Mott-Superfluid transition in bosonic ladders

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(Dated: December 31, 2021)

We show that in a commensurate bosonic ladder, a quantum phase transition occurs between a Mott insulator and a superfluid phase. Large coupling expansions show that this transition is in the Beresinskii-Kosterlitz-Thouless (BKT) universality class at commensurate filling and in the commensurate-incommensurate one for small doping. Various correlation functions such as the single particle one, show universal power law decay at the transition. The transport properties, that we compute can provide a check of the existence of this transition in experimental systems such as the JJ arrays.

We start with the Hamiltonian

\[ H = -t \sum_{i,\alpha} (b_{i,\alpha}^\dagger b_{i+1,\alpha} + \text{h.c.}) + \frac{U}{2} \sum_{i,\alpha} n_{i,\alpha} (n_{i,\alpha} - 1) \]

\[ -\mu \sum_{i,\alpha} n_{i,\alpha} - t_\perp \sum_i (b_{i,1}^\dagger b_{i,2} + \text{h.c.}) \] (1)

where \( \alpha = 1,2 \) is the chain index. \( t \) and \( t_\perp \) are respectively the intra and interchain hopping, \( U \) is the on-site particle interaction, and \( \mu \) is the chemical potential. In the following, unless we specify otherwise, \( \mu \) is chosen to impose one boson per site. To describe the low energy properties of (1) it is convenient to use the density-phase representation of the bosons

\[ \rho(x) \approx \rho_0 - \frac{1}{\pi} \partial_x \phi + \rho_0 \cos(2\phi) \] (2)

\[ \frac{b_i}{\sqrt{\rho_0}} = \Psi(x) e^{i\theta(x)} \sqrt{\rho(x)} \] (3)
\[- \frac{1}{\pi} \delta(x, y) = i \delta(y' - y), \tag{4}\]

where \(\alpha\) is a short distance cut-off of the order of the lattice spacing. Using these variables the single chain Hamiltonian can be rewritten as:

\[
H = H^0 \quad \frac{g_u}{(2\pi)^2} \int dx \cos 2\phi \tag{5}
\]

\[
H^0(u, K) = \frac{u}{2\pi} \int dx \left[ K(\partial_x \theta)^2 + \frac{1}{K}(\partial_x \phi)^2 \right] \tag{6}
\]

All interaction effects are hidden in the Luttinger liquid parameters \(u\), the sound velocity, and \(K\) a coefficient that controls the asymptotic decay of the correlation functions. Free bosons correspond to \(K = \infty\) and hard core ones \((U = \infty)\) to \(K = 1\). Note that for one boson per site, the \(U = \infty\) case is a trivial band insulator. The \(\cos(2\phi)\) term where \(g_u \propto U\) describes the umklapp scattering of the bosons on the lattice and is responsible for the Mott transition. Note that the continuous form (6) is much more general than the microscopic hamiltonian (1) and describes systems with longer range interactions as well. Using the symmetric basis \(\phi_{s,a} = (\phi_1 \pm \phi_2)/\sqrt{2}\), (6) gives:

\[
H = H^0_s(u, K_a) + H^0_a(u, K_a)
\]

\[
\frac{2g_u}{(2\pi)^2} \int dx \cos(\sqrt{2}\phi_a) \cos(\sqrt{2}\phi_a)
\]

\[
\frac{1}{\pi\alpha} \int dx \cos(2\theta_a) \tag{7}
\]

where \(H^0_{s,a}\) are defined by (3). For (1) one has \(u_{s,a} = u\) and \(K_{s,a} = K\).

In (6) there is a competition between the umklapp term, that favors localization of the charge hence order in the field \(\phi_{s,a}\) (and \(\phi_a\)) and the interchain coupling that wants to order the relative superfluid phase \(\theta_a\) between the two chains. Since these two fields are conjugate one can naively expect a transition between the two types of order for the antisymmetric field. The resulting competition affects the symmetric modes, inducing a metal-insulator transition. To investigate this transition we use a renormalization group (RG) method in powers of the umklapp and interchain hopping. The RG equations read:

\[
\frac{dg_u}{dt} = (2 - K_a/2 - K_s/2)g_u
\]

\[
\frac{d\tilde{t}_\perp}{dt} = (2 - K^{-1}_s/2)\tilde{t}_\perp
\]

\[
\frac{dK_a}{dt} = -\frac{K_s^2g_u^2}{16\pi^2} + \frac{\tilde{t}_\perp^2}{8\pi^2}
\]

\[
\frac{dK_s}{dt} = -\frac{K_a^2g_u^2}{16\pi^2}
\]

where \(g_u = g_u/u\) and \(\tilde{t}_\perp = (4\pi^2\alpha)\tilde{t}_\perp/u\) are dimensionless coupling constants. For \(1/4 < K < 2\), (8) show that both \(t\) and \(g_u\) are relevant operators that thus tend to order \(\theta_a\) and \(\phi_a\) respectively. Two different behaviors occur depending on which operator becomes of order unity first: (i) if the umklapp scattering eventually dominates the flow it leads to ordering in \(\phi_a\) and \(\phi_a\) and we recover an insulating behavior similar to the one of a single chain; (ii) if the interchain hopping dominates then \(\theta_a\) orders and the umklapp scattering becomes irrelevant. The only term that can localize the symmetric component is now a term generated to second order of the form \(\cos(\sqrt{8}\phi_a)\). This operator has a dimension \(2K\) instead of \(K\) for a single chain umklapp, and is thus much less relevant. The precise interaction for which this operator is relevant depends on its amplitude that can only be computed reliably when \(g_u \ll 1\). Even if this is not the case, one can show in the large \(\tilde{t}_\perp\) expansion below that there is a range of interactions between \(U_{\text{single chain}}^s\) and \(U = \infty\) for which this operator is indeed irrelevant. Thus at fixed interactions a transition between the Mott insulator and a superfluid for a given value of the interchain hopping occurs. Since both the umklapp and the interchain hopping are relevant operators there is no weak coupling fixed point at the transition, and the RG (8) cannot be used to determine the critical properties of this transition. One can however get qualitatively the transition line as the position where the most relevant operator changes. Using (8) leads to

\[
\tilde{t}_\perp = (g_u)^{\frac{2-1/(2K)}{2-1/(2K)}} \tag{9}
\]

The resulting phase diagram is shown on Fig. 1.

We now turn to the critical properties of the insulator-superfluid transition itself. Since it is difficult to extract from the RG flow, we can only analyse it in specific limits. The first one is the large transverse hopping \(t\gg tU\). On each rung there are two one-particle states, bonding or anti-bonding. The many bosons low lying states correspond to putting every boson in the bonding state. The chemical potential must be such as to ensure a particle-hole symmetry (around two bosons per “site”) in order to have a constant density superfluid-insulator transition. This gives back the familiar problem of one species of bosons on a lattice with a commensurate filling of two bosons per site, with an effective hopping \(t\) and an on site repulsive energy \(U/2\). Since the effective interaction is reduced compared to the single chain the large \(t\) system can be superfluid even if the single chain is Mott insulating. The Mott-superfluid transition is a BKT one with an effective LL parameter \(K_{\text{eff}} = 2\) and a dynamical exponent \(z = 1\). To obtain the LL parameter \(K_s\) of the original ladder one can compute the correlation functions. The one-particle green’s function has a universal power law decay at the transition \(\langle \psi^\dagger(r)\psi(0)\rangle \propto (1/r)^{1/4}\). Using (8) leads to the universal value \(K_s^* = 1\) at the transition. Since for fermionic ladders the large \(t\) limit can lead to different phases than the small \(t\) limit, it is important to check that an identical critical behavior is recovered in another strong coupling limit. We rewrite (8) as the bosonized
form of a different microscopic lattice Hamiltonian than (1), namely two coupled spin one-half chains:

$$H = H^{XXZ}_α + H^{XXZ}_β - J^z_α \sum_i S^z_α,i S^z_β,i$$

$$+ h^x_α \sum_i (-1)^i S^x_α,i$$

$$H^{XXZ} = \sum_i J(S^x_α i S^x_β i + S^y_α i S^y_β i) + J^z S^z_α i S^z_β i$$

(10)

(11)

Using the standard bozonized expressions for the spins (9) from (10) with $h_x \propto t_1$, $J^z_α \propto g_u$, $J^z_β \propto g_a$, $J^z_β \propto g_a$. $J^z_β$ are chosen such as to recover the correct bare Luttinger parameters $K_α$ and $K_β$. The Hamiltonian (10) can be studied in the strong coupling limit $h_x \sim J^z_α \gg J_α,β (t_1 \sim U \gg t)$. Each rung corresponds to a four level system that may be easily diagonalized. Keeping only the two degenerate lowest levels we obtain a pseudo-spin one-half chain. If we denote its spin by $S$ and its couplings by $J$ the correspondence between the spin operators is:

$$S^z_α = \cos(\alpha) \hat{S}^z$$

(12)

$$S^z_β = \hat{S}^z$$

(13)

$$S^z_α = \frac{1}{2} \sin(\alpha) \hat{I}$$

(14)

$$S^z_β = (-1)^{i+1} \sin(\alpha) \hat{S}^z +$$

(15)

$$\cos(\alpha) = \frac{J^z_β}{(J^z_α)^2 + (2h^x_α)^2}$$

(16)

where $I$ is the identity. Using these relations, (10) becomes an XXZ Hamiltonian with the effective couplings:

$$\frac{-J^z_β}{J} = \frac{J^z_β}{J_β} + \left( \frac{J^z_α}{2h^x_α} \right)^2 \left[ J^z_α + J^z_β \right]$$

(17)

A non polarized XXZ chain (corresponding to commensurate filling for the bosons) is in a LL phase for $|J^z_α|/J < 1$ and has a gap otherwise. For the pseudo-spin Hamiltonian this means that as we increase the staggered field the model becomes gapless for a critical value of order $h_x \propto J^z_α$. One recovers the BKT transition with an effective universal critical LL exponent $K_c = 1/2$ and a dynamical exponent $z = 1$. Using (12) and $S^z_β \propto \psi^\dagger_1 \psi^\dagger_2$ for the bosons it is easy to check from (13) that the original bosonic ladder has a universal LL parameter $K^*_s = 1$. The diagonalization on each rung shows that $S^z_α$ has a non-zero mean value, which we interpret as an order in the field $\theta_α$. These results for the transition are coherent with the previous large transverse hopping analysis, which gives some confidence that we indeed capture the correct critical behavior. The two above analysis extend easily to the situation where the chemical potential does not ensure particle hole symmetry. In that case, this leads to either a magnetic field in the spin representation or an extra chemical potential in the effective single bosonic chain limit. In each case the BKT transition becomes a commensurate-incommensurate one with a universal LL parameter $K^*_s = 1/2$ and a dynamical exponent $z = 2$. The other properties at the transition (compressibility, etc.) both for the commensurate and incommensurate case can be obtained in a similar way than for the simple Mott transition for bosons (1). A summary of the critical behavior is shown on Fig. 1.

Various physical observables can be computed. In the superfluid phase the symmetric modes are described by a LL with a parameter $K_s$, whereas the $\theta_α$ mode is gapped. Thus most correlation functions involving the superfluid phase decay as power law. For example

$$\langle \psi^\dagger_α(r) \psi_α(0) \rangle \propto \left( \frac{1}{r} \right)^{\frac{1}{2}}$$

(18)

$$\langle \psi^\dagger_1 \psi^\dagger_2(r) \psi_1 \psi_2(0) \rangle \propto \left( \frac{1}{r} \right)^{\frac{1}{2}}$$

(19)

In the Mott phase $\phi_α$ and $\phi_β$ are ordered so the correlations functions such as (18) decay exponentially. One of the most important difference between the two phases are of course the transport properties. The Drude weight is zero in the Mott insulating phase, whereas it is given by $D = 2u_s K_s$ in the superfluid one, with a discontinuous jump at the transition. Far from the transition one can obtain $K_s$ from the RG. We use a two scale renormalization and cut the renormalization due to the umklapp when the the transverse hopping reaches a value of order one. This gives

$$D = 2u_s K_s \left( 1 - \frac{C}{K_s} \left[ \frac{4K_s (2-K_s)}{4K_s - 2K_s} - 1 \right] \right)$$

(20)
FIG. 2: The curve (a) is a schematic view of the resistivity for the ladder in the mott-insulating state, with an activated behavior for temperatures lower than the charge gap \( \Delta_s \). The curve (b) is for a superfluid ladder (shown for \( K < 1.5 \)) (see text). The dashed part of the curves represents the cross-over region between low and high temperature. The insert shows the optical conductivity (shown for \( K < 1.25 \)).

where \( C \) is a constant of order unity. Thus the Drude weight decreases as one approaches the transition by reducing \( t_\perp \).

The temperature and frequency dependence of the conductivity can also be extracted from the RG. The high frequency behavior may be perturbatively computed from the umklapp scattering operator \( g_u(\cos 2\phi_1 + \cos 2\phi_2) \). This leads to \( \sigma(\omega) \propto g_u^2 \omega^{2K-5} \), similar to the result for a single chain. However for frequencies less than the gap in the antisymmetric mode, \( \Delta_a \), the original umklapp operator has been renormalized nearly to zero. The dominant scattering operator is \( \cos(\sqrt{8} \phi_a) \) leading to \( \sigma(\omega) \propto g_u^2 \omega^{4K_a-5} \). In the Mott phase there is a gap \( \Delta_s \) in the symmetric mode below which these behaviors are cut, whereas it extends to \( \omega = 0 \) in the superfluid phase which has in addition the Drude weight at zero frequency. Similar behavior is obtained for the temperature dependence of the conductivity

\[
\begin{align*}
\rho(T) &\propto T^{2K-3}, & T > \Delta_a \\
\rho(T) &\propto T^{4K-3}, & T < \Delta_a
\end{align*}
\]

In the Mott phase one recovers the familiar activated exponential behavior when \( T < \Delta_s \). Both the dc and ac conductivity are shown on Fig. 2. Note that for \( K_s > 1.5 \) the temperature dependence is non monotonous in the superfluid phase, whereas in the insulating one the resistivity would start to increase with decreasing temperature even well above the Mott gap.

The above predictions could be checked either in numerical simulations or in experimental systems such as the JJ arrays. In numerical simulations the LL parameters could be extracted in a way similar to the one that was used for the single bosonic chain. The gaps, superfluid correlation functions and the Drude weight are probably the most easily checkable quantities. For JJ arrays, as for the single chain the transition we predict should be visible as a metal-insulator transition in a transport experiment. One possible way to control \( t_\perp \) could be to use a magnetic field.

ACKNOWLEDGMENTS

We would like to thank T. Kuehner, H. Monien, E. Orignac and G.T. Zimanyi for useful discussions. This work has been supported in part by NATO grant 971615.

REFERENCES

‡ Electronic address: donohue@lps.u-psud.fr
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1 F. D. M. Haldane, Phys. Rev. Lett. 47, 1840 (1981).
2 M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B 40, 546 (1989).
3 L. Sondhi, S. M. Girvin, J. P. Carini, and D. Shahar, Rev. Mod. Phys. 69, 315 (1997).
4 T. Giamarchi, Physica B 230-232, 975 (1997).
5 G. G. Batrouni, R. T. Scalettar, and G. T. Zimanyi, Phys. Rev. Lett. 65, 1765 (1990).
6 W. Krauth, M. Caffarel, and J. Bouchaud, Phys. Rev. B 45, 3137 (1992).
7 N. Elstner and H. Monien, Phys. Rev. B 59, 12184 (1999).
8 T. D. Kühlner, S. R. White, and H. Monien, Phys. Rev. B 61, 12474 (2000).
9 A. van Oudenaarden and J. E. Mooij, Phys. Rev. Lett. 76, 4947 (1996).
10 R. Fazio and H. van der Zant (2000), cond-mat/0011152.
11 P. Dononue and et al., Phys. Rev. B 63, 045121 (2001), and references therein.
12 K. Le Hur, preprint, cond-mat/0006225 (2000).
13 M. Tsuchiz and et al., preprint, cond-mat/0007503 (2000).
14 E. Orignac and T. Giamarchi, Phys. Rev. B 57, 11713 (1998).
15 E. Orignac and T. Giamarchi, Phys. Rev. B 57, 5812 (1998).
16 H. J. Schulz, Phys. Rev. B 34, 6372 (1986).
17 S. P. Strong and A. J. Millis, Phys. Rev. B 50, 9911 (1994).
18 H. J. Schulz, Fermi liquids and non-Fermi liquids (Elsevier, Amsterdam, 1995), p. 533.
19 H. J. Schulz, Phys. Rev. B 22, 5274 (1980).
20 E. Orignac and T. Giamarchi, preprint, cond-mat/0011497 (2000).