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The one-dimensional extended Bose–Hubbard model[¶]

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Abstract. We use the finite-size, density-matrix-renormalization-group (DMRG) method to obtain the zero-temperature phase diagram of the one-dimensional, extended Bose–Hubbard model, for mean boson density $r = 1$, in the U–V plane (U and V are respectively, onsite and nearest-neighbour repulsive interactions between bosons). The phase diagram includes superfluid (SF), bosonic-Mott-insulator (MI), and mass-density-wave (MDW) phases. We determine the natures of the quantum phase transitions between these phases.

Keywords. Boson systems; quantum statistical theory; ground state; elementary excitations; other topics in quantum fluids and solids; liquid and solid helium.

1. Introduction

The study of systems of interacting bosons has been attracting a lot of attention over the past decade or so. Progress in this field has been driven by an interplay between theory,[1–10] numerical simulations,[11–14] and experiments. The latter include studies of liquid ^{4}He in porous media like vycor or aerogel,[15] Bose–Einstein condensates trapped in optical lattices,[16,17] micro-fabricated Josephson-junction arrays,[18–20] the disorder-driven superconductor-insulator transition in thin films of superconducting materials like bismuth,[21] and flux lines in type-II superconductors pinned by columnar defects aligned with the external magnetic field.[22] Theoretical and numerical studies[2–4,7,11,12] have concentrated on the Bose–Hubbard model which exhibits superfluid (SF) and bosonic-Mott-insulator (MI) phases and, if onsite disorder is included, a Bose-glass (BG) phase too. As we will show below, a mass-density-wave (MDW) phase can also be obtained in an extended-Bose–Hubbard model. Mean-field theories[2–4,6] of such models yield the phases mentioned above and physically appealing pictures of the natures of these phases. However, especially in low dimensions, such mean-field theories cannot always uncover the types of correlations present in these phases or the natures of the transitions between these phases. We have shown earlier[7] that, for *one-dimensional* Bose–Hubbard models, the density-matrix-renormalization-group (DMRG) is a reliable method for the elucidation of such correlations and the universality classes of quantum phase transitions. Here we give a brief overview of our recent calculation of the zero-temperature phase diagram of the extended-Bose–Hubbard model in one dimension by the DMRG method.

[¶]Dedicated to Professor C N R Rao on his 70th birthday
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2. Results and discussion

The Hamiltonian for the extended-Bose–Hubbard model is

$$\Box = -t\sum_{\langle i,j\rangle}(a_i^{\dagger}a_j + hc) + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) + V\sum_{\langle i,j\rangle}\hat{n}_i\hat{n}_j - \sum_i m_i\hat{n}_i, \tag{1}$$

where t is the amplitude for the hopping of bosons between nearest-neighbour pairs of sites $\langle i, j\rangle$, $a_i^{\dagger}$ (a_i) is the boson creation (annihilation) operator at site i, and $\hat{n}_i = a_i^{\dagger}a_i$ the associated number operator with eigenvalues 0, 1, 2,$\cdots$. The onsite interaction U and the nearest-neighbour interaction V are positive (i.e. repulsive). We restrict ourselves to the physically relevant region $V \le U$ and set the energy scale by choosing $t = 1$. The random chemical potential m_i can be used to model onsite disorder.

This model has been studied by a number of groups and several interesting results have been obtained especially in the case $V = 0$.[2,5,7–11] In particular, if $V = 0$ and there is no disorder, only an SF phase is obtained at noninteger densities. For integer densities an MI phase is obtained at large U; as U is lowered the system shows an MI-SF transition, which is of the Kosterlitz–Thouless type[23] in one dimension. The most detailed study of this transition in the Bose–Hubbard model was carried out by us in Ref. [7] by using the DMRG method.

We will not review our DMRG scheme since it has been described in detail elsewhere.[7,24] For our purposes here it suffices to note that, especially in one dimension and with open boundary conditions, the DMRG method allows us to calculate the ground-state energy $E_L^0(N)$, the first-excited-state energy $E_L^1(N)$, and the associated eigenstates $|y_{0L}\rangle$ and $|y_{1L}\rangle$ of models such as (1) as a function of the size L for a system with N bosons. Given these we can calculate the energy gap $G_L \equiv [E_L^0(N+1) + E_L^0(N-1) - 2E_L^0(N)]$, the order parameter for the MDW phase $M_{MDW} \equiv \frac{1}{L}\sum_i(-1)^i\langle y_{0L}|(\hat{n}_i - r)|y_{0L}\rangle$ and the associated correlation function $\Gamma_L^{MDW}(r) \equiv \frac{1}{L}\sum_i(-1)^i\langle y_{0L}|(\hat{n}_i - r)(\hat{n}_{i+r} - r)|y_{0L}\rangle$, where r is the mean density of bosons, the correlation function that characterises the SF phase $\Gamma_L^{SF}(r) \equiv \frac{1}{L}\sum_i\langle y_{0L}|a_i^{\dagger}a_{i+r}|y_{0L}\rangle$ and its second moment $x_L^2 \equiv [\sum_r r^2\Gamma_L^{SF}(r)]/[\sum_r \Gamma_L^{SF}(r)]$. Note that x_L is the correlation length for SF ordering in a system of size L. In a phase with a gap, $\lim_{L\to\infty}G_L = G_\infty > 0$. By contrast, in a critical phase, such as the SF, which has long-range correlations, x_L diverges as $L \to \infty$ and the gap vanishes as $G_L \sim x_L^{-1}$.

The correlation length is extrapolated to the $L \to \infty$ limit by using finite-size scaling.[25] In the critical region,

$$x_L^{-1} \approx L^{-1} f(L/x), \tag{2}$$

where $f(L/x)$ is a scaling function. Thus plots of L/x_L or, equivalently, LG_L, vs U, for different system sizes L, consist of curves that intersect at the critical point, at which the correlation length x_L diverges if $L = \infty$. We show such a plot in figure 1 for $V = 0$. The infinite-system gap $G_\infty > 0$ at large U in the MI phase. However, it vanishes for $U \le U_c \approx 3{\cdot}4$, where the SF phase is obtained. The curves for different values of L coalesce for $U \le U_c \approx 3{\cdot}4$. This indicates that the MI-SF transition is of the Kosterlitz–Thouless (KT) type and that the SF phase is critical. In particular, the SF phase, in this one-dimensional model, has a diverging correlation length, and a vanishing gap. For a full elucidation of the KT nature of the MI-SF transition, we refer the reader to the analysis, via $\boldsymbol{b}$ functions, of Ref. [7]. Note that a d-dimensional, zero-temperature, quantum phase transition lies in the universality class of a finite-temperature phase transition in an associated, classical system in $(d + 1)$ dimensions; here $d = 1$ and the MI-SF transition lies in the universality class of the KT transition in the two-dimensional, classical XY model.

Recently Kühner *et al*[9] have studied model (1) by using the finite-size DMRG[26] (FS-DMRG) method. They have shown that, for $V = 0{\cdot}4$, an SF-MDW transition is obtained for $\boldsymbol{r} = 1/2$; an MI-SF transition is obtained for $\boldsymbol{r} = 1$. We have extended their FS-DMRG calculation to obtain the zero-temperature phase diagram of model (1) in the U–V plane for $U > V$ and for $\boldsymbol{r} = 1$ (figure 2). The number of states in the density matrix is chosen such that the truncation error is always less than 5×10^{-6}. We also restrict the number of bosons per site to 4, which suffices for the values of U we consider (large values of U disfavour large boson numbers at any given site). Further details of our calculation are given in Refs [7, 24].

The phase diagram of figure 2 shows an SF phase at small values of U and V as is to be expected since the bosons interact relatively weakly here. However, as the interaction strengths increase, the MI and MDW phases get stabilised. The former dominates when U is much larger than V whereas the latter dominates if U and V are both large and comparable. This is to be expected since a large, repulsive V disfavours a phase with a uniform density of bosons on nearest-neighbour sites; instead, an MDW phase, with a

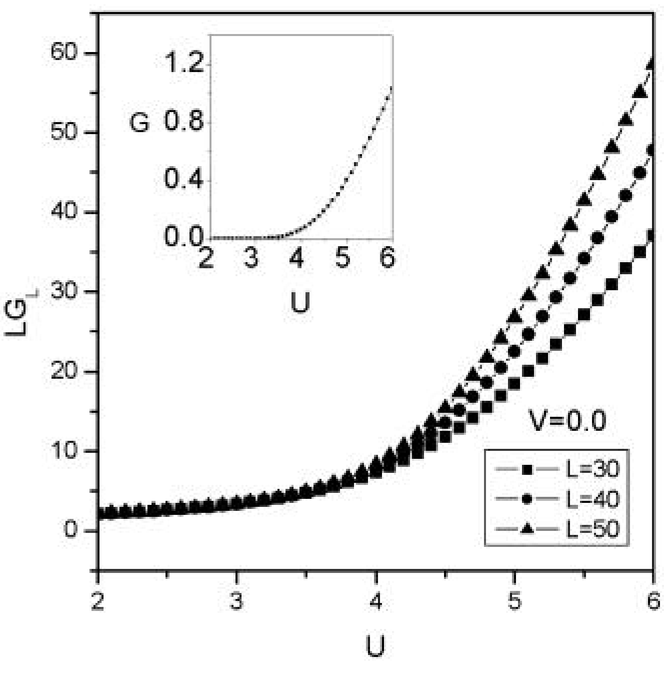

Figure 1. A plot of LG_L as a function of U for different system sizes L for $V = 0$. The coalescence of different curves for $U < 3{\cdot}4$ shows a Kosterlitz–Thouless-type SF-MI transition. The inset shows the infinite-system gap G_∞, obtained by extrapolation, versus U.

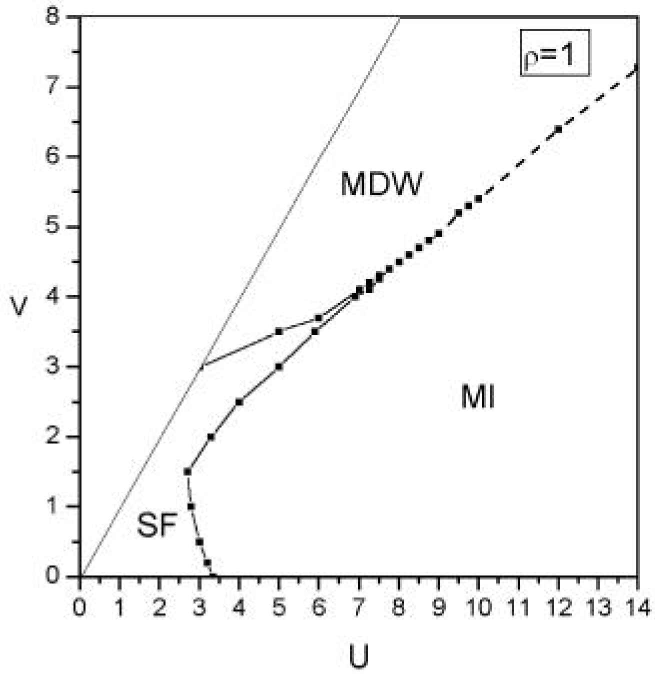

Figure 2. The zero-temperature phase diagram of the extended Bose–Hubbard model (1) obtained, for mean boson density $r = 1$, from our FS-DMRG calculation. Superfluid (SF), bosonic-Mott-insulator (MI), and mass-density-wave (MDW) phases are obtained in the physically relevant region $U > V$ to which we restrict ourselves. The MI-SF phase boundary lies in the Kosterlitz–Thouless (KT) universality class. The MDW-SF phase boundary has both KT and two-dimensional-Ising characters. The MI-MDW phase boundary is first-order (dashed line) at large values of U and V.

periodic variation of the boson density, is stabilised by V. The lattice we consider is bipartite and has two sublattices A and B (say odd-numbered and even-numbered sites); the ground state in the MDW phase is, therefore, doubly degenerate since the peaks in the mass-density wave can lie either on the A or the B sublattice. If the bosons are charged this MDW phase is a charge-density-wave (CDW) phase.

The MI-SF phase boundary in figure 2 lies in the Kosterlitz–Thouless (KT) universality class. We have confirmed this explicitly from plots of LG_L vs U, which coalesce for different values of L as shown in the illustrative plot of figure 3 (compare this with figure 1). This is to be expected for the SF phase of model (1) in one dimension. The MDW-SF phase boundary has both KT and two-dimensional-Ising characters as we have checked explicitly by plots similar to figures 1 and 3. The KT character follows from the XY-symmetry of the SF order parameter; the two-dimensional-Ising character follows from the double degeneracy of the MDW ground state mentioned above. The MI-MDW phase boundary is first-order (dashed line in figure 2) at large values of U and V. This follows from the sharp change in M_{MDW} with V as shown in figure 4 for $U = 12$; we have also checked for this transition that plots of LG_L versus V *do not* intersect or coalesce for different values of L indicating that this is *not* a continuous transition. The precise nature of the multicritical point at which the phase boundaries of figure 2 intersect will be explored elsewhere.[24]

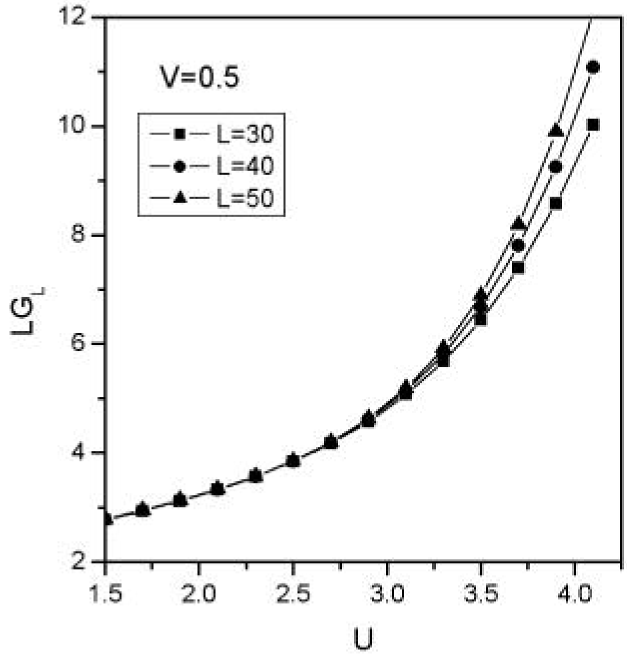

Figure 3. A plot of LG_L as a function of U for different system sizes L for $V = 0{\cdot}5$. The coalescence of different curves for $U < 2{\cdot}9$ shows a Kosterlitz–Thouless-type SF-MI transition (compare figure 1 for the case $V = 0$).

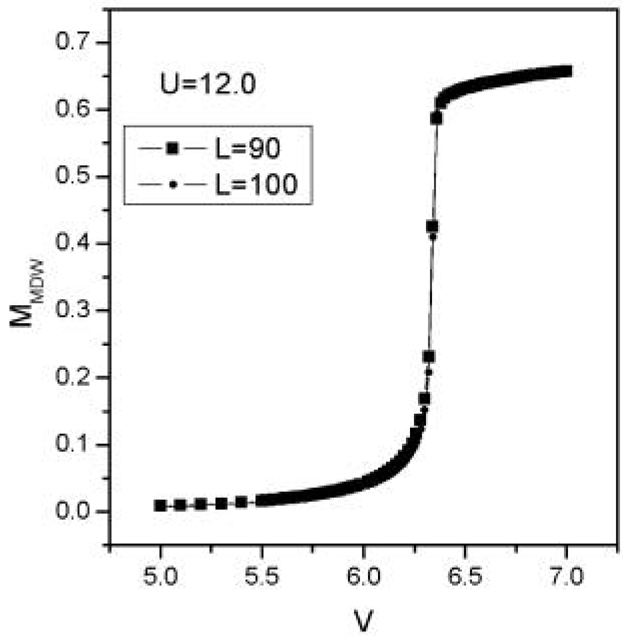

Figure 4. The order parameter of the MDW phase M_{MDW} vs V, for $U = 12$ and $L = 90$ and $L = 100$, showing a sharp jump which indicates that the MI-MDW transition is first order.

3. Conclusions

In conclusion, then, we have studied the complete phase diagram of the one-dimensional, extended Bose–Hubbard model for mean boson density $r = 1$ by using the FS-DMRG method. In addition to the well-known SF and MI phases, we find an MDW phase; we also determine the phase boundaries between these phases. We have looked for, but not found, a supersolid phase which has both SF and MDW order. We hope our study will stimulate experimentalists to look for such MDW phases in systems of interacting bosons.

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