Mott-insulator–superfluid-liquid transition in a 1D boson Hubbard model

V. F. Elesin, V. A. Kashurnikov, and L. A. Openov
Moscow State Engineering–Physics Institute (Technical University), 115409 Moscow, Russia

(Submitted 8 June 1994)
Pis'ma Zh. Eksp. Teor. Fiz. **60**, No. 3, 174–177 (10 August 1994)

The values of the insulator gap Δ in finite 1D systems of interacting bosons, which can be described by a Hamiltonian of the Hubbard type, are calculated numerically through an exact diagonalization of the Hamiltonian matrix. The critical value $(t/U)_c = 0.275 \pm 0.005$ is found through extrapolation to an infinite system. At this critical value, there is a transition from an insulating state to a superfluid state in a chain in which the number of bosons is equal to the number of sites. This value of $(t/U)_c$ is close to the exact result found analytically for a reduced Hamiltonian. The reduced model is a good approximation at $t/U \approx (t/U)_c$. In the critical region we have $\Delta \sim \exp[-b(1-t/t_c)^{-1/2}]$, where $b \approx 0.2$. © *1994 American Institute of Physics.*

Reduced-dimensionality systems of interacting bosons on lattices have recently attracted considerable interest.[1] One reason is that these systems are of importance in their own right, in connection with the theory of quantum phase transitions. Another is the need to interpret specific experiments (see the papers cited in Ref. 1). Yet further interest in the problem is stimulated by the circumstance that the 1D boson Hubbard model remains one of the few 1D problems for which no analytic solution is available.[2]

The Hamiltonian of the 1D boson Hubbard model is[1]

$$H = -t\sum_{i=1}^{N_a} (a_i^+ a_{i+1} + a_i^+ a_{i-1}) + (U/2)\sum_{i=1}^{N_a} n_i(n_i - 1), \tag{1}$$

where the operator a_i^+ (a_i) creates (annihilates) a boson at site i, t is the matrix element for a jump of bosons between nearest sites, U is the repulsion energy of two bosons at a site, N_a is the number of sites in the chain, and $n_i = a_i^+ a_i$ $(0 \leqslant n_i \leqslant N_b$, where N_b is the total number of bosons in the system). Below we assume $U = 1$; i.e., we express all quantities with the dimensionality of an energy in units of U.

A phase transition from an insulating state to a superfluid state occurs[1] in model (1) only if the occupation of the lattice by bosons is commensurate (only if N_b is a multiple of N_a), and t reaches a certain critical value t_c. This critical value t_c was calculated in Refs. 3 for the case $N_b = N_a$ by the Monte Carlo method. The result $t_c = 0.215 \pm 0.01$ was found. An exact analytic solution $t_c = 1/(2\sqrt{3}) \approx 0.2887$ was found in Ref. 4 for a slightly simplified "reduced" Hamiltonian (see the discussion below). That result is quite different from the results found in Ref. 3. A renormalization-group analysis[5] of the reduced Hamiltonian with $N_b = N_a$ yielded $t_c = 0.215$, as did the Monte Carlo method. Bearing in

mind the known limitations of the Monte Carlo method, because of the large error at low temperatures, we would like to find t_c through an exact numerical diagonalization of the Hamiltonian matrix[6] and to thereby resolve the contradictions which we just noted.

In this letter we use the exact-diagonalization method to calculate (for the first time, to the best of our knowledge) the ground-state energies of some finite 1D systems of interacting bosons which can be described by Hamiltonian (1). We find the value $t_c = 0.275 \pm 0.005$, which is close to the exact value for the "reduced" model. We also show that the reduced Hamiltonian is a good approximation at $t \approx t_c$.

As was shown in Ref. 1, the ground state of Hamiltonian (1) is an insulating state only if N_b/N_a is a natural number, and t is sufficiently small. In this case the density (ρ_s) of the superfluid component is zero, and there is an insulating gap $\Delta = \mu_+ - \mu_-$ in the spectrum of excitations. Here the values of μ_+ and μ_- are given by the relations (below, as in Refs. 4 and 5, we consider the particular case $N_b/N_a = 1$ in the thermodynamic limit) $\mu_\perp = E(N_a+1) - E(N_a)$ and $\mu_- = E(N_a) - E(N_a-1)$, where $E(N_b)$ is the ground-state energy of a system of N_b interacting bosons. (The quantity Δ is introduced in the fermion Hubbard model[7] in precisely the same way, i.e., as the difference between the excitation energies upon the addition and removal of one particle.) On the μ–t phase diagram (where μ is the chemical potential), the region of the insulating phase is bounded by the curves $\mu_+(t)$ and $\mu_-(t)$ (Ref. 1). An increase in t leads to a transition to a superfluid state with $\Delta = 0$, $\rho_s \neq 0$. On the μ–t phase diagram, this transition corresponds to a tricritical point. One of the coordinates of this point determines the critical value t_c, at which there is a transition from an insulating state to a superfluid state in a chain in which the number of bosons is a multiple of the number of sites.[1,3–5]

We numerically calculated the energies $E(N_b)$ as a function of t for $N_b = N_a - 1$, N_a, and $N_a + 1$ for chains with $N_a = 4$, 5, 6, 7, 8, and 9 sites, under periodic boundary conditions. The relative error of these calculations was no worse than 10^{-10} in any case. We were thus able to find μ_+, μ_- and Δ for various values of N_a; by extrapolating to $N_a = \infty$ we were able to determine the $\Delta(t)$ dependence in the thermodynamic limit ($N_a \to \infty$, $N_b \to \infty$, $N_b/N_a = 1$).

Figure 1 shows μ–t phase diagrams for $N_a = 4$ and 9. At small values of t, the phase boundaries essentially coincide; i.e., Δ is nearly independent of the dimensions of the system. At $t > 0.15$, the N_a dependence of Δ is very strong. To determine $\Delta_0 \equiv \Delta(N_a = \infty)$ we approximated Δ as a function of $1/N_a$ by a fifth-degree polynomial (on the basis of six exact values of Δ for various values of N_a), and we found Δ_0 as a function of t. Figure 2 shows an example of this approximation; Fig. 3 shows a curve of $\Delta_0(t)$. The critical value t_c, at which Δ_0 vanishes, is 0.275 ± 0.005. For a correct determination of Δ_0 in the case $\Delta_0 < 10^{-3}$ (near t_c), we carried out a more careful approximation of $\Delta(N_a)$ in powers of $1/N_a^\alpha$, where the value of α was chosen to lead to the best agreement of the values of t_c found by extrapolations on the basis of six ($N_a = 4$–9), five ($N_a = 5$–9), four ($N_a = 6$–9), and three ($N = 7$–9) points. We found $\alpha = 0.95 \pm 0.01$.

A phase transition which occurs with increasing t in a 1D system of bosons with $N_b = N_a$ belongs[1] to the universal class of the 2D XY model; i.e., it is a (Berezinskiĭ–) Kosterlitz–Thouless transition. Consequently (Ref. 8, for example), the t dependence of Δ_0 near t_c should be $\Delta_0 \sim \exp[-b(1-t/t_c)^{-1/2}]$ (at $t < t_c$), where b is a nonuniversal

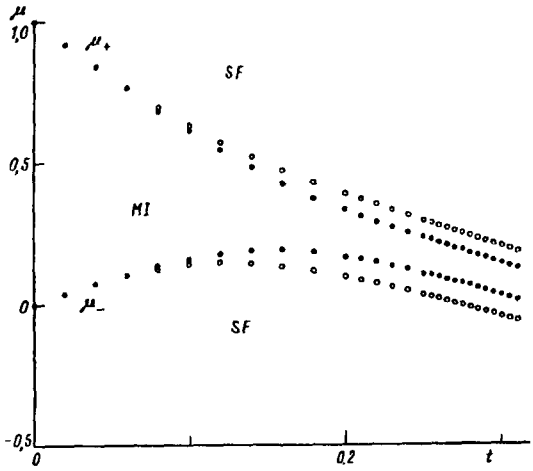

FIG. 1. Plots of μ_+ and μ_- (see the definitions in the text proper) versus t for chains of $N_a=4$ (○) and $N_a=9$ (●) sites ($U=1$). MI—Mott-insulator phase; SF—superfluid-liquid phase.

numerical factor. It can be seen from the inset in Fig. 3 that this is indeed the t dependence which Δ_0 exhibits in the critical region: The logarithm of Δ_0 is a linear function of the quantity $(1-t/t_c)^{-1/2}$ over a broad range of $\ln(\Delta_0)$ values. Here we have $b\approx 0.2$.

The value which we found for t_c is very close to the exact result $t_c=1/(2\sqrt{3})\approx 0.2887$ which has been found analytically[4] for a reduced 1D boson Hubbard model. In this model, the interaction energy of the bosons at a lattice site is [cf. (1)]

$$V(n_i)=\begin{cases} 0 \text{ if } n_i=0 \text{ or } 1, \\ U \text{ if } n_i=2, \\ \infty \text{ if } n_i>2. \end{cases} \tag{2}$$

In other words, there cannot be more than two bosons at one lattice site. To make a more detailed comparison with the results of Ref. 4, we also carried out a numerical study of a reduced Hamiltonian with $V(n_i)$ as in (2). It turned out that the values of t_c for models (1) and (2) agree within the errors, although the range of t_c values (which is governed by

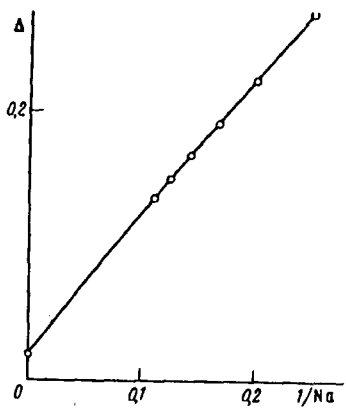

FIG. 2. The insulating gap Δ versus $1/N_a$ for $t=0.23$ ($U=1$). The points for $N_a=4$, 5, 6, 7, 8, and 9 are the results of numerical calculations; the solid curve is an approximation of $\Delta(1/N_a)$ by a fifth-degree polynomial. Here $\Delta_0=\Delta(1/N_a=0)=0.019$.

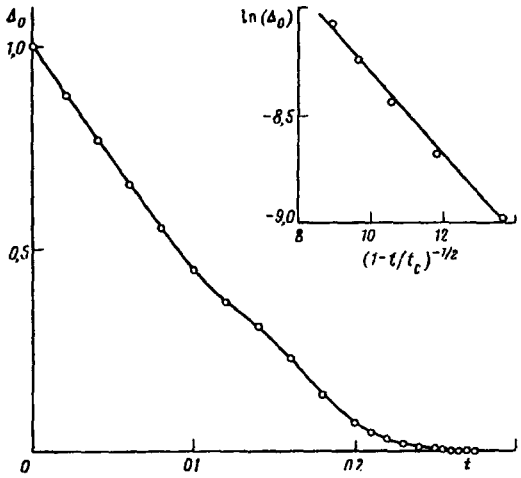

FIG. 3. Plot of Δ_0 versus t ($U=1$). The points are the results of an extrapolation of $\Delta(1/N_a)$ under the condition $t=\text{const}$, as in Fig. 2. Here we have $\Delta_0=0$ at $t_c=0.275$. The inset shows a plot of $\ln(\Delta_0)$ versus $(1-t/t_c)^{-1/2}$.

the extrapolation error) is slightly narrower for model (1) than for model (2). It follows from our calculations that with $N_b=N_a$ and $t\approx t_c$ the probability for the realization of configurations with $n_i>2$ (configurations with more than two bosons at a site) is 0.8% for model (1), in agreement with the data of Ref. 4. This result implies that the simplification in (2) of the original Hamiltonian, (1), actually has only a slight effect on the characteristics of the system at $t\approx t_c$.

As we mentioned earlier, a renormalization-group analysis[5] of reduced model (2) yields $t_c=0.215$. The same value of t_c (with an error ± 0.01) has been found by the Monte Carlo method[3] for Hamiltonian (1). The results of Refs. 3 and 5 differ from our numerical calculations and the exact analytic[4] calculations by 25%. We believe that the agreement of the results of Refs. 3 and 5, within their errors, is only fortuitous. Our reasoning here is that the calculations in Ref. 3, although carried out for large systems ($N_a\geqslant 16$), were carried out for a nonzero temperature ($T=t/2$). This circumstance could substantially increase the calculation error. Furthermore, no detailed analysis of the behavior $\Delta(t)$ near t_c was carried out in Ref. 3. With regard to Ref. 5, we note that Singh and Rokhsar[5] were apparently unable to fully take account of strong fluctuations in the critical region, as is indicated by the finite value, $\nu=4.87$, which they found for the critical exponent of the correlation length ξ. Although this figure is larger than predicted by the mean-field theory ($\nu=0.5$), it is smaller than the actual value [8] $\nu=\infty$. Our calculations, on the other hand, made it possible to find the expected[8] exponential (rather than power-law) dependence $\xi\sim\Delta^{-1}\sim\exp[\text{const}(1-t/t_c)^{-1/2}]$ (see the inset in Fig. 3).

We thus regard the value $t_c=0.275\pm 0.005$ as the most accurate value of t_c for model (1). This value is close to the analytic solution[4] for reduced model (2), which works well at $t\approx t_c$.

We wish to thank A. V. Krasheninnikov and B. V. Svistunov for a discussion of the results. We also thank A. I. Podlivaev for assistance in the numerical calculations. This study was supported by the Russian Fund for Fundamental Research (Project 94-02-05755).

[1] M. P. A. Fisher *et al.*, Phys. Rev. B **40**, 546 (1989).
[2] T. C. Choy and F. D. M. Haldane, Phys. Lett. A **90**, 83 (1982).
[3] G. G. Batrouni *et al.*, Phys. Rev. Lett. **65**, 1765 (1990); G. G. Batrouni and R. T. Scalettar, Phys. Rev. B **46**, 9051 (1992).
[4] W. Krauth, Phys. Rev. B **44**, 9772 (1991).
[5] K. G. Singh and D. S. Rokhsar, Phys. Rev. B **46**, 3002 (1992).
[6] V. F. Elesin *et al.*, Zh. Eksp. Teor. Fiz. **99**, 237 (1991) [Sov. Phys. JETP **72**, 133 (1991)]; **101**, 682 (1992) [**74**, 363 (1992)]; Physica C **195**, 171 (1992).
[7] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).
[8] Yu. A. Izyumov and Yu. N. Skryabin, *Statistical Mechanics of Magnetically Ordered Systems*[in Russian] (Nauka, Moscow, 1987).

Translated by D. Parsons