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Bethe Ansatz Results for Hubbard Chains with Toroidal Boundary Conditions

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We solve exactly the problem of a one-dimensional repulsive-U Hubbard chain with toroidal boundary conditions (HTB) using the Bethe ansatz approach. We calculate analytically the finite-size corrections to the ground-state energy in the half-filled case and use this expression to derive charge and spin stiffnesses with no assumptions. We then use a "particle–hole" transformation to calculate the finite-size corrections for the half-filled *attractive-U* case, and again derive the resulting expressions for the charge and spin stiffnesses. Lastly, we discuss how the repulsive-U corrections relate to those of a Heisenberg model with toroidal boundary conditions.

KEY WORDS: Bethe ansatz; Hubbard model; finite-size corrections.

The Bethe ansatz approach has emerged as one of most powerful techniques for treating 1D quantum systems. The method was first used by Bethe to solve the isotropic Heisenberg Hamiltonian[1] and was subsequently applied to several other models. The approach was developed further in an algebraic manner by Baxter[2] and the Russian school,[3] giving rise to the quantum inverse scattering method (QISM). This algebraic viewpoint made possible the solution of additional models that in principle were very difficult to solve using the traditional, or coordinative Bethe anzatz (CBA), approach. Recently, Sklyanin[4] extended the QISM to include generalized boundary conditions (see also refs. 5 and 6 for the CBA approach). These generalized boundary conditions have proven useful in the study of conformal invariant models.[7] However, one model that remained unsolved by

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the QISM is the Hubbard chain with toroidal boundary conditions (HTB). The Hubbard model with *periodic* boundary conditions was originally solved by Lieb and Wu[8] using the CBA approach. We also use the CBA approach here to solve the HTB, primarily exploring how the boundary conditions affect the Bethe ansatz equations and the finite-size corrections.

The HTB Hamiltonian is defined by

$$H=\sum_{\sigma}\sum_{l=1}^{L-1}(c_{l,\sigma}^{\dagger}c_{l+1,\sigma}+\text{h.c.})+U\sum_{l=1}^{L}c_{l,\uparrow}^{\dagger}c_{l,\uparrow}c_{l,\downarrow}^{\dagger}c_{l,\downarrow}$$
$$+\sum_{\sigma}(e^{i\theta_{\sigma}}c_{L,\sigma}^{\dagger}c_{1,\sigma}+\text{h.c.}) \tag{1}$$

where L is the lattice size; σ refers to the spin indices $\uparrow$ and $\downarrow$; and the θ_{σ} ($\theta_{\uparrow}$ and $\theta_{\downarrow}$) refer to the boundary condition phases on the up and down electrons. In order to diagonalize the model, we use the Bethe ansatz wave function

$$\psi(x_1,\ldots,x_N|Q_1,\ldots,Q_N)=\sum_{P}A(Q|P)\exp\left(i\sum_{j=1}^{N}x_{Q_j}k_{P_j}\right) \tag{2}$$

Here, $(x_1,\ldots,x_N|Q_1,\ldots,Q_N)$ refers to one of the $N!$ permutations $Q=\{Q_1,\ldots,Q_N\}$ of the N components of $(x_1,\ldots,x_N)$, where $(x_1,\ldots,x_N)$ denotes the locations and spin states of the N total number of electrons; the k_{P_j} refer to a permutation $P=\{P_1,\ldots,P_N\}$ of the N conduction electron momenta, given by the N components $(k_1,\ldots,k_N)$; and $A(Q|P)$ is the amplitude associated with the permutations. We take the boundary conditions into account by stipulating

$$\exp(ik_{P_N}L)\,A(Q|P)=\{\exp(i\theta_{\downarrow})\,\delta_{Q_N,N}+\exp(i\theta_{\downarrow})$$
$$\times(1-\delta_{Q_N,N})\}\,A(Q'|P')$$

where Q' and P' are cyclic permutations of Q and P [$Q'=(Q_N,Q_1,\ldots,Q_{N-1})$ and $P'=(P_N,P_1,\ldots,P_{N-1})$]. In analogy to Lieb and Wu,[8] we then obtain the spectrum of the HTB Hamiltonian parametrized in terms of a set $\{\lambda_j,k_j\}$ of variables that satisfy the so-called nested Bethe ansatz equations

$$\exp(ik_j)\exp(i\theta_{\uparrow})=\prod_{\beta=1}^{M}\frac{\sin(k_j)-\lambda_{\beta}+iU/4}{\sin(k_j)-\lambda_{\beta}-iU/4} \tag{4}$$

for $j=1,\ldots,N$ and

$$\exp[i(\theta_{\uparrow}-\theta_{\downarrow})]\prod_{\beta=1,\neq j}^{M}\frac{\lambda_j-\lambda_{\beta}-iU/2}{\lambda_j-\lambda_{\beta}+iU/2}=\prod_{\alpha=1}^{N}\frac{\lambda_j-\sin(k_{\alpha})-iU/4}{\lambda_j-\sin(k_{\alpha})+iU/4} \tag{5}$$

for $j=1,\ldots, M$, where M is the number of down electrons, with the resulting

$$E(\theta_\uparrow, \theta_\downarrow, N, M, L) = -2 \sum_{j=1}^{N} \cos(k_j) \tag{6}$$

As a check on our procedure,[3] we verified that ground-state energies for various fillings were the same as those obtained from exact diagonalizations of four-site and six-site systems.

The phases $\theta_\uparrow$ and $\theta_\downarrow$ enter Eqs. (4) and (5) in a seemingly different way, leading us to explore how the spectrum is changed if $\theta_\uparrow$ and $\theta_\downarrow$ are interchanged. A straightforward manipulation of Eqs. (4) and (5) gives

$$\prod_{j=1}^{N} \exp[i(k_j - k_j') L] = \exp[i(2M-N)(\theta_\uparrow - \theta_\downarrow)] \tag{7}$$

where $k_j = k_j(\theta_\uparrow, \theta_\downarrow)$ and $k_j' = k_j(\theta_\downarrow, \theta_\uparrow)$. In particular, when $N=2M$, $E(\theta_\uparrow, \theta_\downarrow, N, M, L) = E(\theta_\downarrow, \theta_\uparrow, N, M, L)$, in accordance with a simple relabeling of up and down particles.

We note that these equations generalize to a Hubbard chain with arbitrary hopping phases between the sites, given by the Hamiltonian

$$\begin{aligned} H = &\sum_{\sigma} \sum_{l=1}^{L-1} (e^{i\phi_{l,l+1}^{\sigma}} c_{l,\sigma}^{\dagger} c_{l+1,\sigma} + \text{h.c.}) \\ &+ U \sum_{l=1}^{L} c_{l,\uparrow}^{\dagger} c_{l,\uparrow} c_{l,\downarrow}^{\dagger} c_{l,\downarrow} + \sum_{\sigma} (e^{i\phi_{L,1}^{\sigma}} c_{L,\sigma}^{\dagger} c_{1,\sigma} + \text{h.c.}) \end{aligned} \tag{8}$$

This follows from the simple canonical transformation[10]

$$U_{l\sigma} c_{l\sigma} U_{l\sigma}^{-1} = c_{l,\sigma} e^{i\theta_{l\sigma}} \tag{9}$$

for $l=2,\ldots, L$ (the $c_{1,\sigma}$ are unchanged), where

$$\theta_{l\sigma} = -\sum_{m=1}^{l-1} \phi_{m,m+1}^{\sigma} \tag{10}$$

The Hamiltonian of Eq. (8) then reduces to that of Eq. (1) with

$$\theta_\sigma = \phi_{L,1}^{\sigma} + \sum_{l=1}^{L} \phi_{l,l+1}^{\sigma} \tag{11}$$

[3] Similar results, received by us in preprint form after the preparation of the first version of this manuscript, were independently derived by Shastry and Sutherland.[9]

The ground state of the HTB is given by a set of real solutions $\{\lambda_j, k_j\}$ of Eqs. (4) and (5), with finite-size corrections depending explicitly on $\theta_\uparrow$ and $\theta_\downarrow$. In the half-filled sector ($N = L = 2M$), we have used the method developed by De Vega and Woynarovich[11,12] to explicitly calculate these corrections. Omitting here the details of the calculation, we obtain for the leading finite-size correction of the ground-state energy

$$\frac{E_0(\theta_\uparrow, \theta_\downarrow, L)}{L} - e_\infty = -\left(\frac{1}{L^2}\right)\left(\frac{\pi\zeta}{6}\right)\left[1 - 6\left(\frac{\theta_\uparrow - \theta_\downarrow}{2\pi}\right)^2\right] + (\text{higher order}) \quad (12)$$

for $\theta_\uparrow$ and $\theta_\downarrow$ sufficiently small. Here, e_∞ is the ground-state energy per site in the $L \to \infty$ limit and ζ is the sound velocity

$$\zeta = \frac{2I_1(2\pi/U)}{I_0(2\pi/U)}$$

where I_0 and I_1 are the usual modified Bessel functions.

From this correction, we can obtain explicit values for the charge stiffness[13] D_c (also called the Drude weight) and the spin stiffness D_s. For D_c, we recover

$$D_c = \lim_{L\to\infty}\left[\pi L\left\{\frac{\partial^2 E_0(\theta_\uparrow = \theta_\downarrow = \theta, L)}{\partial\theta^2}\right\}_{\theta=0}\right] = 0 \quad (13)$$

as the half-filled Hubbard chain is an insulator. For D_s, we find

$$D_s = \lim_{L\to\infty}\left[\pi L\left\{\frac{\partial^2 E_0(\theta_\uparrow = -\theta_\downarrow = \theta, L)}{\partial\theta^2}\right\}_{\theta=0}\right] = \frac{4I_1(2\pi/U)}{I_0(2\pi/U)} \quad (14)$$

This is the same value that would be obtained by combining a conjecture of Shastry and Sutherland[9] (SS) with the analytic result of Takahashi[14] and Shiba[15] for the half-filled spin susceptibility. SS assume that "the energy $E(\theta)$ remains quadratic... in spite of a level crossing" out to at least $\theta_\uparrow = \pm\theta_\downarrow = \pm\pi$. The energy does *not* in general remain quadratic out to $\theta_\uparrow = \pm\theta_\downarrow = \pm\pi$, precisely because of the level crossing.[16] Rather, the procedure of SS is to "adiabatically" continue the state with $\theta_\uparrow = \theta_\downarrow = 0$ to states with larger values of θ, assuming that in this process $E(\theta)$ always remains quadratic in θ. While this assumption has not been shown to be true in general, comparison with our results, which were obtained without unverified assumptions, indicate that it is at least true at half-filling.

Further, we can use a canonical "particle–hole" transformation to obtain the charge and spin stiffnesses of the *attractive-U* half-filled

Hubbard model. To do so,[17] we set $d_{l,\uparrow} = c_{l,\uparrow}$ and $d_{l,\downarrow} = (-1)^l c^\dagger_{l,\downarrow}$ for all l, converting the Hamiltonian of Eq. (1) to

$$H' = \sum_{\sigma} \sum_{l=1}^{L-1} (d^\dagger_{l,\sigma} d_{l+1,\sigma} + \text{h.c.}) + (-U) \sum_{l=1}^{L} d^\dagger_{l,\uparrow} d_{l,\uparrow} d^\dagger_{l,\downarrow} d_{l,\downarrow}$$
$$+ U \sum_{l=1}^{L} d^\dagger_{l,\uparrow} d_{l,\uparrow} + (e^{i\theta_\uparrow} d^\dagger_{L,\uparrow} d_{1,\uparrow} + \text{h.c.}) + (e^{-i\theta_\downarrow} d^\dagger_{L,\downarrow} d_{1,\downarrow} + \text{h.c.}) \tag{15}$$

This leads directly to the attractive-U corrections at half-filling,

$$\frac{E'_0(\theta_\uparrow, \theta_\downarrow, L)}{L} - e'_\infty = -\left(\frac{1}{L^2}\right)\left(\frac{\pi\zeta}{6}\right)\left[1 - 6\left(\frac{\theta_\uparrow + \theta_\downarrow}{2\pi}\right)^2\right]$$
$$+ (\text{higher order}) \tag{16}$$

From this, we obtain the charge stiffness (or Drude weight)

$$D'_c = \lim_{L\to\infty}\left[\pi L \left\{\frac{\partial^2 E'_0(\theta_\uparrow = \theta_\downarrow = \theta, L)}{\partial\theta^2}\right\}_{\theta=0}\right] = \frac{4I_1(2\pi/U)}{I_0(2\pi/U)} \tag{17}$$

and the spin stiffness

$$D'_s = \lim_{L\to\infty}\left[\pi L \left\{\frac{\partial^2 E'_0(\theta_\uparrow = -\theta_\downarrow = \theta, L)}{\partial\theta^2}\right\}_{\theta=0}\right] = 0 \tag{18}$$

Lastly, we note that the correction of Eq. (12) is analogous to that of the isotropic Heisenberg model with toroidal boundary conditions $S^x_{L+1} \pm iS^y_{L+1} = e^{\pm i\psi}(S^x_1 \pm iS^y_1)$, where S^x and S^y are spin-1/2 Pauli matrices.[7] In fact, as $U \to \infty$, Eqs. (4) and (5) through lowest order in $1/U$ give in the half-filled case decoupled spinless fermions with boundary phase $\theta = (\theta_\uparrow + \theta_\downarrow)/2$, plus an isotropic Heisenberg model with toroidal boundary conditions $\psi = \theta_\uparrow - \theta_\downarrow$, as the value of $\sin(k)$ in Eqs. (4) and (5) is always bounded for real k. However, because a charge gap opens in the half-filled case[8] for *all* values of finite U, charge degrees of freedom then give no contribution to the leading finite-size corrections, and the analogy to the Heisenberg model with toroidal boundary conditions[18] persists for *all* values of U.

In summary, we have derived the Bethe ansatz equations for Hubbard chains with toroidal boundary conditions. We noted that these equations apply to Hubbard chains with arbitrary hopping phases between the sites. Using the equations, we derived the leading finite-size corrections to the ground-state energy in both the repulsive-U and attractive-U half-filled cases. We then utilized these corrections to obtain analytic expressions for

the charge stiffness (Drude weight) and the spin stiffness of the repulsive-U and attractive-U models at half-filling. Lastly, we discussed how the repulsive-U corrections relate to those of a Heisenberg chain with toroidal boundary conditions. Future work may include generalizations to Hubbard systems with higher degeneracy.

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REFERENCES

1. H. A. Bethe, *Z. Phys.* **71**:205 (1931).
2. R. J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic Press, London, 1982).
3. L. D. Faddeev, *Soviet Scientific Reviews* (Harvard Academic, London, 1980).
4. E. K. Sklyanin, *J. Phys. A* **21**:2375 (1988).
5. M. Gaudin, *Phys. Rev. A* **4**:386 (1971).
6. H. Schulz, *J. Phys. C* **8**:581 (1985).
7. F. C. Alcaraz, M. N. Barber, M. T. Batchelor, R. J. Baxter, and G. R. W. Quispel, *J. Phys. A* **20**:6397 (1981).
8. H. E. Lieb and F. Y. Wu, *Phys. Rev. Lett.* **20**:1445 (1968).
9. B. S. Shastry and B. Sutherland, *Phys. Rev. Lett.* **65**:243 (1990).
10. N. Byers and C. N. Yang, *Phys. Rev. Lett.* 7:46 (1961).
11. H. J. De Vega and F. W. Woynarovich, *Nucl. Phys. B* **251**:439 (1985).
12. F. Woynarovich and H. P. Eckle, *J. Phys. A* **20**:L97, L443 (1987).
13. W. Kohn, *Phys. Rev.* **133**:A171 (1964).
14. M. Takahashi, *Progr. Theor. Phys.* **43**:1619 (1970).
15. H. Shiba, *Phys. Rev. B* **6**:930 (1972).
16. R. M. Fye, M. J. Martins, D. J. Scalapino, J. Wagner, and W. Hanke, *Phys. Rev. B*, submitted.
17. H. Shiba, *Prog. Theor. Phys.* **48**:2171 (1972).
18. F. C. Alcaraz and F. Wreszinki, *J. Stat. Phys.*, to appear.