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Thermodynamics of Non-Relativistic Scattering Theory

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We use the thermodynamic Bethe ansatz to study the nonrelativistic scattering theory of low-energy excitations of the 1D Hubbard model using the S-matrices proposed by Eßler and Korepin. This model can be described by two types of excitation states, holons and spinons, as asymptotic states. In the attractive region, the spinon is massive while the holon is massless. The situation is reversed with a repulsive coupling. We show that the central charge of the Hubbard model in the IR limit is $c = 1$ due to the massless degree of freedom, i.e., the holon for the attractive region, and the massive mode decouples completely. This result is consistent with various known results based on lattice Bethe ansatz computations. Our results make it possible to use the S-matrices of the excitations to compute more interesting quantities like correlation functions.

There has been considerable interest in the interplay of integrable quantum field theory and statistical mechanics [1]. In particular, a lot of progress in this relationship has been made in two-dimensional models. One of the most useful methods in these models is the factorizable S-matrix theory [2]. In $1+1$-dimensional integrable field theories where an infinite number of conservation laws exist, the S-matrices are factorizable into two-body elastic S-matrices, which satisfy the Yang-Baxter equation. With known particle spectra and additional symmetries, one can determine the S-matrices exactly [2] by solving the Yang-Baxter equation. Another method is to diagonalize the Hamiltonian using Bethe ansatz and find physical particle states and their S-matrices [3]. In addition to their importance as physical amplitudes of scattering between asymptotic particle states, exact S-matrices can give other interesting quantities like the central charges of underlying conformal field theories (CFT's) from the finite size effects, conformal dimensions of the operators, and even the correlation functions.

Our motivation is to establish the S-matrix approach for studying the non-relativistic lattice models like the 1D Hubbard model [4]. Although the Bethe ansatz method is quite useful in finding eigenvalue spectra, excitation states, and their thermodynamic properties, it is not so useful in finding other important quantities, in particular, correlation functions. Recently, Eßler and Korepin derived the S-matrices for low lying excitations of the 1D Hubbard model [5]. What concerns us here, as a first step towards the complete S-matrix bootstrap of the low lying excitations of the Hubbard model, is how to confirm the validity of these matrices. For this purpose, we employ the thermodynamic Bethe ansatz (TBA) for 2D quantum field theory (QFT) which is now a standard tool [6] for checking the S-matrices. In the original formulation of factorizable scattering theory, one is interested in the scattering of relativistic excitations. In interacting 1-D quantum systems, such as the Hubbard model, there are in general several low-energy excitations with complicated dispersion relations and with different Fermi velocities. However, as T goes to zero, the relativistic invariance is recovered with the Fermi velocities as the effective speed of light [7]. Therefore, we can apply the relativistic TBA to our non-relativistic scattering problem in the IR limit. In this letter, we will compute the central charge in the IR limit and compare it with the result of the finite size effect [8]. The central charge is related to the specific heat of the system [7].

Among the lattice models of strongly correlated electron systems in low dimensions, it is believed that the two-dimensional Hubbard model provides some of the properties of high-T_c superconductivity [9]. Furthermore, a strong quantum fluctuation in low dimensions suggests common features in the 2D and the 1D Hubbard models.

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Fortunately, the 1D Hubbard model can be exactly diagonalized via the Bethe-ansatz technique [4]. Its thermodynamic properties, such as the susceptibility, the magnetization, and the low-temperature specific heat, for the repulsive ($U > 0$) and the attractive ($U < 0$) on-site interactions have been studied in the literature [10]. It is noticeable that the excitation spectrum is described by the spin and charge excitations, i.e., spinons and holons, and that the spin (charge) excitation possesses a gap in the attractive (repulsive) Hubbard model as long as the on-site interaction U exists. The low-energy charge (spin) excitations for the attractive (repulsive) case are proportional to those for the antiferromagnetic Heisenberg chain irrespective of the strength of the interaction and of the electron filling. Woynarovich and Eckle [8] have analyzed the finite-size corrections in the Hubbard model for the repulsive and half-filled case, and their analysis yields the central charge of the Virasoro algebra $c = 1$ which is contributed by the spin excitations, while the contribution of the charge excitations is negligible only if the on-site repulsion U is not so weak.

Let us now examine the dispersion relations of the excitations in the attractive case. Note that the results for the repulsive case can be obtained from the attractive case by interchanging the roles of holons and spinons. The holon energy in terms of the rapidity λ is given by

$$E_c(\lambda) = 2\int_0^\infty \frac{d\omega}{\omega}\frac{J_1(\omega)\cos(\omega\lambda)}{\cosh(\omega U)}, \tag{1}$$

whereas the momentum is given by

$$P_c(\lambda) = -\int_0^\infty \frac{d\omega}{\omega}\frac{J_0(\omega)\sin(\omega\lambda)}{\cosh(\omega U)}, \quad -\frac{\pi}{2} \le P_c(\lambda) \le \frac{\pi}{2}. \tag{2}$$

In the above, U is the coupling constant of the on-site interaction of the 1D Hubbard model. Notice that the holon is massless and $E_c = v_c P_c$ as $\lambda \to \infty$, where v_c, the Fermi velocity, is given by $v_c = E_c'(\infty)/P_c'(\infty)$.

The spinon has the following dispersion relations for the energy and the momentum, respectively:

$$E_s(k) = 2|U| - 2\cos k + 2\int_0^\infty \frac{d\omega}{\omega}\frac{J_1(\omega)\cos(\omega\sin k)}{\cosh(\omega U)}\exp(-|\omega U|), \tag{3}$$

and momentum,

$$P_s(k) = k - \int_0^\infty \frac{d\omega}{\omega}\frac{J_0(\omega)\sin(\omega\sin k)}{\cosh(\omega U)}\exp(-|\omega U|), \quad -\frac{\pi}{2} \le P_s(k) \le \frac{\pi}{2}. \tag{4}$$

We see that the spinon stays massive for finite U for all values of the rapidity.

Recently, using these dispersion relations, Eßler and Korepin derived the scattering matrices of the Hubbard model from the Bethe ansatz solution by generalizing the method of extracting the S-matrix from the asymptotics of the wave functions of the scattering state [5]. These S-matrices of the excitations on the lattice are well-defined as long as the wave packets of two excitations are well-separated. The complete scattering matrix is 16×16 dimensional and is in a block diagonal form consisting of 4 blocks. Each of the blocks describe holon-holon, spinon-holon, holon-spinon, and spinon-spinon scatterings, respectively, as follows:

$$S = \begin{pmatrix} S_{cc}(u) & 0 & 0 & 0 \\ 0 & S_{sc}(w) & 0 & 0 \\ 0 & 0 & S_{cs}(w) & 0 \\ 0 & 0 & 0 & S_{ss}(v) \end{pmatrix}, \tag{5}$$

where the holon-holon scattering amplitude is

$$S_{cc}(u) = -\frac{\Gamma\left(\frac{1+iu}{2}\right)\Gamma\left(1-\frac{iu}{2}\right)}{\Gamma\left(\frac{1-iu}{2}\right)\Gamma\left(1+\frac{iu}{2}\right)}\left(\frac{u}{u+i}\mathbf{I} + \frac{i}{u+i}\mathbf{P}\right), \quad u = \frac{\lambda-\lambda'}{2|U|}, \tag{6}$$

with Γ being the gamma function. In the above $\mathbf{I}$ and $\mathbf{P}$ are the 4×4 identity and permutation matrices, respectively. This S-matrix has the same form as that of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet and of the $SU(2)_1$ WZNW model [11]. The spinon-spinon scattering amplitude is

$$S_{ss}(v) = \frac{\Gamma\left(\frac{1-iv}{2}\right)\Gamma\left(1+\frac{iv}{2}\right)}{\Gamma\left(\frac{1+iv}{2}\right)\Gamma\left(1-\frac{iv}{2}\right)}\left(\frac{v}{v-i}\mathbf{I} - \frac{i}{v-i}\mathbf{P}\right), \quad v = \frac{\sin k - \sin k'}{2|U|}, \tag{7}$$

and can be obtained from S_{cc} by setting $u \to -v$. The spinon-holon scattering amplitude is

$$S_{sc}(w) = -i\frac{1+i\exp(\pi w)}{1-i\exp(\pi w)}\mathbf{I}, \quad w = \frac{\lambda - \sin k}{2|U|}. \tag{8}$$

We have the same form for the holon-spinon scattering amplitude S_{cs}. Notice that S_{sc} and S_{cs} approach constant values as $w \to \infty$.

Let us now apply the TBA to non-relativistic scattering as $T \to 0$. The TBA computes the Casimir energy of a theory on a circle of length R with S-matrices and the particle spectrum as input data [6]. With a temperature $T = 1/R$, the configuration of minimizing free energy gives the ground state energy of the system, which is again related to the central charges of the underlying CFT by

$$E_{\text{ground}}(R) \sim -\sum_i \frac{\pi c_i}{6 v_i R} \tag{9}$$

where v_i are Fermi velocities for excitations in the system and c_i are the corresponding effective central charges.

Consider N particles in a box of length L with a periodic boundary condition(PBC). Moving a k-th particle of type a with energy $E_a(\theta_k)$ and momentum $P_a(\theta_k)$ all the way by exchanging with other particles and coming back to the original configuration using a PBC, we get

$$e^{-iLP_a(\theta_k)}\prod_{i=1, i\neq k}^{N} S_{aa_i}(\theta_k - \theta_i) = 1 \tag{10}$$

where the index a_i specifies species of the i-th particle. In general, the product of S-matrices is a large size matrix called a transfer matrix, and one should diagonalize this by some technique. However, we consider a diagonal scattering theory first because the non-diagonal case can be understood as a slight modification. Taking logarithms on both sides of Eq. (10) gives

$$-LP_a(\theta_k) + \sum_{i=1}^{N} \frac{1}{i} \ln S_{aa_i}(\theta_k - \theta_i) = 2\pi n_k, \tag{11}$$

with an arbitrary integer n_k. In the thermodynamic limit, N, $L \to \infty$, one can express Eq. (11) in terms of the density of states as

$$2\pi\rho_a(\theta) = -LP'_a(\theta) + \sum_b \int d\theta' \rho_b^1(\theta')\phi_{ab}(\theta - \theta') \tag{12}$$

where $\rho_a(\theta)$ and $\rho_a^1(\theta)$ are the densities of the allowed and the occupied states, respectively, and ϕ_{ab} is the logarithmic derivatives of S-matrices S_{ab}. In terms of the 'pseudo-energies' ϵ_a defined by $e^{-\epsilon_a} = \rho_a^1/(\rho_a - \rho_a^1)$, one can express the ground state energy by

$$E_{\text{ground}}(R) = -\frac{1}{R}\sum_a \int_{-\infty}^{\infty} \frac{d\theta}{2\pi} RP'_a(\theta)L_{\epsilon_a}(\theta) \tag{13}$$

where $L_\epsilon(\theta) = \ln[1+e^{-\epsilon(\theta)}]$. ϵ_a is determined by the minimizing condition of the free energy which is the following set of nonlinear equations:

$$\epsilon_a(\theta) = RE_a(\theta) - \sum_b \phi_{ab} * L_{\epsilon_b}(\theta) \tag{14}$$

where $*$ denotes rapidity convolution, $f*g(\theta) = \int_{-\infty}^{\infty} d\theta'\, f(\theta-\theta')g(\theta')$. As we mentioned above, the sum in Eq. (13) for non-diagonal theories has to been taken with care. Diagonalization of the transfer matrix brings in additional 'massless' particles, which do not contribute to the central charge directly in the sum due to their masslessness, but which, nevertheless, affect the massive particle distributions. Additional care must be taken for non-relativistic scattering because the participating particles can have different Fermi velocities, unlike the relativistic case where all have the light speed as the Fermi velocity.

For the non-diagonal theories, the product of the S-matrices in Eq. (10) is replaced by the eigenvalues of the transfer matrix. For the 1D Hubbard model the non-diagonal matrices S_{cc} and S_{ss} are of the six vertex model type:

$$S_\alpha = \begin{pmatrix} a_\alpha & 0 & 0 & 0 \\ 0 & b_\alpha & c_\alpha & 0 \\ 0 & c_\alpha & b_\alpha & 0 \\ 0 & 0 & 0 & a_\alpha \end{pmatrix}, \quad \alpha = c, s. \tag{15}$$

The eigenvalues of the transfer matrices and the associated constraint equations can be derived by the algebraic Bethe Ansatz method to be

$$\Lambda_\alpha(\theta) = \prod_{i=1}^{N} a_\alpha(\theta - \theta_i) \prod_{r=1}^{M} \frac{a_\alpha(y_r - \theta)}{b_\alpha(y_r - \theta)} + \prod_{i=1}^{N} b_\alpha(\theta - \theta_i) \prod_{r=1}^{M} \frac{a_\alpha(\theta - y_r)}{b_\alpha(\theta - y_r)}, \tag{16}$$

and

$$\prod_{i=1}^{N} \frac{b_\alpha(y_k - \theta_i)}{a_\alpha(y_k - \theta_i)} \prod_{r=1}^{M} \frac{b_\alpha(y_r - y_k)}{a_\alpha(y_r - y_k)} \frac{a_\alpha(y_k - y_r)}{b_\alpha(y_k - y_r)} = -1. \tag{17}$$

From the S-matrices Eqs. (6) and (7), one can read off the corresponding matrix elements to evaluate the explicit eigenvalues. The holon and the spinon sectors are coupled by the diagonal scattering matrix S_{sc}.

We have two kinds of the periodic conditions for the Bethe wave functions of holons and spinons in terms of Λ_c, Λ_s, and S_{cs} and two sets of the constraint equations. For simplicity, we concentrate on the holon sector first and will generalize the argument to spinons. From Eqs. (6) and (17), the constraint equation for the holon sector becomes

$$\prod_{i=1}^{N} \frac{\beta_k - \theta_i - i|U|}{\beta_k - \theta_i + i|U|} \prod_{r=1}^{M} \frac{\beta_k - \beta_r + 2i|U|}{\beta_k - \beta_r - 2i|U|} = -1, \tag{18}$$

where we have introduced the shifted rapidities $\beta_i = y_i - i|U|$ to have the unitary form. It is well known from the analogy in the antiferromagnetic Heisenberg chain that in the thermodynamic limit, $N \to \infty$, the general solutions of these equations are the strings consisting of n-pseudoparticles of roots $\beta_r^{n,j} = \beta_r^0 + i|U|(n + 1 - 2j)$, where β_r^0 is real, $j = 1, \cdots, n$, and $n = 1, \cdots, \infty$. Such a string is a bound state of n-pseudoparticles and can be interpreted as a fictitious massless particle of real rapidity β_r^0. Since the length of the strings can be infinitely long, there are an infinite number of such massless particles. Similarly the constraint equations for spinons can be understood in the context of another kind of pseudoparticles designated by the rapidities α's which also form the string-solutions in the thermodynamic limit. Therefore, what we have is a diagonal scattering theory of holons, spinons and an infinite number of massless particles associated with them. The scattering amplitudes of the n-th massless particle with a holon is

$$S_n(\theta) = \frac{\theta - in|U|}{\theta + in|U|}, \tag{19}$$

and the scattering amplitudes between the massless particles are

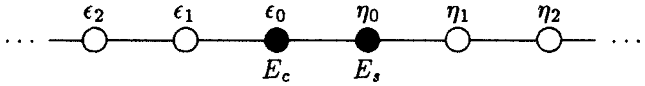
$$S_{nm}(\theta) = \left[\frac{\theta + i|n-m||U|}{\theta - i|n-m||U|}\right] \times \left[\frac{\theta + i(|n-m|+2)|U|}{\theta - i(|n-m|+2)|U|} \cdots \frac{\theta + i(n+m-2)|U|}{\theta - i(n+m-2)|U|}\right]^2 \times \left[\frac{\theta + i(n+m)|U|}{\theta - i(n+m)|U|}\right]. \tag{20}$$

For the spinons, the corresponding scattering amplitudes are obtained by the replacement $\theta \rightarrow -\theta$.

The minimizing condition of the free energy, using the above mentioned S-matrices, leads to an infinite set of non-linearly coupled equations. It is a standard procedure to use Fourier transformation on the TBA equations and to simplify the equations in terms of a unified kernel $\varphi = \left(4|U| \cosh \frac{\pi\theta}{2|U|}\right)^{-1}$ [12]:

$$\begin{aligned} RE_c(\theta) &= \epsilon_0(\theta) + \varphi * (L_{\epsilon_1} + L_{\eta_0})(\theta) \\ 0 &= \epsilon_n(\theta) + \varphi * (L_{\epsilon_{n-1}} + L_{\epsilon_{n+1}})(\theta), \quad n \geq 1 \\ RE_s(\theta) &= \eta_0(\theta) + \varphi * (L_{\eta_1} + L_{\epsilon_0})(\theta) \\ 0 &= \eta_n(\theta) + \varphi * (L_{\eta_{n-1}} + L_{\eta_{n+1}})(\theta), \quad n \geq 1. \end{aligned} \qquad (21)$$

These TBA equations have the incidence structure of an infinite chain, where a pair of semi-infinite chains of SU(2)-invariant, factorized scatterings are joined together as shown in the following picture:



These TBA equations can be solved easily as $R \rightarrow \infty$. When U is finite, the spinons become massive and do not contribute to the central charge because the pseudo-energy $\eta_0(\theta) \sim RE_s(\theta) \rightarrow \infty$ for all values of θ. After decoupling the spinon sector, we have only the semi-infinite chain of the holon sector. For a finite value of θ, $E_c(\theta)$ is non-zero, and from Eq. (21), $\epsilon_0(\theta)$ becomes infinite. Therefore, only non-vanishing contribution to the central charge comes from the $\theta \rightarrow \infty$ limit. In this limit, taking a derivative on Eq. (14) and substituting P_c' with E_c'/v_c into Eq. (13), we can now invoke the standard TBA analysis to evaluate the central charge in terms of the pseudo-energies at $\theta = 0$ and ∞. Note that the Fermi velocity in the denominator of Eq. (9) is canceled by the v_c in the above substitution. The final result for the central charges is

$$c_{\text{eff}} = \frac{6}{\pi^2} \sum_{n=0}^{\infty} \left[\mathcal{L}\left(\frac{x_n^\infty}{1+x_n^\infty}\right) - \mathcal{L}\left(\frac{x_n^0}{1+x_n^0}\right) \right] \qquad (22)$$

where $\mathcal{L}(x)$ is the Rogers dilogarithmic function

$$\mathcal{L}(x) = -\frac{1}{2} \int_o^x dt \left[\frac{\ln(1-t)}{t} + \frac{\ln t}{(1-t)} \right] \qquad (23)$$

and we have defined $x_n^\infty = \exp[-\epsilon_n(\infty)]$ and $x_n^0 = \exp[-\epsilon_n(0)]$. The TBA equations, Eq. (21), can be rewritten as a set of algebraic equations for x_n's:

$$\left.\begin{aligned} x_0^\infty &= (1+x_1^\infty)^{\frac{1}{2}} \\ x_n^\infty &= (1+x_{n-1}^\infty)^{\frac{1}{2}}(1+x_{n+1}^\infty)^{\frac{1}{2}} \end{aligned}\right\} \quad n \geq 1,$$

$$\left.\begin{aligned} x_0^0 &= 0 \\ x_n^0 &= (1+x_{n-1}^0)^{\frac{1}{2}}(1+x_{n+1}^0)^{\frac{1}{2}} \end{aligned}\right\} \quad n \geq 1. \qquad (24)$$

These have solutions $x_n^\infty = (n+2)^2 - 1$ and $x_n^0 = (n+1)^2 - 1$. Since $x_n^0 = x_{n-1}^\infty$, only x_∞^∞ survives to give $c_{\text{eff}} = 1$ after using $\mathcal{L}(1) = \frac{\pi^2}{6}$.

As we claimed in the beginning, the central charge we computed comes from the holon sector while the spinon sector decouples. This is what happens for finite U, but seems valid even for vanishing U as long as $U > 1/R$. In the literature, a discontinuity between $U \rightarrow 0$ and $U = 0$ has been predicted such that if $U = 0$, the central charge will be 2 because the model is nothing but a theory with four free fermions. Physically, this discontinuity arises in the specific heat since the central charge is proportional to it and is due to a gap in the excitation spectrum [10]. Discontinuities in the excitation spectrum around $U = 0$ have previously been reported by Woynarovich [13]. In our analysis, we use the holon and the spinon S-matrices which are valid for non-vanishing U. Within this validity, our result is what has been seen in the literature from different computations. With this confirmation for the Eßler-Korepin S-matrices, we have established the S-matrix program for non-relativistic models where the massless degree of freedom survives and gives the correct central charges in the $T \rightarrow 0$ limit. We hope our result can be a starting point for the application of the S-matrices to various lattice problems. We are particularly interested in computing the correlation functions using the form-factor approach [14]. In this scenario, the correlation functions of any local operator are expressed in terms of the form-factors which can be computed from the exact S-matrices. Although one needs to sum an infinite number of terms, this can be realized as the sum converges very fast. We hope to report this result elsewhere.

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