Quantum Phase Transitions for Bosons in One Dimension

Reinhard Baltin and Karl-Heinz Wagenblast

Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe, Germany

(February 24, 2018)

Abstract

We study the ground state phase diagram and the critical properties of interacting Bosons in one dimension by means of a quantum Monte Carlo technique. The direct experimental realization is a chain of Josephson junctions. For finite-range interactions we find a novel intermediate phase which shows neither solid order nor superfluidity. We determine the location of this phase and study the critical behaviour of the various transitions. For on-site interaction only, we map out the phase diagram as a function of the hopping strength and the chemical potential.

PACS numbers: 05.30.Jp, 67.40.Db, 67.90.+z
One dimensional systems attracted strong interest over the past years. The major work focused on Fermionic models where a breakdown of Landau’s Fermi-liquid theory opens an avenue for new investigations. Bosonic models deserve our attention for several reasons: The close analogy between Fermions and Bosons in 1D, the study of enhanced quantum fluctuations in low dimensions, and the possibility of experimental investigation.

A good candidate for experimental studies is $^4$He, which has been investigated in the bulk and on surfaces [1]. Another class are superconductors. The phase of the superconducting order-parameter is a Bosonic quantum variable. Nanofabricated circuits, especially Josephson junction networks show these quantum effects. Mott transitions have been observed in two dimensions [4] and recently also in one-dimensional systems [3]. The low-energy Hamiltonian of a Josephson chain coincides with that of a Luttinger liquid [4].

The interplay between the interactions and the hopping gives rise to various ground states which are separated by quantum phase transitions. A superconductor–insulator transition separates a Mott-insulating phase with localized particles from a phase with delocalized particles and superfluid response. The critical value of the hopping strength depends on the chemical potential. The inclusion of finite-range interactions enriches the picture, opening the possibility for various commensurate Mott-insulating phases with a solid-type ordering of the particles. Mean-field studies [5] and numerical investigations of two-dimensional systems [6–8] showed that the transition from a Mott-insulating solid phase to the superfluid phase splits into two separate transitions with intermediate supersolid phases. In these supersolid phases superfluidity and long-range solid order coexist. No such supersolid phase has been found in 1D [4].

We study the quantum-phase model in 1D by means of a quantum Monte Carlo method. For on-site interactions we determine the phase diagram with lobe-shaped Mott-insulating phases in good agreement with a $t/U$-expansion of Freericks and Monien [10], as shown in Fig. 1a). With on-site and nearest-neighbour interactions the transition between solid phases, where the site-occupancy alternates between $N$ and $N + 1$, and superconducting phase splits into two separate transitions as displayed by the scaling plot in Fig. 2. This
gives rise to a novel intermediate phase which shows neither superfluidity, nor a solid order. We determine the location of this phase and discuss its properties. We extract the critical behaviour of the transitions in agreement with predictions of order-parameter descriptions for the onset of superfluidity \[11,12\].

The quantum-phase model describes Bosons on a lattice. Its Hamiltonian is given by

\[
H = \sum_i \left[ \frac{U_0}{2} n_i^2 + U_1 n_i n_{i+1} - \mu n_i - t \cos(\phi_{i+1} - \phi_i) \right].
\]  

Two key ingredients are incorporated in this model: The interaction of the Bosons (on-site \(U_0\) and nearest-neighbours \(U_1\)), and the hopping \(t\). The chemical potential \(\mu\) tunes the number of particles on the lattice. Phase \(\phi_i\) and number \(n_i\) of this model are non-commuting operators, i.e. \([n_i, \phi_j] = i\delta_{ij}\). The variable \(i\) labels the lattice sites. The essential physics is thus dominated by the competition between phase-coherence and solid order. This gives rise to quantum fluctuations and quantum phase-transitions at zero temperature. The properties of this model are periodic in \(\mu\) with a period of \(U_0 + 2U_1\). The quantum-phase model directly represents a chain of Josephson junctions with \(n_i\) being the excess number of Cooper pairs on site \(i\), the Coulomb interactions \(U\), and the Josephson coupling \(t\). A gate voltage can be applied to tune the chemical potential \[^{[6]}\]. The quantum-phase model is equivalent to the Bose-Hubbard model in the limit of a large number of Bosons per site \[^{[6]}\].

We use the mapping of a \(d\)-dimensional quantum model onto a \(d+1\)-dimensional classical model to study the Hamiltonian of Eq. \[^{[1]}\]. The 1D quantum-phase model has a current-loop representation in 1+1 dimensions with the partition function \[^{[2]}\]

\[
Z = \sum_{\{J^x, J^\tau\}} \delta(\partial_{\tau} J^\tau + \partial_x J^x) \exp \left\{ -K \sum_{i, \tau} \left[ (J^\tau_{i,\tau})^2 + \frac{U_1}{U_0} J^\tau_{i,\tau} J^\tau_{i+1,\tau} - \frac{\mu}{U_0} J^\tau_{i,\tau} + (J^x_{i,\tau})^2 \right] \right\}. \tag{2}
\]

A discrete two-component current \((J^x, J^\tau)\) flows on a \((1+1)\)-dimensional space-time lattice. The constraint \(\partial_{\tau} J^\tau + \partial_x J^x = 0\) allows only divergence-free current loops. The imaginary time is discretized with the time-spacing \(\epsilon\). The mapping is explained in detail in Ref. \[^{[3]}\]. The effective coupling constant \(K\) plays the role of the inverse temperature of the classical model and is given by \(K = \epsilon U_0/2 = \ln [I_0(\epsilon t)/I_1(\epsilon t)]\), where \(I_0, I_1\) are the modified Bessel
functions. The time spacing $\epsilon$ is chosen to be of the order of the inverse Josephson plasma-frequency, $\epsilon \approx 1/\sqrt{\mu_0}$, such that the couplings in $x, \tau$-direction are isotropic. The time component of the current $J^\tau_i$ can be identified as the number of excess Bosons on site $i$.

The key quantities in our study are the superfluid stiffness $\rho_0$ and the structure factor $S(k)$. The former measures superfluid correlations in the system. The latter indicates whether the particles are arranged periodically, i.e. whether the system is in a solid ground state. Both quantities can be expressed in terms of the currents $J$ on a lattice of size $L \times L_{\tau}$:

$$\rho_0 = \frac{1}{LL_{\tau}} \sum_{i,\tau} \langle J^x_{i,\tau} J^x_{0,0} \rangle,$$

$$S(k) = \frac{1}{LL_{\tau}} \sum_{i,\tau} \langle J^\tau_{i,\tau} J^\tau_{0,0} \rangle \exp\{ikr_i\}.$$  (4)

Nearest-neighbour interactions give rise to solid phases with a finite $\pi$-component of the structure factor $S_{\pi} = S(k = \pi)$.

An order-parameter description for the onset of superfluidity predicts a dynamical critical exponent $z = 1$ in the particle-hole symmetric case at the tips of the lobes in the $t-\mu$ plane and a Kosterlitz-Thouless (KT) transition. For broken particle-hole symmetry away from these symmetry lines, $z = 2$ and a power law critical behaviour follows from these considerations. A Ginzburg-Landau description for the transition to a finite $S_{\pi}$ was developed in Ref. [13]. In the absence of a superfluid background this action implies the dynamical critical exponent $z = 1$.

The simulation is confined to rather small system sizes, and we use finite-size scaling for determining critical properties of our model. For power-law critical behaviour we use the scaling Ansatz:

$$\rho_0 = L^{1-z} \tilde{\rho}(L^{1/\nu}(t - t_c), L_{\tau}/L^z),$$

$$S_{\pi} = L^{-2\beta/\nu} \tilde{S}(L^{1/\nu}(t - t_c), L_{\tau}/L^z),$$  (6)

where $\beta$ is the critical exponent of the order parameter, $\nu$ is the critical exponent for the correlation length, and $\tilde{\rho}, \tilde{S}$ are scaling functions.
A KT critical point can be determined using the jump of the stiffness, characteristic logarithmic corrections, and the behaviour of the exponentially diverging correlation length \[14\].

We also investigated the possibility of a first order transition by studying the energy histogram. We find no evidence for a first order transition in the phase diagram.

We simulate the model of Eq. (2) with periodic boundary conditions using the Metropolis algorithm. The current loops can be divided into two classes. Local loops represent a current around a single plaquette on the lattice. Global loops describe a net current through the whole system. In each Monte Carlo sweep we try to create a local loop on each lattice site and global loops throughout the lattice. Each Monte Carlo run for one data point consists of \(2 \cdot 10^5 - 2 \cdot 10^6\) sweeps for equilibration and \(10^6 - 10^7\) sweeps for measurement, depending on the lattice size and the coupling \(t/U_0\).

We now present our numerical data, first for on-site interaction \((U_1 = 0)\). For non-integer values of \(\mu/U_0\) particle-hole symmetry is broken and according to Eq. (3) the scaled data \(L\rho_0\) vs. \(t\) for different lattice sizes should cross at the critical coupling \(t_c\) provided \(L^2/L_\tau\) is kept constant. Fig. 1b) shows the scaled superfluid stiffness vs. the coupling for \(\mu/U_0 = 0.3\). The curves for different lattices cross at \(t_c/U_0 = 0.207 \pm 0.003\). The critical exponent \(\nu\) is fitted such that plots of \(L\rho_0\) vs. \(L^{1/\nu}(t - t_c)\) collapse onto one curve, the scaling function \(\tilde{\rho}\), as shown in the inset of Fig. 1b). We find \(\nu = 0.6 \pm 0.1\) which agrees with results from \[12\]. At \(\mu/U_0 = 0.4\) the critical coupling is \(t_c/U_0 = 0.10 \pm 0.005\). For \(\mu/U_0 = 0.2\) we find \(t_c/U_0 = 0.325 \pm 0.01\). The critical exponent \(\nu\) is independent of the chemical potential in the range \(0.2 \leq \mu/U_0 \leq 0.4\). At integer values of \(\mu/U_0\), the system has particle-hole symmetry. Here we use the universal jump of the superfluid stiffness characteristic for a KT transition to determine the transition point \[14\]. From the simulations with quadratic lattices \((L, L_\tau \leq 24)\) we obtain \(t_c/U_0 = 0.83 \pm 0.07\).

The resulting phase diagram consists of Mott-insulating lobes with fixed integer density in the \(t-\mu\) plane, see Fig. 1a). The cusp-like shape of the lobes is also found in the phase diagram of the related 1d Bose-Hubbard model analyzed in Ref. \[9\]. In the vicinity of the
symmetry lines at integer values of $\mu/U_0$ we find deviations from the predicted finite-size scaling of the superfluid stiffness of Eq. (3). We argue that this is due to the vicinity of the KT transition which introduces another length scale in the scaling relation. Asymptotically for large systems we expect to recover a scaling according to Eq. (5). The solid lines in Fig. 1a) are the phase boundary obtained by a third order $t/U$-expansion for the Bose-Hubbard model of Freericks and Monien [10] in the limit of a large number of Bosons per site which is in good agreement with our data. In Ref. [10] it is argued that the deviation near the tips of the lobes is due to the KT transition whose physics cannot be described in perturbation theory of finite order.

When nearest-neighbour interaction is included the phase diagram is richer, including solid, superfluid and novel intermediate phases. We find Mott-insulating lobes where the site occupancy alternates periodically between $N$ and $N+1$, i.e. solid order with a finite structure factor $S_\pi$, a superfluid phase with $\rho_0 \neq 0$, and a compressible intermediate phase with $S_\pi = 0$ and $\rho_0 = 0$. We focus in our studies on the case of broken particle-hole symmetry where we can use the scaling relations of Eq. (5) and Eq. (6). The dynamical exponent for the onset of superfluidity is thus $z = 2$. For the transition to a finite $S_\pi$ we use $z = 1$, and fit the ratio $2\beta/\nu$ such that the scaled data cross in one point. We estimate for $2\beta/\nu = 0.12 \pm 0.02$. Fig. 2 shows the scaled data of $\rho_0$ and $S_\pi$ vs. coupling for $U_1/U_0 = 0.4$ and $\mu/(U_0 + 2U_1) = 0.6$. We obtain for the superfluid transition $t_c/U_0 = 0.130 \pm 0.006$ and for the transition to the solid phase $t_c/U_0 = 0.112 \pm 0.005$. In between there is an intermediate phase in which the system neither is superfluid nor solid. We address this lack of order at $T = 0$ to the enhanced fluctuations in 1D. There are corrections to the scaling relation of the superfluid stiffness, since the curves in Fig. 2 do not exactly cross in one point. A detailed investigation of these corrections, which we address again to the vicinity of the KT transition, is beyond our numerical resolution.

The absence of both, superfluidity and solid order, may imply the existence of a normal phase of the Bosons with metallic response. A study of the superfluid stiffness as a function of the Matsubara frequencies and an analytic continuation can yield insight into the response
properties [13]. Within the accuracy of our results we are not able to prove or disprove the existence of a finite d.c. conductivity [16]. There are general objections to a normal phase for Bosons at zero temperature by Leggett [17]. The arguments are based on the absence of nodes of the many body ground state wave function for Bosons in the continuum. These arguments are not directly applicable to our case as we study a lattice model. Furthermore, Leggett himself argued that the existence of a normal ground state of Bosons cannot be ruled out completely in 1D. The question of the response of the intermediate phase remains open and subject to further studies. A very recent work predicts the existence of a repulsive Luttinger liquid intervening the solid and superfluid phase [18].

In conclusion we determined the phase diagram of the quantum-phase model in 1D by means of a quantum Monte Carlo method. For repulsive on-site interaction we mapped out the phase diagram as a function of the hopping strength and the chemical potential. Finite-range interactions give rise to new phases. The insulating phases with half-integer filling have solid order with a unit cell of two lattice spacings. Our simulations show an intermediate phase where both, solid and superfluid order are destroyed by the strong quantum fluctuations in 1D.

We would like to thank Rosario Fazio, Anne van Otterlo, Gerd Schön, and Gergely T. Zimanyi for stimulating discussions. This work is within the SFB195 of the “Deutsche Forschungsgemeinschaft”.
REFERENCES

* Present address: Max-Planck-Institut für Kernphysik, Postfach 103980, D-69029 Heidelberg, Germany.

[1] *The Physics of Liquid and Solid Helium*, edited by K.H. Bennemann and J.B. Ketterson (Wiley, New York, 1976).

[2] L.J. Geerligs *et al.*, Phys. Rev. Lett. 63, 326 (1989); P. Delsing *et al.*, Phys. Rev. B 50, 3959 (1994); A.J. Rimberg *et al.*, Phys. Rev. Lett. 78, 2632 (1997).

[3] A. van Oudenaarden and J.E. Mooij, Phys. Rev. Lett. 76, 4947 (1996).

[4] R. Fazio, K.-H. Wagenblast, C. Winkelholz, and G. Schön, Physica B 222, 364–369 (1996).

[5] K. Liu and M.E. Fisher, J. Low Temp. Phys. 10, 655 (1973).

[6] A. van Otterlo and K-H. Wagenblast, Phys. Rev. Lett. 72, 3598 (1994); A. van Otterlo, K-H. Wagenblast, R. Baltin, C. Bruder, R. Fazio, and G. Schön, Phys. Rev. B 52, 16176 (1995).

[7] G.G. Batrouni, R.T. Scalettar, G.T. Zimanyi, and A.P. Kampf, Phys. Rev. Lett. 74, 2527 (1995); R.T. Scalettar *et al.*, Phys. Rev. B 51, 8467 (1995).

[8] E. Roddick and D.H. Stroud, Phys. Rev. B 51, 8672 (1995).

[9] G.G. Batrouni, R.T. Scalettar, and G.T. Zimanyi, Phys. Rev. Lett. 65, 1765 (1990); G.G. Batrouni *et al.*, Phys. Rev. B 46, 9051 (1992); P. Niyaz, R.T. Scalettar, C.Y. Fong, and G.G. Batrouni, Phys. Rev. B 50, 362 (1994).

[10] J.K. Freericks and H. Monien, Europhys. Lett. 26, 545 (1994); J.K. Freericks and H. Monien, Phys. Rev. B 53, 2691 (1996).

[11] S. Doniach, Phys. Rev. B 24, 5063 (1981).
[12] M.P.A. Fisher, B.P. Weichman, G. Grinstein, and D.S. Fisher, Phys. Rev. B 40, 546 (1989).

[13] E.S. Sørensen, M. Wallin, S.M. Girvin and A.P. Young, Phys. Rev. Lett. 69, 828 (1992); M. Wallin et al., Phys. Rev. B 49, 12115 (1994);

[14] H. Weber and P. Minnhagen, Phys. Rev. B 37, 5986 (1988).

[15] E. Frey and L. Balents, Phys. Rev. B 55, 1050 (1997).

[16] R. Baltin, Diplomarbeit Universität Karlsruhe (1996).

[17] A.J. Leggett, Physica Fennica 8, 125 (1973).

[18] A.I. Larkin and L.I. Glazman, cond-mat/9705169.
FIG. 1. Results for on-site interaction. 

(a) Phase diagram. The phase boundary separates the Mott-insulating (MI) phase from the superfluid phase (SF). The symbols are our Monte Carlo results, the solid line is the result of a third order $t/U$-expansion from Ref. [10].

(b) Scaled data for the superfluid stiffness at $\mu/U_0 = 0.3$. The intersection of the curves gives the transition point at $t_c = 0.207U_0$. Array sizes $L \times L_r$: (1) $6 \times 9$, (2) $8 \times 16$, (3) $10 \times 25$, (4) $12 \times 36$. The inset shows the scaling of the data to a single function according to Eq. (5), with $\nu = 0.6$. 
FIG. 2. Scaled data for the structure factor (left) and the superfluid stiffness (right) for $U_1/U_0 = 0.4$ and $\mu/(U_0 + 2U_1) = 0.6$. In the intermediate phase for $0.112 < t/U_0 < 0.130$ the system shows neither solid order nor superfluidity. Array sizes $L \times L_\tau$ for the superfluid stiffness: (1) 6 × 9, (2) 8 × 16, (3) 10 × 25, (4) 12 × 36. For the structure factor: $L = L_\tau = 8$ (a), 10, 12, 14, 16, 18, and 20 (b).