconfinement transition between a 1D Mott insulator and a 3D superfluid for commensurate fillings and a dimensional crossover for the incommensurate case. We determine the phase diagram and excitations of this system and discuss the consequences for Bose condensates loaded in 2D optical lattices.

PACS numbers: 03.75.Kk, 05.30.Jp, 71.10.Pm

Loading optical lattices with ultracold atoms is providing new types of many-body systems as well as new ways to look at hard problems such as quantum phase transitions in strongly interacting systems. The recent observation of the superfluid-Mott insulator transition has demonstrated the large degree of tunability offered by these setups. This will allow the exploration of e.g. spin-1 atoms, fermions, and Bose-Fermi mixtures, where strong interactions may lead to novel quantum many-body states. They offer also the possibility to realize anisotropic traps and thus to explore the physics of interacting particles in reduced dimensions. Recently, two dimensional (2D) optical lattices have been realized, where at each lattice site, a 1D tube of ultracold atoms is trapped. Such systems thus provide a unique way to obtain strongly interacting 1D Bose gases, of which the Tonks gas is the best known example (see e.g. 1-3).

In 1D, interactions cause more drastic effects than in higher dimensions and lead, both for fermions and bosons, to a very peculiar state known as Tomonaga-Luttinger liquid (TLL), which by now is theoretically well understood. However, despite the intense theoretical and experimental activity in fermionic systems or spin chains, much less is known when a collection of such 1D systems is coupled. In general, one can expect a dimensional crossover where the system goes from a TLL at high temperature to an anisotropic 3D system with more conventional properties (e.g. a Fermi liquid for fermions, a superfluid for bosons) at low temperature.

The transition is even more drastic and less well understood when, due to the existence of an axial periodic potential (thereafter called “Mott potential”), the 1D system becomes a Mott insulator (MI) [4,11,12]. Quite generally, the competition between Mott localization and superfluidity leads to interesting phenomena [13]. For coupled 1D chains the competition between the Mott insulating physics and interchain tunneling changes the dimensional crossover into a deconfinement transition where the system goes from a 1D insulator towards a 3D metal or superfluid. For fermions this transition remains a theoretical challenge [14] and has been observed in coupled chain systems such as the organic conductors [15]. For bosons, much less is known even though the problem has been tackled in the context of spin chains (i.e. hard core bosons) [16] or for a bosonic ladder [17]. In general, however, comparison between theory and experiments is rendered difficult by the complex nature of the solid-state materials.

In this paper, motivated by the clean and tunable realization of coupled 1D gases offered by 2D optical lattices [4,16], we investigate their phases and phase diagram (see Fig. 1). For the lattice without the axial Mott potential, we show that the system exhibits, as a function of temperature, a dimensional crossover from a strongly anisotropic normal gas to a 3D Bose-Einstein condensate (BEC) or superfluid, which can have a large quantum depletion. For this 3D superfluid (SF), we obtain the condensation temperature, the zero-temperature condensate fraction, the excitation spectra, and the momentum distribution in the thermodynamic limit. When an axial Mott potential is present, we show that its tendency to deplete. For this 3D superfluid (SF), we obtain the condensation temperature, the zero-temperature condensate fraction, the excitation spectra, and the momentum distribution in the thermodynamic limit. When an axial Mott potential is present, we show that its tendency to

\[ H = \sum_{\mathbf{R}} \int_{0}^{L} dx \left\{ \frac{\hbar^{2}}{2M} \partial_{x} \Psi_{\mathbf{R}}^{\dagger}(x) \partial_{x} \Psi_{\mathbf{R}}(x) + u(x) \rho_{\mathbf{R}}(x) \right\} + \sum_{\mathbf{R}} \frac{1}{2} \int_{0}^{L} dx \int_{0}^{L} dx' v(x - x') \rho_{\mathbf{R}}(x) \rho_{\mathbf{R}}(x') \]

\[ - \frac{J}{2} \sum_{\mathbf{R},\mathbf{R'}} \int_{0}^{L} dx \left[ \Psi_{\mathbf{R}}^{\dagger}(x) \Psi_{\mathbf{R'}}(x) + h.c. \right]. \] (1)

\[ \Psi_{\mathbf{R}}(x) \] is the bosonic field operator at \( x \) (the axial co-
Using \( \Psi_R(x) \approx \sqrt{\Delta_{S\text{F}}} e^{i\phi R(x)} \) and \( \rho_R(x) = [\rho_0 + \partial_x \theta_R(x)/\pi] \sum_m e^{2i m [\theta_R(x) + \pi \rho_0 x]} \), Eq. (1) becomes

\[
H_{\text{eff}} = \frac{\hbar v_s}{2\pi} \sum_R \int_0^L dx \left[ \frac{1}{K} (\partial_x \theta_R(x))^2 + K (\partial_x \phi_R(x))^2 \right] \\
+ \frac{\hbar v_s g_u}{2\pi a^2} \sum_R \int_0^L dx \cos (2\theta_R(x) + \delta \pi x) \\
- \frac{\hbar v_s g_j}{2\pi a^2} \sum_{(R,R')} \int_0^L dx \cos (\phi_R(x) - \phi_{R'}(x))
\]

where \( \delta = 2\rho_0 - G/\pi \) is the mismatch between the density \( \rho_0 \) and the periodicity of \( u(x) = u_0 \cos (Gx) \). The dimensionless couplings \( g_j = 2\pi J(\rho_0^a) A/\hbar v_s \rho_0 \), and \( g_u = 2\pi u_0(\rho_0^a)/\hbar v_s \rho_0 \), where \( a \approx \hbar v_s/\mu \) is the short-distance cut-off and \( A \approx (K/\pi)^1/2K \). Results and asymptotic expressions for \( K \) and the sound velocity \( v_s \) in terms of \( \gamma = M_{\text{TM}_3}/h^2 \rho_0 \) can be found in Ref. [7]. Interestingly, an anisotropic version of the Bose-Hubbard model [13], (i.e. with axial hopping \( J_z \gg J \)) also leads to Eq. (2), but the relationship of the microscopic parameters (namely \( J_z, J \) and \( U \)) to \( K, v_s, g_u \) and \( g_j \) is not easy to estimate. But if instead \( K \) and \( g_u \) are regarded as phenomenological parameters, our results directly apply to this model as well.

First we consider the case \( u_0 = 0 \) (i.e. \( g_u = 0 \)). This includes the incommensurate case \( \delta \neq 0 \) for which the periodic potential \( u(x) \) has no effect at low temperatures [14, 15, 16]. In the absence of tunnelling, the system is then a set of isolated TLL’s with no true condensate and a power-law decay of phase correlations [17]. Tunneling thus induces, at a temperature \( T_c \), a dimensional crossover from the TLL behavior at \( T > T_c \) towards a 3D superfluid or BEC at low temperatures. To study the crossover, we treat the tunneling term in a mean-field (MF) approximation, taking \( \psi_0 = \langle \Psi_R(x) \rangle \) to be the (square root of the) condensate fraction. The problem then reduces to a sine-Gordon (SG) model [18, 19, 20], describing an effective 1D system. Above \( T_c, \psi_0 = 0 \). Therefore, \( T_c \) is found by the existence of a non-zero solution for \( \psi_0 \). We get, in agreement with [20],

\[
\left( \frac{2\pi T_c}{\hbar v_s \rho_0} \right)^{-1/2K} = f(K) \frac{4J}{\hbar v_s \rho_0},
\]

where \( f(K) = A \sin \left( \frac{K}{2} \right) B^2 \left( \frac{K}{2}, 1 - \frac{K}{2} \right) \) and \( B(x) \) is the Beta function. Below \( T_c, \psi_0 \) is found by minimizing the free energy density. At \( T = 0 \) one minimizes \( \mathcal{E}_{\text{MF}}(\psi_0) = 4J \psi_0^2 - \Delta_{\text{SF}}(\psi_0) \tan^2 \frac{\pi}{8\hbar v_s K} \), where the second term is the SG model energy density [21], and \( \Delta_{\text{SF}}(\psi_0) \) the soliton gap (the excitations of the SG model are gapped solitons and breathers [21, 22]). Thus we find that the condensate fraction \( \psi_0(T = 0) \sim \rho_0 (J/\mu)^{1/4K-1} \), whereas the soliton gap \( \Delta_{\text{SF}} \sim \mu (J/\mu)^{2K/(4K-1)} \).

In the broken-symmetry (superfluid) phase the system possesses two modes. The Goldstone mode (i.e. oscill-
tions of the order parameter phase) is gapless as a consequence of (global) gauge invariance. The other mode corresponds to oscillations of the order parameter amplitude. To obtain these modes we compute the gaussian fluctuations around the MF solution (random-phase approximation, RPA). Using known properties of correlation functions of the SG model [8, 21], and within the single-mode approximation (SMA: taking into account only the lowest breather mode) [16], we obtain:

$$\omega^2(q, Q) = v^2_s q^2 + \frac{\Delta^2_0}{2\hbar^2} F(Q)$$  \hspace{1cm} (4)

$$\omega^2_s(q, Q) = \Delta^2_0 + v^2_s q^2 + \left(\frac{\Delta^2_0}{2\hbar^2} F(Q)\right)$$  \hspace{1cm} (5)

where $\Delta^2_0 = \Delta^2_0 (8K - 2)/8K - 1$ and $q$ (resp. $Q$) is the momentum along (resp. perpendicular to) the chains. $\Delta_n = \Delta_s \sin(n\pi/2(8K - 1))$ is the energy gap for the $n$-th breather ($n = 1, 2, \ldots$), and $F(Q) = \sum_{j=x,y,z} (1 - \cos Q_j b)$. For weakly interacting bosons ($K \gg 1$), the use of SMA may be questioned because the breather excitations of the mean-field SG model proliferate [8, 21]. Therefore, we have employed a variational approach previously used for coupled spin chains [22], and found the same dependence on $J/\mu$ for the dispersion as in [4]. With this approach, we have also calculated the momentum distribution of the superfluid phase (in the absence of a trap). At $T = 0$ and small momenta ($\ll \pi/b$), $\Psi_R(x) \approx \rho_0^{1/2} e^{i\phi_R(x)}$ and $\omega^2(q, Q) \approx v^2_s q^2 + v^2_{\perp} Q^2$, $(v_{\perp} \sim \mu b (J/\mu)^{2K/(4K - 1)}/\hbar$, cf. Eq. [4]), we find an anisotropic generalization of the Bogoliubov result [24]:

$$\frac{n(q, Q)}{w(Q)} \approx \frac{\psi^2_0 b Q^2}{4k}\delta(q) + \frac{\pi b^2 \psi^2_0 / 2K}{\left[q^2 + (v_{\perp} Q/v_s)^2\right]^{1/2}},$$ \hspace{1cm} (6)

which is valid for arbitrary interactions within the tubes. $w(Q)$ is the Fourier transform of the Wannier orbital, which varies slowly with $Q$.

We next consider the case of a finite axial Mott potential, i.e. $u_0 \neq 0$ and $\delta \approx 0$. In the absence of tunneling, the individual tubes would be 1D MI’s: even for a weak Mott potential, an integer number of bosons are localized to each well of the Mott potential [10, 11]. Increasing the tunneling will thus lead to deconfinement (i.e. 1D MI to 3D SF transition). To study the competition between the the Mott potential ($g_u$) and the Josephson coupling ($g_J$), we have used the renormalization group (RG) method. Since the Hamiltonian in [2] defines an effective field theory, its couplings ($K$, $g_u$, $g_J$, etc.) depend on the cut-off energy scale, which is typically set by the temperature for $T < \mu$. Thus, as the temperature is decreased, the couplings $K$, $g_u$, $g_J$ are renormalized, due to virtual transitions to high energy states. The nature of the ground state is thus determined by the dominant coupling as $T \to 0$. Using perturbative RG, we find the following RG flow equations:

$$\frac{dg_F}{dt} = \frac{g^2_F}{K}, \hspace{1cm} \frac{dg_J}{dt} = \left(2 - \frac{1}{2K}\right) g_J + \frac{g_J g_F}{2K},$$ \hspace{1cm} (7)

$$\frac{dg_u}{dt} = (2 - K) g_u, \hspace{1cm} \frac{dK}{dt} = 4g_J^2 - g_u^2 K^2,$$ \hspace{1cm} (8)

where $\ell \approx \ln \mu/T$. The coupling $g_u$ is generated by the RG and describes an interaction between bosons in neighboring tubes; $g_u$ and $g_J$ compete for $1/4 < K < 2$: the relative magnitude of their initial (i.e. bare) values determines which coupling grows faster. The faster growth of one coupling inhibits the other’s growth via the renormalization of $K$: If $g_u$ grows faster, $K$ flows towards 0, leading to the 1D MI, while if $g_J$ grows faster, $K$ also grows and leads to the 3D SF. To estimate the phase boundary between the 1D MI and the 3D SF, we integrate these equations (at fixed $g_u(0)$) with various $g_J(0)$ till the couplings are of order one. The resulting phase boundary is the continuous curve in Fig. 1. Via a separate mean field calculation at a specific $K$ value (see [19]), we showed that the condensate fraction $\psi^2_0$ grows continuously from zero at the phase boundary.

Finally, we turn to finite-size effects. First the finite extent of trapped cloud (either longitudinally or transversely) limits the minimum momenta of the modes. Thus the energy of the lowest modes in the 3D SF phase can be directly estimated from our results by using the minimum available momentum in [4]. For instance, for a finite 2D lattice containing $M_y \times M_z$ tubes (i.e. an atom cloud of size $L \times M_y b \times M_z b$) the lowest available momentum is $\sim \pi/(M_y b)$. Putting this value into [4], we find the frequency of the lowest transverse modes decreases with decreasing $J$. This is in qualitative agreement with the hydrodynamic analysis of Ref. [27]. However, unlike this hydrodynamic analysis, our results apply to the strongly interacting regime of the superfluid near the transition where depletion of the condensate can be large (as shown e.g. by the power-law behavior of the condensate fraction, $\psi^2_0 \sim \rho_0 (J/\mu)^{1/(4K - 1)}$). In addition, we are also able to describe the transition to the Mott insulating regime. Note that for finite size systems the phase transitions described above become crossovers. Furthermore, for harmonically trapped systems in the MI regimes an inhomogeneous state arises where the the SF and MI coexist [4, 12], and $\psi_0$ decreases slowly across the phase boundaries.

A second type of finite size effects comes from the finite size and hence discrete spectrum of each tube. In the experiments in 2D optical lattices loaded with ultracold atoms [4, 5], there are typically $N_0 \sim 10^2 - 10^3$ atoms per tube. At low temperatures, if $J$ is made very small (i.e. the lattice potential very deep), each 1D tube will behave as an atomic “quantum dot” characterized by a charging energy $E_C = \hbar \pi v_s / K L$ [7]. This is to be
balanced against the hopping energy $E_J$, which is not just $JN_0$ as the hopping amplitude is renormalized by the creation of virtual sound waves within the 1D tubes. Thus, to study this effect for $u_0 = 0$, we integrate out the phonons perturbatively in $J$ and obtain a quantum-phase model:

$$H_{QP} = -E_J \sum_{\langle R, R' \rangle} \cos (\phi_{R} - \phi_{R'}) + \frac{E_C}{2} \sum_{R} (N_R - N_0)^2 - \mu \sum_{R} N_R,$$

where $N_R$ (resp. $\phi_R$) is the particle-number (reps. phase) operator of tube $R$ (hence $[N_R, \phi_R] = i\delta_{RR'}$).

The renormalized hopping $E_J = J(N_0) \simeq JN_0^{1-\frac{1}{K}}$. The model \cite{2} has been extensively studied in the literature in connection with 2D arrays of Josephson junctions. It exhibits a 2D MI-SF at a critical value of $E_J/E_C$. For commensurate filling $N_0 (\mu = 0)$, a Monte Carlo (MC) calculation \cite{26} gives $(E_J/E_C)c \simeq 0.15$. In our case this reduces to $(J/\mu)c \simeq 0.3N_0^{-3/2}$ in the Tonks limit ($K \simeq 1$) and to $(J/\mu)c \simeq 0.15N_0^{2}$ for weakly interacting bosons ($K \gg 1$). Away from commensurate filling ($\mu \neq 0$), the critical $J/\mu$ is reduced as shown in the insert of Fig. 1, obtained using the MC data from Ref. \cite{26}. Note that in the 2D MI, only the phase coherence between different tubes of the 2D lattice is lost. There is no gap (apart from the finite size gap) to excitations within each 1D system. This is different from the 1D MI described above, where all excitations are gapped and any order (even quasilong range) in the phase is absent. For finite $u_0$, when $K \gtrsim 2$, $g_u$ flows to zero and the consideration above applies (hence the horizontal and vertical dashed lines in Fig. 1). Otherwise ($K \lesssim 2$), $g_f$ flows to zero and the 1D MI is as described above.

The above predictions can be directly tested in 2D optical lattices \cite{3,4}. In presence of the Mott potential, the deconfinement transition is of course the easiest to check. Even without the Mott potential, $\psi_0^2$ and $T_c$ as functions of $J/\mu$, and the change in the momentum distribution from the 1D TLL to the 3D superfluid should be accessible, by releasing the trap and the optical lattice, then measuring the expansion images. Finally, the excitation spectra of the superfluid can be measured with Bragg spectroscopy at low momentum transfer.

We thank T. Esslinger, A. Nersesyan, and M. Gunn for useful conversations/correspondence. AFH and MAC thank the hospitality of the University of Geneva where this work was started. AFH is funded by EPSRC (UK), MAC by Gipuzkoako Foru Aldundia (Basque Country). This work was supported in part by the Swiss National Science Foundation through MaNEP.

Note Added.- After this Letter was submitted, we received a preprint from Esslinger \cite{27} reporting on experimental results for the system we have considered here. The reported results are at least qualitatively consistent with our predictions.

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[28] The precise relationship \cite{21} between $\Delta$ and the coupling of the SG term allows us to obtain the full dependence of $\psi_0$ on $K$ and the non-universal ratio $\Lambda/\langle \rho_{\text{SG}} \rangle^{1-1/2K}$. The full expression will be given elsewhere \cite{21}.
[29] This is analogous to the Coulomb blockade phenomenon.
in mesoscopic physics.