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Thermodynamics of correlated electrons with bond charge and Hubbard interaction in one dimension

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Abstract. The integrable model of one-dimensional electrons with bond charge and Hubbard interaction is investigated at finite temperatures. The approach based on the quantum transfer matrix is employed. The specific heat and compressibility are calculated showing interesting structures at intermediate temperatures. In the low-temperature regime the Luttinger liquid picture is verified.

Systems of strongly correlated electrons in low dimensions are subjects of considerable current interest. In particular, the discovery of high-T_C superconducting materials [1] has triggered extensive studies of various systems such as the Hubbard model, the t–J model, etc.

In one dimension the powerful tool of the Bethe ansatz (BA) method has unveiled several fundamental properties of these models. Especially, the combination of the BA method with methods of conformal field theory (CFT) resulted in a satisfactory picture for the zero temperature properties. However, the finite temperature properties are yet to reach the same quality.

The scope of the traditional thermodynamical Bethe ansatz (TBA) is not sufficiently wide to provide interesting quantities beyond the free energy such as finite temperature correlation lengths. Moreover, due to technical reasons the TBA usually causes troubles even in numerical evaluations of the free energy. A novel approach combining several developments in the theory of exactly solvable lattice models has been proposed that does not have the previously mentioned drawbacks [2–7]. More recently, the application to highly correlated electron systems such as the Hubbard model [8] and the supersymmetric t–J model turned out to be successful [9].

In this communication, we will study the finite temperature properties of a generalized Hubbard model [10] for electrons in one-dimensional space adopting the novel scheme. The model is characterized by a so-called correlated-hopping term, on-site Coulomb interaction and a pair-hopping term

$$\mathcal{H} = -\sum_{j=1}^{L}\sum_{\sigma=\uparrow,\downarrow}(c^{\dagger}_{j,\sigma}c_{j+1,\sigma} + c^{\dagger}_{j+1,\sigma}c_{j,\sigma})\exp(-\tfrac{1}{2}(\eta-\sigma\gamma)n_{j,\sigma} - \tfrac{1}{2}(\eta+\sigma\gamma)n_{j+1,-\sigma}) + U\sum_{j} n_{j,\uparrow}n_{j,\downarrow} + t_p\sum_{i}(c^{\dagger}_{j+1,\uparrow}c^{\dagger}_{j+1,\downarrow}c_{j,\uparrow}c_{j,\downarrow} + c^{\dagger}_{j,\uparrow}c^{\dagger}_{j,\downarrow}c_{j+1,\uparrow}c_{j+1,\downarrow}) \quad (1)$$

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which we study on a ring of length L with periodic boundary conditions. The solvable manifold we are going to discuss is given by $U/2 = t_p = \sinh\gamma/\sinh\alpha\gamma$, $\exp(-\eta) = \sinh(\alpha+1)\gamma/\sinh\alpha\gamma$, $\gamma \geqslant 0$ and α is either greater than 0 or smaller than -1. We note that this model does not comprise the pure Hubbard model ($\eta = \gamma = t_p = 0$), but several other models of interest: the pure correlated-hopping model ($|\alpha| \to \infty$), the supersymmetric t–J model ($\alpha \to 0, \gamma = 0$), and a model of hard core particles of three species ($\alpha \to -1$). The ground-state properties of the system have been analysed in [10]. Generally, for finite γ the spin excitations (spinons) possess a gap, while the charge excitations (holons) are gapless as in the Emery model. For $\gamma = 0$, both spinon and holon are massless for the repulsive case, while only pair excitations are massless for the attractive case. The crossover behaviour from dominant density–density correlations to dominant pair correlations manifests the superconducting properties of the model. In view of the latter properties the model deserves further studies, especially on finite temperature properties. The TBA construction has been applied to the rational case ($\gamma = 0$), resulting in an infinite set of coupled equations [11]. The complexity of the resultant equations defies, however, the further analysis of finite temperature properties. In the following we will present an alternative and comprehensive investigation of the thermodynamics of the model.

Besides properties of physical interest, the model also possesses rich mathematical structures. The symmetry underlying the solvability of this model has been clarified in terms of a four-dimensional representation of $U_q(gl(2|1))$, $q = \mathrm{e}^{\gamma}$. In the rational limit ($\gamma \to 0$) four supersymmetric generators (including an appropriate chemical potential term) exist which commute with the Hamiltonian. Thus, the model exhibits supersymmetry under suitable boundary conditions without taking the continuum limit. In this sense the model is quite unique. We refer to [12, 13] for the diagonalization of the associated row-to-row transfer matrix. Below, we will show that the partition function of the quantum transfer matrix enjoys a simple factorization property as a function of the spectral parameter.

In this report, we restrict ourselves to the repulsive case ($\alpha > 0$). The studies of the attractive case as well as a complete derivation of the key equations will be given in a separate publication.

We quickly review the novel approach to finite temperature studies utilizing the quantum transfer matrix. Here we adopt a most sophisticated formalism. Let $T(v)$ denote the transfer matrix of the classical vertex model [14] corresponding to our quantum system. The local Boltzmann weights, $R(v)$, depend on a so-called spectral parameter which labels the commuting family of transfer matrices $[T(v_1), T(v_2)] = 0$. Similarly, let $\overline{T}(v)$ be the transfer matrix consisting of $\pi/2$ rotated vertices. The standard initial condition then implies

$$\lim_{N\to\infty} (T(u)\overline{T}(u))^{N/2} = \exp(-\beta\mathcal{H}') \qquad \text{with } u = g\frac{\beta}{N} \tag{2}$$

where N is often referred to as the Trotter number and g is a (trivial) normalization to be specified later. We are now dealing with a virtually two-dimensional classical system of horizontal and vertical extension L and N, respectively. We define the so-called quantum transfer matrix as the column-to-column transfer matrix. This matrix can be embedded in a family of commuting operators $T_Q(v)$ which are defined by alternating products of vertices $R(v+u)$ and rotated vertices $\widetilde{R}(v-u)$. Therefore, we have a 'finite temperature Baxter's formula'

$$-\beta f = \lim_{N\to\infty} \log \Lambda_Q^{\max}(0) \tag{3}$$

where $\Lambda_Q^{\max}(v)$ is the largest eigenvalue of $T_Q(v)$, and the interchangeability of the limits of infinite system size and Trotter number is assumed, see also [15]. Similarly we can reduce

the evaluation of several thermodynamic quantities to that of other eigenvalues of $T_Q(v)$. As mentioned we adopt the 36 vertex $U_q(gl(2|1))$ model [14] as the classical counterpart of Hamiltonian (1) which is recovered after a trivial shift of the ground-state energy and chemical potential $\mathcal{H}' = \mathcal{H} + 2\cosh(\alpha+1)\gamma\mathcal{N}_e - 2L\cosh(\alpha+1)\gamma$, where $\mathcal{N}_e$ denotes the total number of electrons and the normalization $g = \sinh(\alpha+1)\gamma/\sinh\gamma$.

Through some calculations based on the quantum inverse scattering method, we find the following eigenvalue expression for $\Lambda_Q(v)$

$$\begin{aligned}\Lambda_Q(v) = {} & \phi_1(v)\frac{q_1(v+\mathrm{i}\gamma(2\alpha+1)/2)}{q_1(v+\mathrm{i}\gamma/2)}\mathrm{e}^{2\mu\beta} + \phi_2(v)\frac{q_1(v+\mathrm{i}\gamma(2\alpha+1)/2)q_2(v+\mathrm{i}\gamma)}{q_1(v+\mathrm{i}\gamma/2)q_2(v)}\mathrm{e}^{\mu\beta} \\ & + \phi_2(v)\frac{q_1(v+\mathrm{i}\gamma(2\alpha+1)/2)q_2(v-i\gamma)}{q_1(v-\mathrm{i}\gamma/2)q_2(v)}\mathrm{e}^{\mu\beta} + \phi_3(v)\frac{q_1(v+\mathrm{i}\gamma(2\alpha+1)/2)}{q_1(v-\mathrm{i}\gamma/2)}\end{aligned} \tag{4}$$

where we have introduced a chemical potential term $-\mu\mathcal{N}_e$ where μ is measured from the bottom of the band. The functions ϕ are defined by

$$\begin{aligned}\phi_1(v) &= \left(\frac{\sinh(\mathrm{i}v+u)\sinh(\mathrm{i}v+\alpha\gamma-u)\sinh(\mathrm{i}v-\gamma+u)}{\sinh(\mathrm{i}v-(\alpha+1)\gamma+u)\sinh(\mathrm{i}v+\alpha\gamma+u)\sinh(\mathrm{i}v-\alpha\gamma-u)}\right)^{N/2} \\ \phi_2(v) &= \left(\frac{\sinh(\mathrm{i}v+u)\sinh(\mathrm{i}v-u)}{\sinh(\mathrm{i}v-(\alpha+1)\gamma+u)\sinh(\mathrm{i}v-\alpha\gamma-u)}\right)^{N/2}\end{aligned} \tag{5}$$

and $\phi_3(v,\alpha) = \phi_1(-v, \alpha\to-\alpha-1)$. The functions $q(v)$ are given in terms of Bethe ansatz rapidities $v_j^{(i)}$: $q_i(v) = \prod_j \sin(v - v_j^{(i)})$. The location of these rapidities is determined by nested Bethe ansatz equations (BAE) which are derived from the analyticity of $\Lambda_Q(v)$. We avoid solving the BAE directly. Instead, we reformulate the analyticity condition in the form of nonlinear equations for conveniently defined auxiliary functions.

Let us introduce

$$a_0(v) = \frac{\lambda_1(x)(\lambda_3(x)+\lambda_4(x))}{\lambda_2(x)(\lambda_1(x)+\lambda_2(x)+\lambda_3(x)+\lambda_4(x))} \qquad a_1(v) = \frac{\lambda_1(x)}{\lambda_2(x)+\lambda_3(x)+\lambda_4(x)} \tag{6}$$

where λ_i denotes the ith summand on the right-hand side of (4) and the argument has been shifted according to $x = v + \mathrm{i}\frac{\alpha\gamma}{2}$. We are now interested in the largest eigenvalue. Through extensive numerical and analytic calculations we have verified remarkable properties of the corresponding distribution of the BA rapidities. Certain additive combinations of the λ-functions factorize in terms of the q-functions. As an example we note the $a_0(v)$ function

$$a_0(v) = \frac{(\sinh(\mathrm{i}v+\alpha\gamma-u)\sinh(\mathrm{i}v-\gamma+u))^{N/2}}{1+\mathrm{e}^{-\beta\mu}}\frac{\overline{q}_2(v-\mathrm{i}(\alpha+1)\gamma)}{\overline{q}_1(v-\mathrm{i}(\alpha+\frac{1}{2})\gamma)q_2(v+\mathrm{i}\gamma)} \tag{7}$$

where the upper-line denotes the complex conjugation $\overline{f}(v) = \overline{f(\overline{v})}$. As a direct corollary $\Lambda_Q^{\max}(v)$ takes a simple form

$$\begin{aligned}\Lambda_Q^{\max}(v) &= \ell_Q(v)\overline{\ell_Q}(v) \\ \ell_Q(v) &= \frac{(\mathrm{e}^{\beta\mu}+1)q_1(v+\mathrm{i}(\alpha+\frac{1}{2})\gamma)}{(\sinh(\mathrm{i}v+(\alpha+1)\gamma-u)\sinh(\mathrm{i}v+\alpha\gamma+u))^{N/2}}\end{aligned} \tag{8}$$

i.e. it factorizes into 'holomorphic' (v) and 'anti-holomorphic' ($\overline{v}$) parts. To our knowledge, such a factorization of the partition function in terms of dressed functions has never been observed before for one-dimensional quantum systems at finite temperature.

The following nonlinear integral equations are immediate consequences of this property

$$\begin{aligned}\log a_0 &= \beta\psi_{[-\mathrm{i}\delta]} + \beta\mu + k_{[-\mathrm{i}\delta]} * \log A_1 + k_{[-2\mathrm{i}\delta]} * \log \overline{A}_0 \\ \log a_1 &= \beta(\psi + \overline{\psi}) + 2\beta\mu + k_{[-\mathrm{i}\delta]} * \log \overline{A}_0 + \overline{k}_{[+\mathrm{i}\delta]} * \log A_0 + (k + \overline{k}) * \log A_1\end{aligned} \tag{9}$$

where we have introduced the notation for shifted functions $f_{[x]}(v) = f(v + x)$, the convolution $A * B = \frac{1}{\pi}\int_{-\pi/2}^{\pi/2} A(v - v')B(v')\,\mathrm{d}v'$, and

$$\psi(v) = \frac{\sinh^2((\alpha+1)\gamma)}{\sinh(\mathrm{i}v + \alpha\gamma/2)\sinh(\mathrm{i}v - (\alpha+2)\gamma/2)} \qquad k(v) = \frac{\sinh\gamma}{2\sinh\mathrm{i}v\sinh(\mathrm{i}v - \gamma)}. \tag{10}$$

Furthermore, a positive parameter δ of the order of γ has been introduced to render the integrands analytic. Note that the final results do not depend on this parameter thanks to Cauchy's theorem. We also remark the similarity of the above (nonlinear) integral equations to the (linear) dressed energy equations. This relation can be established quantitatively in the low-temperature limit [16, 17]. After solving (9) the eigenvalue $\Lambda_Q(v)$ is given by

$$\begin{aligned}&\Lambda_Q(v) = \Lambda_0(v) + \zeta * \log A_0 + \overline{\zeta} * \log \overline{A}_0 + (\zeta + \overline{\zeta}) * \log A_1 \\ &\Lambda_0(0) = 2\beta\cosh(\alpha+1)\gamma \qquad \zeta(v) = -\frac{\beta\psi(-v)}{\sinh(\alpha+1)\gamma}.\end{aligned} \tag{11}$$

As emphasized already, we have to deal with only two integral equations in contrast to the infinite number of coupled equations in the case of TBA. In principle and practice, the free energy for arbitrary temperature and chemical potential can be obtained by numerical calculations of (9) achieving a much higher precision.

Before presenting results of our numerical computations, let us mention some consistency relations we have checked. For instance, the high-temperature limit of the entropy is correctly reproduced as well as the limiting cases of free fermions ($\gamma \to 0$, $\alpha \to \infty$) and the t–J model ($\gamma \to 0$, $\alpha \to 0$) for which the nonlinear integral equations (9) actually coincide with those for the t–J model [9, 17]. Finally, we observe the consistency with the Luttinger liquid predictions for the low-temperature asymptotics.

In figure 1 numerical results are shown for the specific heat and compressibility of the system with parameters $\gamma = 0$ and $\alpha = \frac{1}{2}$. Quite generally, we observe a linear temperature dependence of the specific heat $c(T)$ in the low-temperature limit and a finite compressibility $\kappa(T)$ for $T = 0$ unless the particle density approaches the extremal values of 0 and 2. For small particle densities, the specific heat resembles that of the t–J model which actually corresponds to $\alpha = 0$. Two structures are visible corresponding to charge and spin excitations, the latter one being dominant for densities close to 1. There exists, however, several features different to the t–J model. Due to the pair-hopping term, the model has a massless dispersion relation for such coherent movings. Therefore, the double peak structure, observed for the t–J model, is smoothed out and hardly seen for $n \sim 1$. More significantly, the present system allows for densities larger than 1, in contrast to the t–J model. After further increase of n the 'spin' maximum of $c(T)$ is suppressed in height and shifted to lower temperatures, because of a decreasing density of unpaired spins. Simultaneously, pairs of electrons, i.e. doubly occupied sites, begin to dominate the dynamics via the Hubbard and pair-hopping mechanisms in (1). The corresponding structure of $c(T)$ is located at about $T \simeq t_p = 2$. For densities close to the maximum value the specific heat approaches a flat curve. Also the compressibility shows an interesting dependence on temperature and particle density. For densities $0 < n < 1$ this quantity shows a maximum at a temperature corresponding to the charge 'peak' in the specific heat. At larger densities a double peak structure is developed corresponding to the two types of charge excitations of the system (single particles and pairs).

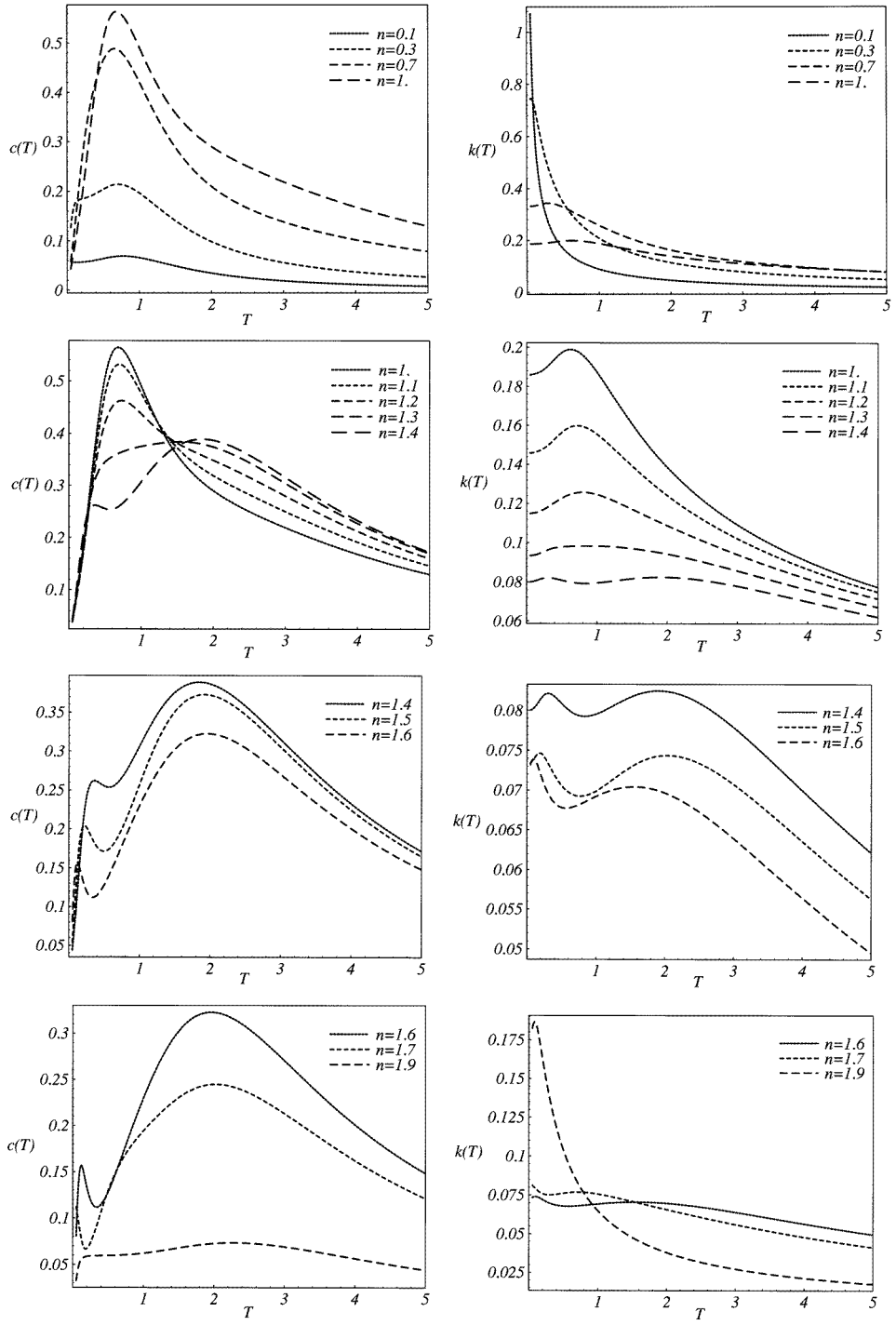

Figure 1. Specific heat and compressibility in dependence on temperature, T, for different particle densities, n, and fixed interaction parameters $\gamma = 0$, $\alpha = \frac{1}{2}$. Note the different offsets and scales of the diagrams.

Therefore, we have presented the exact thermodynamics of a solvable generalized Hubbard model. The remarkable factorization property of the eigenvalue function of the quantum transfer matrix enabled us to derive nonlinear integral equations. The low-temperature behaviour for the repulsive case, $\gamma = 0$ and small values for α and n is found to be governed by the t–J universality class. We also observe an exotic behaviour at high electron densities.

Similar studies for the model with attractive interaction and for the sub-case of the correlated-hopping model [18] are in progress. Also, we would like to report on the evaluation of the correlations at finite temperatures in the near future.

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