Bethe ansatz for the one-dimensional boson Hubbard model

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The Bethe ansatz (BA) for the one-dimensional boson Hubbard model is studied. Even though the model cannot be solved exactly by this method, it is argued that it gives an excellent approximation for densities $\rho \lesssim 1$. This claim is substantiated by a detailed study of the internal consistency of the BA solution, and by comparison with quantum Monte Carlo simulations.

The Bethe ansatz[1] (BA) has been an extremely successful method to study and solve exactly one-dimensional (1D) quantum many-body systems with a δ-function pair potential (in the continuum) or an on-site interaction (on the lattice). One of the big successes of the method was the exact solution of the 1D Hubbard model,[2] a fermionic lattice version of the continuum Bose gas, solved by Lieb and Liniger.[3]

In the last few years, boson-type Hubbard models have been investigated actively in the context of superfluidity in constrained geometries and short-coherence-length superconductors.[4-8] The commonly used model is described by the Hamiltonian

$$H = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + \text{H.c.}) + \frac{U}{2} \sum_{i=1}^{L} n_i (n_i - 1), \qquad (1)$$

where a_i is a *boson* annihilation operator on site i ($i = 1, \ldots, L$), and n_i is the number operator ($\sum_{i=1}^{L} n_i = N$). As usual, I set $t = 1$; the other definitions are standard. The model is especially interesting close to integer densities $\rho = N/L$ at which it undergoes a superfluid–Mott-insulator transition for a finite value of the interaction U, even in one dimension.

In one dimension, the boson Hubbard model equation (1) is simply a lattice version of the model of Lieb and Liniger, retaining the original statistics. The Bethe ansatz for this model was first studied by Haldane.[9] It was found[10] that there are subtle problems with the multiply (i.e., more than doubly) occupied sites, which are not treated correctly in this approach. Perhaps because of these shortcomings, work on the BA for this very rich model was not pursued farther. The 1D model has recently been studied in numerical simulations by Batrouni, Scalettar, and Zimanyi.[7]

If the BA is only approximate for the boson Hubbard model (except if $U = \infty$ or $\rho \rightarrow 0$, when multiply occupied sites play no role), it is clear that the density of multiply occupied sites will be very small in the insulating, solid Mott phase at $\rho = 1$. Therefore, the BA *approximation* may be excellent and render the true qualitative and quantitative aspects of the model for all but the smallest values of U. The investigation of this hypothesis has been the motivation of the present work.

In the following, a fairly complete analysis of the BA approximation at densities $\rho \lesssim 1$ and comparison with exact numerical simulations will be given. The general finding is that the BA solution is "almost" consistent: it

has the presumably correct critical exponents for the compressibility and the superfluid density ρ_s/ρ as $\rho \rightarrow 1$, satisfying the hyperscaling relation. At integer density, the superfluid density is constant for low values of the interaction U, and identical equal to zero above the transition point. At the transition, ρ_s/ρ is discontinuous, as it should be for a superfluid at a Kosterlitz-Thouless (KT) phase transition.[11] Close to the transition, however, on the superfluid side, the BA approximation would predict a diverging ρ_s/ρ, thus violating the bound that $\rho_s/\rho \leq 1$.

Direct comparison with the numerical simulations is very favorable. The energy and chemical potential are in excellent agreement with the numerical results,[7] which were mostly obtained on systems of very small size ($L = 16$). Around U_c, the simulations became plagued by large finite-size effects (due to the logarithmic interaction at the KT phase-transition point), and it is very difficult to obtain a good numerical estimate of U_c. Rather, I have tested the consistency of the BA numerically at the predicted value of U_c. Using our own exact quantum Monte Carlo code,[5,6] I find that the density of multiplicity occupied sites is indeed very low. At the critical point, $p(n_i \geq 3) \sim 0.008$.

Some of the calculations (divergence of the energy, chemical potential) are rather standard, and I will only quote the results here. The calculation of the superfluid density, however, is interesting, as it needs a higher-order approach to the BA equations. I have been able to do this calculation analytically (see also Ref. 12 for a similar approach to the problem). The analytical work above U_c is especially simplified by the fact that the BA integral equations can be solved *exactly* in the insulating phase, as shown by Haldane.[9]

Consistency equations can be written in the usual way to ensure that the BA wave function

$$\Psi(r_1, \ldots, r_N) = \sum_P a(P)$$

$$\times \exp\left[i \sum_{j=1}^{N} k_{P(j)} r_j\right] (r_1 < r_2 < \cdots < r_N)$$

is a correct solution of the Hamiltonian equation (1), even if two of the arguments are identical. These BA consistency conditions for the boson Hubbard model follow straightforwardly from the continuum Bose gas:[3,9]

$$\theta_{sj} = -2 \arctan[(2/U)(\sin k_s - \sin k_j)] \qquad (2)$$

and

$$(-)^{N-1}\exp(-ik_jL)=\exp\left[i\sum_{s=1}^{N}\theta_{sj}+\Theta\right] \qquad (3)$$

where the parameters θ_{sj} are related to the prefactors $a(p)$. The total energy of the system is $E=-2\sum_{i=1}^{N}\times\cos k_i$. In Eq. (3), which fixes the boundary conditions (B.C.) of the wave function, Θ is zero for a stationary ring (periodic B.C.) and takes on the value $\Theta=v/L$ for a ring which is set into rotation with a velocity equal to v (twisted B.C., cf. Ref. 13 for related work on the fermion Hubbard model). The superfluid density ρ_s/ρ (at $T=0$) is defined precisely by the change of the ground-state energy with a small rotation.[14-16]

$$\rho_s/\rho:=\lim_{\Theta\to 0}N\frac{E(\Theta)-E(0)}{\rho\Theta^2}. \qquad (4)$$

In the thermodynamic limit, I assume $\Theta\sim O(1)$ and expect in this case no problem with the exchange of limits $N\to\infty$ and $\Theta\to 0$. It is evident from Eq. (4) that the energy change per particle $[E(\Theta)-E(0)]/N$ of the system then has to be determined up to order $O(1/L^2)$. In order to achieve this precision, finite-size corrections are taken into account.[17]

For the ground state (with $\Theta=0$), the (ordered) pseudomomenta in Eq. (3) are symmetrically distributed between values $-\pi\le K-\sigma/L$ and $K+\sigma/L\le\pi$. The distribution of momenta is written as

$$\frac{k_{j+1}-k_{j-1}}{2}=L^{-1}/f(k_j)+L^{-2}g(k_j). \qquad (5)$$

Using the trapezoid rule, I get the following rule for the replacement of sums by integrals:

$$1/L\sum_{j=1}^{N}z(k_j)=\int_{-K}^{K}dx\,z(x)f(x)+L^{-1}\left[(z_1+z_N)/2+\sigma f(K)-\int_{-K}^{K}dx\,z(x)\mathcal{A}(x)\right]+O(L^{-2}), \qquad (6)$$

with $z(k_j)$ any sufficiently smooth function and with $\mathcal{A}(x)=f^2(x)g(x)$. To derive the integral equations for f and $\mathcal{A}$, we have to use

$$z(k_j)=\theta_{sj-1}-\theta_{sj+1}$$
$$=-2\cos k_j\,\Omega(k_j,k_s)[L^{-1}/f(k_j)+L^{-2}g(k_j)],$$

with

$$\Omega(x,y)=1/[U^2/4+(\sin x-\sin y)^2].$$

The integral equation for f is

$$2\pi f(x)=1+U\cos x\int_{-K}^{K}dy\,f(y)\Omega(x,y). \qquad (7)$$

K is fixed by the condition $\rho=\int_{-K}^{K}dx\,f(x)$, as can be seen from Eq. (6) with $z(x)=1$. Equation (7) is an inhomogeneous Fredholm integral equation which can easily be solved by iteration. It is more convenient[9] to consider the transformation

$$2\pi f(x)=1+\cos x[|\cos x|^{-1}-f^*(\sin x)].$$

f^* then obeys the integral equation

$$f^*(z)=(1-z^2)^{-1/2}-\frac{U}{\pi}\int_{-1}^{1}dx\frac{1}{(1-x^2)^{1/2}}\Omega'(x,z)$$
$$-\frac{U}{2\pi}\int_{-x_0}^{x_0}dx\,f(x)\Omega'(x,z), \qquad (8)$$

with $x_0=\sin K$ and $\Omega'(x,y)=[U^2/4+(x-y)^2]^{-1}$. At unit density $\rho=1$, the maximum momentum goes from $K=0$ (at $U=0$) to $K=\pi$ at $U\ge U_c=2\sqrt{3}$. Above U_c, an explicit solution to the integral equation is given by

$$2\pi f^*(x)=(1-x^2)^{-1/2}-[(U/2-ix)^2+1]^{-1/2}$$
$$-[(U/2+ix)^2+1]^{-1/2}.$$

For values just below $U=U_c$, $\sin K$ will be small, and the solution of Eq. (8) can be simultaneously expanded in U_c-U and $\pi-K$. The two small parameters are related to each other by the condition $1\equiv\rho=\int_{-K}^{K}dx\,f(x)$. I find $K=\pi-2(3^{1/2}/7^{1/4})(U_c-U)^{1/2}$. Using this result, it can

be shown that the energy and its first two derivatives remain continuous at U_c.

What is the nature of the system above U_c? As explained in Ref. 4, the system, above U_c, should be a Mott insulator, i.e., have vanishing compressibility and superfluid density. Furthermore, as the Mott insulating state is approached (at fixed $U>U_c$), the compressibility and the superfluid density should have mean-field critical exponents $\kappa=\partial\rho/\partial\mu\sim[\mu(1)-\mu(\rho)]^{-\alpha}$ and $\rho_s/\rho\sim|1-\rho|^{z-1}$, with $\alpha=\frac{1}{2}$ and $z=2$. All these properties can be obtained within the BA approximation, as I will show in the remainder of the paper.

In the BA framework the chemical potential $\mu(N,L)=E(N,L)-E(N-1,L)$ is calculated from the change of the k_j's as the particle number is incremented.[2] Denoting by a prime the momenta in the system with $N-1$ particles, I can calculate the change in the individual quasimomenta as $k'(j)=k(j)+L^{-1}\phi(j)$ with $\phi=O(1)$. It is easy to derive the integral equation for $J(x)\equiv\phi(x)f(x)$ as

$$2\pi J(x)=\pi-2\arctan[(2/U)(\sin K-\sin x)]$$
$$+U\int dy\cos y\,J(y)\Omega(x,y). \qquad (9)$$

As before, this integral equation at $\rho=1$ and $U>U_c$ is transformed by incorporating the inhomogeneity into the definition of J:

$$2\pi J(x)=\pi-2\arctan[2/U(\sin K-\sin x)]+UJ^*(\sin x).$$

For $U>U_c$ at $\rho=1$, J^* is zero, and the chemical potential is given by

$$\mu=-\frac{4}{\pi}\int_{-\pi}^{\pi}dx\sin x\arctan\left[\frac{2}{U}\sin x\right]+2. \qquad (10)$$

Equation (10) can be explicitly compared with the numerical data of Batrouni, Scalettar, and Zimanyi,[7] who display results for the chemical potential in their Fig. 1. I have plotted Eq. (10), and have found very good quantita-

tive agreement with their data. Close to the transition, the differences seem to be of the order of a few percent. They may well be attributable to a combination of large finite-size effects close to the Kosterlitz-Thouless transition, systematic errors (of the order of a few percent[7]), and to the approximate nature of the BA solution.

The integral equation for $J^*(x)$ can be expanded into a series in $1-\rho$ for densities ρ close to 1 allowing the calculation of the chemical potential for $\rho \lesssim 1$. This yields the result

$$1-\rho = \sqrt{\mu(1) - \mu(\rho)} \pi [1 - 4/(4+U^2)^{1/2}] .   (11)$$

It then follows that the compressibility $\kappa = \partial\rho/\partial\mu$ diverges with the (correct) mean-field exponent $\alpha = \frac{1}{2}$ for all values of the interaction $U > U_c$.

I now turn to the calculation of the superfluid density in the BA approximation. Here, the change of the k_j's is due to the introduction of a phase, rather than an extra particle. Denoting with a prime quantities in the rotating system, I have to calculate

$$(k_j' - k_j)L = -\sum_{s=1}^{N} (\theta_{sj}' - \theta_{sj}) + \Theta ,   (12)$$

writing $k_j' = k_j + \omega(k_j)/L + v(k_j)/L^2$, and expanding $\theta_{sj}' - \theta_{sj}$ to second order in $1/L$ [cf., Eq. (2)] the integral equations for $\omega(x)$, depending on Θ, and for $v(x)$, which depends on $\omega(x)$, can be derived. Now one has to proceed carefully, since in the derivation of the integral equation for $\omega(x)$ the terms of order L^{-1} [cf., Eq. (6)] have to be kept. They contribute to the equation for $v(x)$. Therefore, the function $\mathcal{A}$ has to be evaluated first. An integral

equation of the familiar form can be deduced from Eq. (6) and from the formula for $\theta_{sj-1} - \theta_{sj+1}$:

$$2\pi\mathcal{A}(y) = Z(y,\sigma) + U\cos y \int_{-K}^{K} \mathcal{A}(x)\Omega(x,y) ,   (13)$$

with

$$Z(y,\sigma) = -U\cos y \{ \Omega(y,K)$$
$$+ \Omega(y,-K)[1/2 + \sigma f(K)] \} .   (14)$$

σ has to be determined by the consistency equation for the density to order $1/L$: $N/M = \rho + \tau/L$. Choosing $\tau = 0$, I get

$$1 + 2\sigma f(K) = \int \mathcal{A}(x)dx .   (15)$$

It can be seen easily that the consistent solution of Eqs. (13)–(15) is given by $1 + 2\sigma f(K) = 0$, which implies $\mathcal{A}(x) = 0$. I am unaware of a simple way of deducing this result from general principles without the help of extra hypotheses. It has two direct implications: (i) The finite size corrections to K are linear $k_N = K + \sigma/L$ with $\sigma = -1/2f(K)$ anywhere except at $U = U_c$, where $f(K) = 0$. (ii) The energy per particle is $E/N = $const $+ O(1/L^2)$.

Now I can write down the integral equations for the function $P(x) = f(x)\omega(x)$ and $Q(x) = f(x)v(x)$

$$2\pi P(x) = \Theta + U\int_{-K}^{K} dy \cos y P(y)\Omega(x,y) ,   (16)$$

$$2\pi Q(x) = R(x) + U\int_{-K}^{K} dy \cos y Q(y)\Omega(x,y) ,   (17)$$

with

$$R(x) = -U\int_{-K}^{K} dy\, f(y)\{[\omega(y)\cos y - \omega(x)\cos x]^2[\sin y - \sin x]\Omega(x,y)^2 + \omega^2(y)\sin y\,\Omega(x,y)/2\}$$
$$+ \frac{2\pi f(x) - 1}{2}\omega^2(x)\tan x .   (18)$$

As before, by incorporating the inhomogeneities into the definitions of the functions P and Q, these equations can be solved analytically above U_c. Explicitly, I find

$$2\pi P(x) = \Theta;$$

$$2\pi Q(x) = R(x) + \frac{U}{2\pi}\int_{-\pi}^{\pi} dy\, R(y)\cos y\,\Omega(x,y) .   (19)$$

For any U, $P(x)$ is an even function $P(x) = P(-x)$, therefore, there is no contribution to order $O(1)$ to the change of the total energy, as it should be. The second-order change in the energy is

$$E(\Theta) - E(0) = 2/L\int_{-K}^{K} dx\, f(x)[\omega^2(x)/2\cos x + v(x)\sin x] .   (20)$$

Equations (19), (20), and (4) now yield a completely explicit formula for the superfluid density at $U > U_c$, $\rho = 1$. I have not succeeded in determining all the integrals analytically, but I find (with seven significant digits) that $E(\Theta) - E(0) = 0$, therefore, the superfluid density vanishes. The two terms which contribute to the energy shift diverge as $U \to U_c$, but cancel exactly.

In Fig. 1, I show the numerically calculated values for the superfluid density as a function of U around the critical point. For $U \to U_c$, the superfluid density diverges (in the BA approximation) in violation of the bound $\rho_s/\rho \leq 1$, which can be obtained by a generalization of the well-
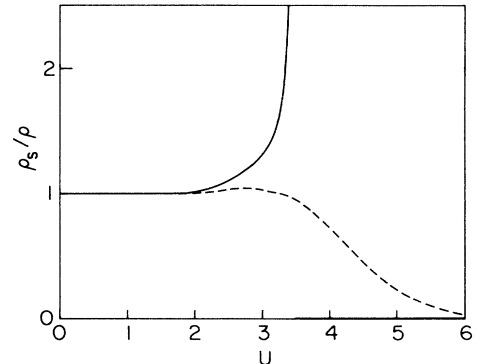

FIG. 1. Superfluid density ρ_s/ρ in the Bethe ansatz approximation for $N = \infty$ (solid line) at density $\rho = 1$ and for a finite system with 19 bosons on 19 sites (dashed line).

known variational argument[14] to the case of a lattice. To check the result, I have also calculated the exact, numerical solution of the BA consistency equations for finite systems and the result for 19 bosons on 19 sites is also shown. Even there, it can be seen that the predicted value is larger than 1 close to U_c. This behavior is the only indication of an inconsistency that I have been able to see in the BA approximation.

The critical exponent z for the superfluid density can now also be determined from Eqs. (16)–(18). For simplicity, I have determined ρ_s/ρ from the numerical solution of the integral equations for small values of $1 - \rho$. The results are consistent with the critical exponent z (to three significant digits), even though the scaling region is very small as $U \rightarrow U_c$ from above, as it should be. At $U = 4$, for example, $\rho_s(\rho)$ is linear for $\rho \gtrsim 0.995$ only. For larger U, as those considered in Ref. 7, the scaling regime is much larger also.

In conclusion, I have presented an analysis of the Bethe ansatz approximation for the 1D boson Hubbard model. I have calculated the chemical potential and the superfluid density in this approximation, and compared it to recent numerical work of Batrouni, Scalettar, and Zimanyi. ρ_s is determined by four connected integral equations (for f, g, ω, and v). Above U_c, the solution of all these integral equations can be obtained explicitly, with the result $\rho_s = 0$. The BA approximation would be exact if the probability of multiply occupied sites were zero. Monte Carlo calculations of this quantity show that, at the critical point U_c, this probability is very low, in support of the original hypothess that the BA approximation is excellent.

It would be very interesting to be able to raise this calculation to the status of a true variational calculation, by calculating the expectation value and especially the variance of the BA wave function's local energy $H\Psi/\Psi$, as is usually done with a variational wave function. Another interesting calculation would concern a direct calculation of the probability of multiply occupied sites. Finally, I would like to note that the large degree of consistency of the BA approximation is somewhat mysterious and may still hide some surprises.

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