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Efficient thermodynamic description of multicomponent one-dimensional Bose gases

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We present a method of obtaining nonlinear integral equations characterizing the thermodynamics of one-dimensional multicomponent gases interacting via a δ-function potential. In the case of the repulsive two-component Bose gas we obtain a simple system of two nonlinear integral equations, allowing for an efficient numerical implementation, in contrast with the infinite number of coupled equations obtained by employing the thermodynamic Bethe ansatz. Our technique makes use of the quantum transfer matrix and the fact that, in a certain continuum limit, multicomponent gases can be obtained from appropriate anisotropic spin chains.

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Introduction. Recent advances in magnetic and optical trapping of ultracold quantum gases have opened new possibilities in investigating the physics of strongly interacting particles in one dimension [1]. Coupled with the fact that the strength of the atomic interaction can be controlled using magnetic Feshbach resonances or state-dependent dressed potentials [2], these new experiments provide a fertile ground for testing the theoretical predictions obtained from the study of various integrable models solvable by Bethe ansatz. As a result, we have witnessed the experimental realization of the Lieb-Liniger model [3] using bosonic ^{87}Rb atoms [4–8] and, moreover, the measured thermodynamics [9] is described very well by the Yang-Yang thermodynamics, which was developed in [10], using what we call nowadays the thermodynamic Bethe ansatz (TBA) [11]. In the case of integrable multicomponent one-dimensional (1D) gases, TBA produces an infinite number of integral equations [11,12], which makes the extraction of physical information and comparison with prospective experimental data difficult. In this Rapid Communication, we propose a solution to this problem using the quantum transfer matrix [13,14] and the connection between multicomponent gases and anisotropic spin-chains. Our method has the advantage of providing a finite number of nonlinear integral equations (NLIEs), which are extremely suited for numerical computations, in stark contrast with the TBA result.

Model. We consider a 1D system of M bosons, of equal mass $m = 1/2$, with n internal degrees of freedom, interacting via a δ-function potential. The many-body Hamiltonian is

$$\mathcal{H} = -\sum_{i=1}^{M} \frac{\partial^2}{\partial x_i^2} + 2c \sum_{i<j} \delta(x_i - x_j) - \sum_{i=1}^{n} \mu_i M_i, \qquad (1)$$

where c is the coupling constant and we consider $\hbar = k_B = 1$. The first and the second term in the Hamiltonian (1), represent the kinetic and and the interaction energy, while the third is the Zeeman term, where M_i is the number of particles in the hyperfine state $|i\rangle$ and μ_i the respective chemical potential. The interaction is attractive for $c < 0$ and repulsive for $c > 0$. The model is integrable and was solved in [3,15–17].

Despite the fact that the model is integrable, computing the thermodynamics is still an incredibly difficult task. The first attempt was done by Yang and Yang [10] for the spinless bosons using the TBA. TBA has proved to be an extremely useful technique and was used to obtain information about the thermodynamics of various exactly solvable models [11]; however, it has one big shortcoming: For a large class of models it produces an infinite number of coupled NLIE. This is also the case for our model, with the exception of the spinless case ($n = 1$). From a very simplified point of view this is due to the fact that the spectrum of the theory contains infinitely many branches. The numerical implementation of this system of equations requires various truncations, which introduce an uncontrollable source of numerical errors and makes the extraction of relevant physical information extremely difficult. Therefore, it is highly desirable to devise a numerically efficient method, which provides a finite number of NLIE.

Fortunately, in the case of lattice models such a method exists. Developed in [13,14], the quantum transfer matrix (QTM) approach was successfully applied to a large class of integrable spin chains and even models of strongly correlated electrons. Within this approach, the thermodynamic properties of the model are obtained from the largest eigenvalue of the QTM, which in the thermodynamic limit gives the free energy. Even though there is no equivalent of the QTM for continuum models, it is well known [18,19] that a large class of integrable models can be obtained from lattice models in suitable continuum limits. We say that an integrable model is the continuum limit of a lattice integrable model if, by performing this limit in the Bethe equations and energy spectrum of the lattice model one obtains the Bethe equations and energy spectrum of the continuum model. The natural consequence is that the thermodynamics of the continuum model can be obtained from the thermodynamics of the lattice model if we take the same limit. This method is used in this Rapid Communication, allowing us to obtain an efficient thermodynamic description of the two-component Bose gas (for the single-component case, see [20]).

In this publication we study and give results for the Hamiltonian (1) in dimensionless units; however, physical units can be restored easily. For particles with mass m and contact interaction strength g (see, for example, (1) in [21]), the units of temperature, chemical potential, magnetic field, particle density and susceptibility, compressibility, heat capacity, and entropy per length are $T_0 = \hbar^2/(2ma^2k_B)$, $\mu_0 = h_0 = \hbar^2/(2ma^2)$, $d_0 = 1/a$, $\chi_0 = \kappa_0 = 2ma/\hbar^2$, $c_0 = S_0 = k_B/a$, respectively. The quantity a is a length scale that can be chosen freely, yielding the dimensionless coupling constant $c = mga/\hbar^2$ appearing in (1). In all figures presented

in this paper, physical data are shown in the given units and for dimensionless coupling $c = 1$, which is realized for any parameter values of m and g with a suitably chosen $a = \hbar^2/(mg)$.

Method. The general strategy is as follows. First, we identify the spin-chain from which we will obtain in the appropriate continuum limit our model of interest. The next step is the investigation of the thermodynamics of the lattice model using the QTM technique, which will provide a finite number of NLIE. Finally, the desired result is obtained by taking the continuum limit in the equations for the lattice model. Let us make these general considerations more precise. In the case of the repulsive two-component Bose gas, the relevant lattice model is the $U_q(\widehat{sl}(3))$ Perk-Schultz spin chain [22–26], with periodic boundary conditions characterized by the Hamiltonian

$$H = J\sum_{j=1}^{L}\left(\cos\gamma\sum_{a=1}^{3}e_{aa}^{(j)}e_{aa}^{(j+1)} + \sum_{\substack{a,b=1\\a\neq b}}^{3}e_{ab}^{(j)}e_{ba}^{(j+1)} - i\sin\gamma\sum_{\substack{a,b=1\\a\neq b}}^{3}\mathrm{sgn}(a-b)e_{aa}^{(j)}e_{bb}^{(j+1)}\right) - \sum_{j=1}^{L}\sum_{a=1}^{3}h_a e_{aa}^{(j)}, \tag{2}$$

where $\gamma \in (0,\pi)$ determines the anisotropy, $(q = e^{i\gamma})$, L is the number of lattice sites, $J > 0$ fixes the energy scale, h_a are chemical potentials, and $e_{ab}^{(j)} = I^{\otimes j-1}\otimes e_{ab}\otimes I^{\otimes L-j}$, with e_{ab} the 3-by-3 matrix with elements $(e_{ab})_{ij} = \delta_{ai}\delta_{bj}$. This Hamiltonian is the sum of two terms, H_b (in the brackets), and the chemical potential term H_c, which does not break the integrability of the model [24]. The $U_q(\widehat{sl}(3))$ Perk-Schultz spin chain can be obtained as the fundamental spin model (see [27]) associated with the trigonometric Perk-Schultz R matrix [24], $\mathsf{R}(v) = \sum_{a,b,c,d=1}^{3}\mathsf{R}_{bd}^{ac}(v)e_{ab}\otimes e_{cd}$, with $\mathsf{R}_{aa}^{aa}(v) = \frac{\sin(\gamma+v)}{\sin\gamma}, \mathsf{R}_{ab}^{ab}(v) = \frac{\sin v}{\sin\gamma}$, $(a\neq b), \mathsf{R}_{ab}^{ba}(v) = e^{i\,\mathrm{sgn}(a-b)v}$, $(a\neq b)$, and all the other elements zero. The transfer matrix $\mathsf{T}(v)$ is the 3^L-by-3^L matrix with elements $\mathsf{T}_{\mathbf{b}}^{\mathbf{a}}(v) = \sum_{\{\mathbf{c}\}}\prod_{j=1}^{L}\mathsf{R}_{c_j\ b_j}^{c_{j+1}a_j}(v)$, where $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ are multiple indices; that is, $\mathbf{a} = (a_1,\ldots,a_L)$ and the sum is over all $\mathbf{c}$ with $c_1 = c_{L+1}$. The H_b part of the Hamiltonian can be obtained as the logarithmic derivative of the transfer matrix $H_b = J\sin\gamma\,\frac{\partial\ln\mathsf{T}(v)}{\partial v}|_{v=0}$. In order to treat the model at finite temperature we introduce the 3^N-by-3^N QTM with elements

$$(\mathsf{T}_{\mathrm{QTM}})_{\mathbf{b}}^{\mathbf{a}}(v) = \sum_{\{\mathbf{c}\}}e^{\beta h_{c_1}}\prod_{j=1}^{N/2}\mathsf{R}_{c_{2j}\ b_{2j}}^{c_{2j+1}a_{2j}}(v+iu)\tilde{\mathsf{R}}_{c_{2j-1}b_{2j-1}}^{c_{2j}\ \ a_{2j-1}}(iu-v),$$

where $c_1 = c_{N+1}$, $\tilde{\mathsf{R}}_{bd}^{ac}(v) = \mathsf{R}_{da}^{cb}(v)$, $u = -J\beta\sin\gamma/N$, with N the Trotter number and $\beta = 1/T$. The largest eigenvalue of the QTM, from which the free energy of the model can be obtained, has the form $\Lambda_{\mathrm{QTM}}(v) = \sum_{j=1}^{3}\lambda_j(v)$ [28], with

$$\lambda_j(v) = \phi_-(v)\phi_+(v)\frac{q_{j-1}(v-i\gamma)}{q_{j-1}(v)}\frac{q_j(v+i\gamma)}{q_j(v)}e^{\beta h_j},$$

where $\phi_\pm(v) = (\frac{\sinh(v\pm iu)}{\sin\gamma})^{N/2}$ and

$$q_j(v) = \begin{cases}\phi_-(v) & j = 0,\\ \prod_{r=1}^{N/2}\sinh\left(v - v_r^{(j)}\right) & j = 1,2,.\\ \phi_+(v) & j = 3.\end{cases}$$

The two sets of parameters, $\{v_r^{(j)}\}$, are the Bethe roots of the QTM and satisfy the Bethe equations $\lambda_j(v_r^{(j)})/\lambda_{j+1}(v_r^{(j)}) = -1$, $r = 1,\ldots,N/2$. The Bethe roots are distributed in certain strips of the complex plane which are independent of temperature and Trotter number. This type of specific distribution allows for the definition of auxiliary functions and the use of Cauchy's theorem in deriving NLIE for the largest eigenvalue [14,29–32]. Our results, which in the continuum limit produce Eqs. (3) and (4), can be understood as the multicomponent generalization of the equations presented in [32].

Main result. In order to obtain the thermodynamics of the two-component Bose gas we have to perform a particular continuum limit in the NLIE obtained for the $U_q(\widehat{sl}(3))$ spin chain. The spin chain is characterized by the following parameters: lattice constant δ, number of lattice sites L, anisotropy γ, strength of the interaction J, and chemical potentials h_1,h_2,h_3. The two-component Bose gas is obtained by performing the limit $\gamma = \pi - \epsilon$, $\delta \to O(\epsilon^2)$, $L \to O(1/\epsilon^2)$, $J \to O(1/\epsilon^4)$, $h_1 \to O(1/\epsilon^2)$, with $\epsilon \to 0$. Performing this limit in the Bethe equations and energy spectrum of the $U_q(\widehat{sl}(3))$ spin chain, we obtain the Bethe equations and energy spectrum of a two-component Bose gas characterized by the parameters: length $l = L\delta$, coupling constant $c = \epsilon^2/\delta$, mass of the particles $m = J\delta^2$, and chemical potentials $\mu_1 = J\epsilon^2 + h_2 - h_1$, $\mu_2 = h_3 - h_2$. In order to simplify the formulas, we are going to consider $J\delta^2 = 1$ (mass of the particles equal to 1/2) and introduce $\mu = (\mu_1+\mu_2)/2$ and an effective magnetic field $h = (\mu_1-\mu_2)/2$, where $\mu_{1,2}$ are the chemical potentials of the spin-up and -down particles. We are now ready to state the main result of this Rapid Communication. The thermodynamics of the two-component repulsive Bose gas is completely characterized by the following system of NLIEs:

$$\ln a_1(k) = -\beta(k^2-\mu-h) + [K_0 * \ln A_1](k) + [K_1 * \ln A_2](k+i\epsilon), \tag{3a}$$

$$\ln a_2(k) = -\beta(k^2-\mu+h) + [K_2 * \ln A_1](k-i\epsilon) + [K_0 * \ln A_2](k), \tag{3b}$$

where $A_i(k) = 1 + a_i(k)$, $K_0(k) = 2c/(k^2+c^2)$, $K_1(k) = c/[k(k+ic)]$, $K_2(k) = c/[k(k-ic)]$, and $[f*g](k) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}f(k-k')g(k')\,dk'$. The grandcanonical potential per

length is given by

$$\phi = -\frac{T}{2\pi}\int_{-\infty}^{+\infty} [\ln A_1(k) + \ln A_2(k)]\, dk, \qquad (4)$$

from which all the other thermodynamic quantities can be obtained. Equations (3) and (4) constitute an efficient thermodynamic description for a multicomponent continuum integrable model at all values of the relevant parameters (temperature, chemical potentials and coupling constant).

Analytic limits. First, we consider the limit $c \to 0$. Then, we have $\lim_{c\to 0} c/(k^2 + c^2) = \pi\delta(k)$ and $\lim_{c\to 0} c/[k(k \pm ic)] = 0$ and the integral equations decouple:

$$\ln a_1(k) = -\beta(k^2 - \mu - h) + \ln[1 + a_1(k)],$$
$$\ln a_2(k) = -\beta(k^2 - \mu + h) + \ln[1 + a_2(k)].$$

These equations are easily solvable, and we find

$$\phi = \frac{T}{2\pi}\int_{-\infty}^{+\infty} \ln[(1 - e^{-\beta(k^2-\mu-h)})(1 - e^{-\beta(k^2-\mu+h)})]dk,$$

which is exactly the grand-canonical potential of two noninteracting bosonic gases at different chemical potentials.

In the case of an extremely strong magnetic field, $h \to \infty$, we expect that the system will become fully polarized and we should obtain the Yang-Yang thermodynamics [10] of the repulsive one-component Bose gas. In this limit $a_2(k) \sim 0$ and we obtain

$$\ln a_1(k) = -\beta(k^2 - \mu - h) + [K_0 * \ln(1 + a_1)](k),$$

and $\phi = -\frac{T}{2\pi}\int_{-\infty}^{+\infty} \ln[1 + a_1(k)]dk$, which is the result obtained in [10]. The same result is obtained in the low-temperature limit ($T \ll \mu,h,c$), when the magnetic field is finite and fixed, which shows the ferromagnetic (fully polarized) nature of the ground state.

As we have mentioned, the numerical implementation of the infinite number of coupled NLIE obtained with the help of TBA [12] is extremely difficult and encounters serious problems in the regime of low magnetic field ($h \ll T,\mu,c$) or low temperature limit ($0 < T \ll h,\mu,c$). In contrast, Eqs. (3) are easily implementable and provide reliable results in a larger domain of the parameters space. We have checked our results with available numerical data obtained by using the much more involved TBA equations [33] and found perfect agreement. In our case, the regime in which the accuracy is decreasing, is given by the low temperature and low magnetic-field limit ($T \to 0, h \to 0$). This is a consequence of a first-order phase transition and the coexistence of fully polarized phases at T and h equal to 0, respectively. It can be seen clearly in Figs. 1 and 2 that, in the absence of the magnetic field, the population levels, $d_i = -(\frac{\partial\phi}{\partial\mu} + (-1)^{i-1}\frac{\partial\phi}{\partial h})/2$, $i = 1,2$, are equal and, consequently, the polarization defined as $P = (d_1 - d_2)/d$ with $d = d_1 + d_2$ is zero. In the presence of the magnetic field the ground state is ferromagnetic; therefore, the polarization at $T = 0$ is $+1$, for any positive field (-1 for negative field) and it decreases at higher temperatures. The ferromagnetic nature of

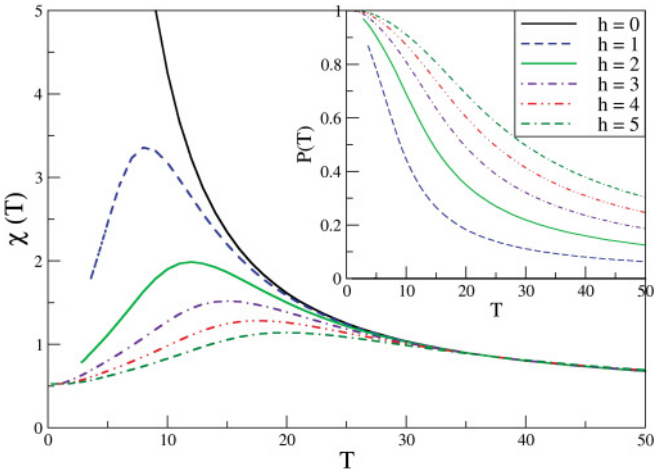

FIG. 2. (Color online) Susceptibility χ as a function of temperature T for $\mu = 15$, $c = 1$, and various effective magnetic fields h (in units of χ_0, T_0, μ_0, and h_0). (Inset) Polarization as a function of temperature for the same parameters. In the absence of the magnetic field the polarization is zero.

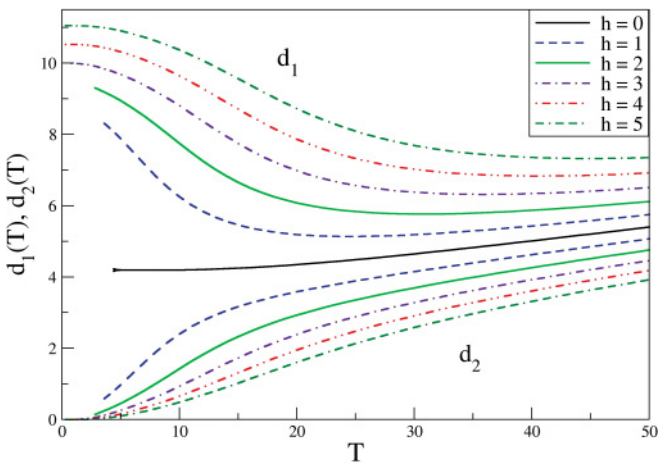

FIG. 1. (Color online) Population densities d_1, d_2 in the upper, lower part of the figure, respectively, as functions of temperature T for $\mu = 15$, $c = 1$, and various effective magnetic fields h (in units of d_0, T_0, μ_0, and h_0).

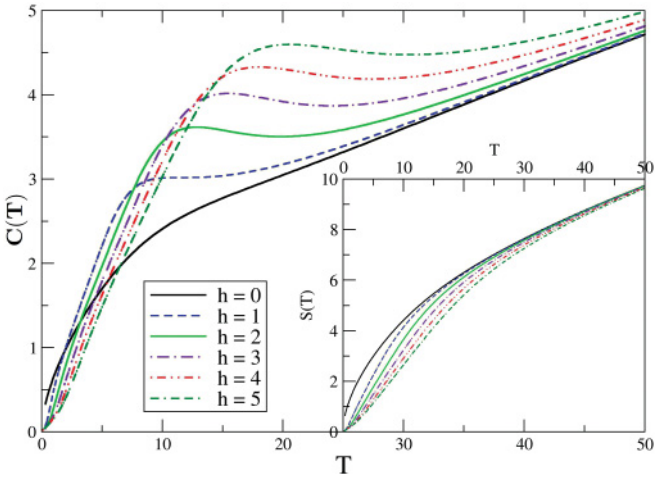

FIG. 3. (Color online) Specific heat C as a function of temperature T for $\mu = 15$, $c = 1$, and various effective magnetic fields h. (Inset) Entropy $S = -\frac{\partial\phi}{\partial T}$ as a function of temperature for the same parameters. (All quantities in units of c_0, T_0, μ_0, h_0, and S_0.)

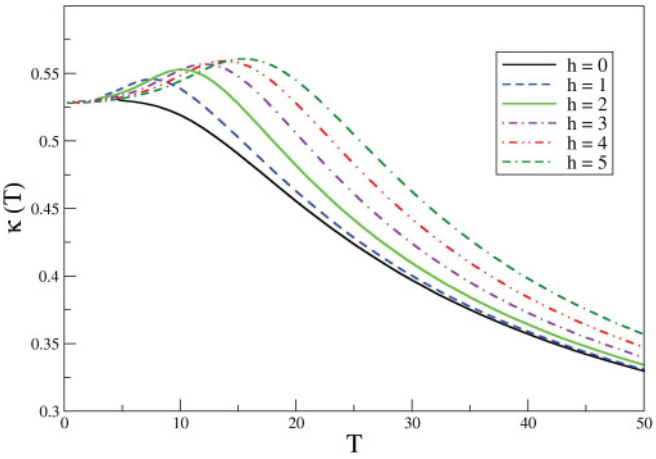

FIG. 4. (Color online) Compressibility κ as a function of temperature T for $\mu = 15$, $c = 1$, and various effective magnetic fields h (in units of κ_0, T_0, μ_0, and h_0).

the ground state, which can also be seen in the $T^{1/2}$ behavior of the specific heat $C = T\frac{\partial S}{\partial T}$ at zero magnetic field (see Fig. 3), is in accordance with a more general theorem of Eisenberg and Lieb [34] on systems with spin-independent interactions (see also [21]). Another consequence of the phase transition is the divergence of the zero-field susceptibility, $\chi = -\frac{\partial^2\phi}{\partial h^2}$, a feature which can be seen in Fig. 2. The specific heat, magnetic susceptibility, and compressibility, $\kappa = -\frac{\partial^2\phi}{\partial\mu^2}$ (see Fig. 4), present a nonmonotonic behavior with local maxima shifting to higher temperatures as the magnetic field increases.

In conclusion, we have presented a method of obtaining a finite number of NLIE characterizing the thermodynamics of integrable multicomponent 1D Bose gases, which allows for an efficient numerical treatment and has significant advantages over the TBA result. Fermionic gases can be treated in a similar fashion, but in this case the relevant lattice model for the n-component system is the $U_q(\widehat{sl}(n|1))$ Perk-Schultz spin chain. The derivation and a detailed analysis of Eqs. (3) and (4) will be presented in a future publication.

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