Asymptotic Spin-Spin Correlations of the $U \to \infty$ One-Dimensional Hubbard Model

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The large-distance behavior of the spin-spin correlation function of the one-dimensional repulsive Hubbard model is evaluated analytically in the strong-coupling regime at quarter filling. In this case, its power-law decay is characterized by an exponent $\gamma=\frac{3}{2}$. We have found that this behavior is generally valid at *any* nonzero doping, although our argument is not mathematically rigorous away from quarter filling. These results strongly suggest that the renormalization-group scaling to the Tomonaga-Luttinger model is exact in the $U\to\infty$ Hubbard model.

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Much of our present understanding of the physics of highly correlated electron systems is closely tied up with the Hubbard model (HM). The one-dimensional HM has been the subject of particular interest since the well-known exact solution of Lieb and Wu[1] who formally obtained the ground-state wave function and the energy spectrum of the HM Hamiltonian,

$$H=-\sum_{i,\sigma}(c_{i,\sigma}^{\dagger}c_{i+1,\sigma}+\text{H.c.})+U\sum_i n_i^{\uparrow}n_i^{\downarrow}\,. \tag{1}$$

From the exact solution, several properties, like chemical potential and magnetic susceptibility, have been explicitly calculated both at finite U (Refs. 1 and 2) and in the strong-coupling regime where also finite-temperature thermodynamic quantities have been found.[3] In spite of these remarkable successes, however, many crucial open problems remain, even in 1D. In particular, the long-distance behavior of the spin-spin correlation function is known only in two limits: the noninteracting electron gas and the half-filled system for $U\to\infty$. In both cases it has the asymptotic form

$$\langle \mathbf{S}(0)\cdot\mathbf{S}(r)\rangle \sim \cos(2k_F r)/r^{\gamma}\,, \tag{2}$$

where $\gamma=2$ for $U=0$ and $\gamma=1$ (with logarithmic corrections) at $U\to\infty$ and half filling.[4,5] Away from these two limits, no exact results are known about spin-spin correlations in the 1D HM.

In this Letter, we present an exact analytical evaluation of the asymptotic spin-spin correlations of the $U\to\infty$ 1D HM away from half filling.

We start from the exact ground-state wave function of a system of N (even) electrons in a L site chain with periodic boundary conditions, originally obtained by Lieb and Wu.[1] Ogata and Shiba[6] have shown that, in the $U\to\infty$ limit, it simplifies in the following form:

$$\psi(x_1,\dots,x_N,y_1,\dots,y_M)=\psi_{\text{SF}}(x_1,\dots,x_N)\phi_H(y_1,\dots,y_M)\,, \tag{3}$$

where $x_1,\dots,x_N$ denote the spatial coordinates of the N electrons, and the $y_1,\dots,y_M$ "coordinates" label the positions of the $M=N/2$ spin-up electrons on a "lattice" whose sites are $x_1,x_2,\dots,x_N$. In the following M will be taken as an odd integer. With these notations $\phi_H(y_1,\dots,y_M)$ is the same function appearing in the Bethe ground-state wave function of a Heisenberg N-site chain. Moreover, in expression (3) ψ_{SF} is the ground-state wave function of a free spinless Fermi gas with antiperiodic boundary conditions. Equation (3) is derived from the Bethe *Ansatz* solution of the Hubbard model by explicitly taking the limit $U\to\infty$ in the Lieb and Wu equations. In this case, following the notation of Ref. 1, the coefficients $[Q,P]$ appearing in the Bethe *Ansatz* are determined by the equation $[Q,P]=-[Q,P']$ which implies complete antisymmetry with respect to the label P. Moreover, the eigenvalue equations for the two sets of quantum numbers k_j and Λ_α decouple in the $U\to\infty$ limit, giving

$$Lk_j=2\pi I_j\,,$$
$$-N\theta(2\Lambda_\alpha)=2\pi J_\alpha-\sum_{\beta=1}^{M}\theta(\Lambda_\alpha-\Lambda_\beta)\,,$$

where the quantum numbers I_j and J_α are half odd integers and integers, respectively. The first equation reproduces the spectrum of a spinless fermion gas with antiperiodic boundary conditions, while the second one is exactly the consistency condition in the Bethe *Ansatz* solution of the Heisenberg chain with periodic boundary conditions. A careful analysis of the wave function then leads to Eq. (3).

The spin-spin correlations in this state can be written as

$$\langle \mathbf{S}(0)\cdot\mathbf{S}(r)\rangle=\sum_{j=2}^{r+1}P_{\text{SF}}^{r}(j)S_H(j-1)\,, \tag{4}$$

where $P_{\text{SF}}^{r}(j)$ is the probability of finding j particles in $(0,r)$ with one particle at 0 and another at r in the spinless Fermi gas:

$$P_{\text{SF}}^{r}(j)=\langle n_0 n_r\delta(N_r-j)\rangle_{\text{SF}}\,, \tag{5}$$

where $\delta(n)$ is Kronecker's δ function, $N_r\equiv\sum_{l=0}^{r}n_l$, and the symbol $\langle\,\rangle_{SF}$ indicates the quantum average over the spinless fermion ground state. The Heisenberg spin-spin correlation function $S_H(j)$ appearing in Eq. (4) is known to have an antiferromagnetic short-range order:

$$S_H(j)=(-1)^j f(j)\,, \tag{6}$$

where $f(j)\to\Gamma[\log^{\sigma}(j)/j]$ for large j. A recent analysis[7] has shown that $\sigma=\frac{1}{2}$. Neglecting the non-asymptotic contributions to $f(j)$, it is easy to verify that the function $f(j)$ satisfies the following inequality for any $j>j'\geq r$:

$$\left|\frac{f(j)-f(j')}{j-j'}\right|\leq M(r)=\frac{2\Gamma}{r^2}\log^{\sigma}(r)\,. \tag{7}$$

Inequality (7) is valid in the $r\to\infty$ limit, provided that either the corrections to the asymptotic behavior of $f(j)$ are "sufficiently smooth," or they vanish faster than $\log^{\sigma}(r)/r^2$. In the following we assume that this is the case. Our analysis is then exact only to leading order in r.

The evaluation of the full probability function $P^r_{SF}(j)$ is a difficult task even for a free fermion gas, because it is a highly nonlocal correlation function. In order to gain some intuition on the behavior of this quantity, it is convenient to analyze some of its general properties. In the following we will take the thermodynamic limit ($N\to\infty$, $L\to\infty$, $\rho=N/L$) at fixed r in order to eliminate finite-size effects. Therefore the inequality $N\gg r$ will be always understood. $P^r_{SF}(j)$ is a positive-definite function normalized to

$$Z=\sum_{j=2}^{r+1}P^r_{SF}(j)=\langle n_0 n_r\rangle_{SF}=\rho^2+O(1/r^2)\,, \tag{8}$$

where $\rho=N/L$ is the average electron density. The first two moments of this distribution can be evaluated analytically yielding, to leading order,

$$\langle j\rangle=Z^{-1}\sum_j jP^r_{SF}(j)=r\rho+1\,,$$
$$\langle j^2\rangle=Z^{-1}\sum_j j^2P^r_{SF}(j)=\langle j\rangle^2+\frac{1}{\pi^2}\ln r\,. \tag{9}$$

The previous asymptotic forms follow from the direct evaluation of three- and four-body correlation functions on the spinless fermion ground state, and can be easily verified by use of Wick's theorem. The second equation is valid to order $\ln r$ for every density away from half filling. These results indicate that the function $P^r_{SF}(j)$ is strongly peaked around $j\sim\rho r$ with a spread of the order $\Delta j\sim(\ln r)^{1/2}/\pi$. Therefore only a small neighborhood of the value $j=\rho r$ gives a significant contribution to the sum in Eq. (4) for large r. This suggests that the asymptotic behavior of Eq. (4) can be obtained even without the evaluation of the full probability distribution $P^r_{SF}(j)$. It is possible to give a simple formal proof of this statement.

Given a normalized probability distribution $P^r_{SF}(j)$ satisfying Eqs. (9) and given $f(j)$ bounded and satisfying Eq. (7), the quantity $\sum_{j=2}^{r+1}P^r_{SF}(j)(-1)^j f(j)$ differs from $[\sum_{j=2}^{r+1}P^r_{SF}(j)(-1)^j]f(\langle j\rangle)$ by terms vanishing faster than $\log^{|\sigma|+1}(r)/r^2$.

In fact, let us consider the difference R between the two considered quantities, and split up the sum in two pieces $R=R_1+R_2$ with

$$R_1=\sum_{j=2}^{\langle j\rangle/2}P^r_{SF}(j)(-1)^j[f(j)-f(\langle j\rangle)]\,,$$
$$R_2=\sum_{j=\langle j\rangle/2+1}^{r+1}P^r_{SF}(j)(-1)^j[f(j)-f(\langle j\rangle)]\,.$$

From the boundeness of $f(j)$ [say, $|f(j)|\leq A$]:

$$R_1\leq 2A\sum_{j=2}^{\langle j\rangle/2}P^r_{SF}(j)\,. \tag{10}$$

The term appearing on the right-hand side of Eq. (10) can be easily bounded by means of the variance of j:

$$\frac{\langle j\rangle^2}{4}\sum_{j=2}^{\langle j\rangle/2}P^r_{SF}(j)\leq\sum_{j=2}^{r+1}P^r_{SF}(j)(j-\langle j\rangle)^2\,. \tag{11}$$

Hence, from Eqs. (9)-(11) we get $R_1\leq\text{const}\times\log(r)/r^2$. The second term R_2 can be bounded using Eq. (7) and the Schwarz inequality:

$$R_2\leq M\left(\frac{\langle j\rangle}{2}\right)\sum_{j=\langle j\rangle/2}^{r+1}|j-\langle j\rangle|P^r_{SF}(j)$$
$$\leq M\left(\frac{\langle j\rangle}{2}\right)\left(\sum_{j=2}^{r+1}(j-\langle j\rangle)^2P^r_{SF}(j)\right)^{1/2}.$$

Finally, using (9) and the previous bound on R_1 we get the desired result.

Such an asymptotic evaluation when applied to Eq. (4) gives

$$\langle\mathbf{S}(0)\cdot\mathbf{S}(r)\rangle\to -C_r\Gamma\frac{\ln^{\sigma}\rho r}{\rho r}+O\left(\frac{\ln^{|\sigma|+1}r}{r^2}\right), \tag{12}$$

where C_r is the $k=\pi$ component of the Fourier transform of $P^r_{SF}(j)$ defined by

$$C_r=\sum_{j=2}^{r+1}P^r_{SF}(j)\exp(i\pi j)=\langle n_0 n_r e^{i\pi N_r}\rangle_{SF}\,.$$

Because of the algebraic properties of the density operators n_r, the function C_r can be written as a linear combination of the simpler quantity $D(r)$:

$$C_r=\tfrac{1}{4}[D(r-2)-2D(r-1)+D(r)]\,, \tag{13}$$

with

$$D(r)=\langle e^{i\pi N_r}\rangle_{SF}\,.$$

In order to evaluate this average, we note that the spinless fermion ground state is a Slater determinant (SD) of

N plane-wave orbitals with antiperiodic boundary conditions $\varphi_n(x)=L^{-1/2}\exp[2\pi(n+\frac{1}{2})x/L]$. This action of the operator $\exp(i\pi N_r)$ on such a state gives another SD of orbitals $\varphi_n'(x)$ differing from φ_n only in the interval $(0,r)$ where $\varphi_n'=-\varphi_n$. Hence, the quantity $D(r)$ is given by the determinant of the $N\times N$ overlap matrix A between $\varphi_n(x)$ and $\varphi_m'(x)$:

$$A_{n,m}=\delta_{n,m}-\frac{2}{L}\sum_{x=0}^{r}e^{2\pi ix(n-m)/L}.$$

This matrix, being separable, has only $r+1$ eigenvalues different from unity[8] and therefore its determinant can be reduced to that of a $(r+1)\times(r+1)$ matrix B. Taking the thermodynamic limit at fixed r, B can be written as

$$B_{j,l}=B(j-l)=\begin{cases}-(2/\pi)\sin\pi\rho(j-l)/(j-l), & j\neq l,\\ 1-2\rho, & j=l.\end{cases} \tag{14}$$

The limiting case $\rho=1$ is particularly simple because the matrix B becomes diagonal, leading to $C_r=(-1)^{r+1}$. This result, when substituted into Eq. (12), gives just the Heisenberg spin-spin correlations, appropriate for the half-filled system.

In the following we will extend the analysis to the case $\rho\neq 1$. Note that in the matrix B all the elements $B_{j,l}$ depend just on the difference $(j-l)$, i.e., B is a Toeplitz matrix.[9] This class of matrices has been extensively studied in many problems of statistical mechanics including the evaluation of the correlation functions of the 2D Ising model. However, the basic theorem leading to the asymptotic expansion of the determinant of a Toeplitz matrix cannot be applied directly in our case because $B(n)$ decays too slowly for large n. The problem simplifies in the case $\rho=\frac{1}{2}$ where the spinless fermion state is invariant under charge conjugation. This canonical transformation changes the fermion creation operators into annihilation operators with an overall sign which depends on the sublattice they belong to: $c_i^\dagger\to(-1)^i c_i$. Under this symmetry, the operator $\exp(i\pi N_r)$ changes according to

$$\exp(i\pi N_r)\to\exp[-i\pi(N_r-r-1)] =(-1)^{r+1}\exp(i\pi N_r),$$

yielding $D(r)=0$ for even r. Now we proceed to the evaluation of $D(r)$ for odd $r=2p-1$. As a first step we note that the matrix $B_{j,l}$ can be cast into the form

$$\begin{bmatrix}0 & F^+\\ F^- & 0\end{bmatrix}. \tag{15}$$

This is achieved by use of the unitary transformation which interchanges the rows and columns of the original matrix B collecting the even (odd) indices together. The matrices $F^\pm$ in Eq. (15) are $p\times p$ Hilbert matrices defined by

$$F_{n,m}^{\pm}=\mp\frac{1}{\pi}\frac{1}{n-m\pm\frac{1}{2}}.$$

The determinant of Hilbert matrices can be analytically computed.[9] The behavior for large p of the determinant of (15) is given by

$$D(r=2p-1)=(-1)^p\det F^+\det F^- =A^2\frac{(-1)^p}{p^{1/2}}+O\left(\frac{1}{p^{5/2}}\right),$$

where the numerical constant $A=0.645\,002\,448\ldots$ is formally given by

$$\ln A=\sum_{l=1}^{\infty}l\left[\ln\left(1-\frac{1}{4l^2}\right)+\frac{1}{4l^2}\right]-\frac{1}{4}(1+\gamma)$$

and γ is the Euler constant.

Having determined the asymptotic form of $D(r)$, we substitute our result into the right-hand side of Eq. (13) which gives

$$C_r=-\frac{1}{\sqrt{2}}A^2\frac{\cos(2k_Fr)}{r^{1/2}},$$

where $k_F=\pi\rho/2$ is the Fermi momentum of the interacting electron gas. This result together with Eq. (12) gives the long-range behavior of the spin-spin correlation function in the Hubbard model at $\rho=\frac{1}{2}$,

$$\langle\mathbf{S}(0)\cdot\mathbf{S}(r)\rangle\to A^2\sqrt{2}\Gamma\cos(2k_Fr)\frac{\ln^{\sigma}(r/2)}{r^{3/2}} +O\left(\frac{\ln^{|\sigma|+1}r}{r^2}\right). \tag{16}$$

Equation (16) is the main result of this paper. It shows that the spin-spin correlations of the HM at quarter filling have a power-law decay characterized by an exponent $\gamma=\frac{3}{2}$. This can be contrasted to the Heisenberg result $\gamma=1$, valid for the $U\to\infty$ HM at half filling. The physical origin of the change in the exponent γ upon doping can be attributed to the umklapp process, present only at half filling, which enhances the antiferromagnetic correlations.

Although the derivation we have given in this Letter strictly applies to the $\rho=\frac{1}{2}$ case, we have found that the same power-law decay is generally valid at any density away from half filling. However, in this case our derivation is not so simple and rigorous as in the quarter-filled case because standard techniques for the asymptotic expansion of a Toeplitz determinant cannot be applied for the matrix $B_{j,l}=B(j-l)$ of Eq. (14). The main problem is that the Fourier transform of the function $B(n)$ is discontinuous, and this spoils the derivation of the basic theorem (Szegö's theorem) which governs the asymptotic expansion of a Toeplitz determinant.[9] In order to circumvent this problem, we might regularize $B(n)$ by introducing an additional parameter Λ which smoothens the discontinuity in its Fourier transform. In this way Szegö's theorem can be applied but we are forced to interchange the order of the two limiting procedures $r \to \infty$ and $\Lambda \to 0$. Assuming that the leading term in the evaluation of the singular Toeplitz determinant (14) does not depend on the order in which the limits are taken, the same power-law decay $r^{-3/2}$ is obtained at all densities. Although we have not tried to demonstrate that such an asymptotic expansion is mathematically rigorous, we have verified that the leading behavior $C_r \propto \cos(2k_F r)/r^{1/2}$ does not depend on the possible choices of the regularization. This fact supports our previous assumption.

In summary, we have given the first analytical evaluation of an important correlation function of the 1D HM at strong coupling. Previous renormalization-group (RG) studies[10] predicted that, in the weak-coupling regime, the HM for $\rho \neq 1$ scales to the exactly solvable (spin-isotropic) Tomonaga-Luttinger model (TLM) with renormalized coupling constants. According to this analysis the HM is a marginal conductor for $\rho \neq 1$ (without a well-defined Fermi surface) characterized by a power-law singularity at k_F,

$$n(k) \sim n(k_F) - c\,|k - k_F|^{\theta} \operatorname{sgn}(k - k_F) .$$

RG also predicts power-law decay of the density-density and spin-spin correlation functions as in the TLM. In the TLM all these singularities are related by scaling laws (valid for any value of the coupling constants):

$$4\gamma = \beta + 4, \quad 16\beta\theta = (\beta - 4)^2 , \tag{17}$$

where the exponent β characterizes the long-range decay of the $4k_F$ oscillations present in the density-density correlation function. Numerical studies[6,11] have provided indirect indications that scaling to the Tomonaga-Luttinger model might be exact at $U \to \infty$.

Now we are in the position to check, for the first time, the validity of such a hypothesis in the strong-coupling limit of the HM. In fact, from Eq. (3), it is clear that the density-density correlation function at $U \to \infty$ coincides with that of free spinless fermions, yielding $\beta = 2$. This, together with our previous result $\gamma = \frac{3}{2}$, is consistent with the Tomonaga-Luttinger exponents (17) predicted by the RG weak-coupling analysis. Therefore this result strongly suggests that even for $U \to \infty$ the HM scales to the TLM.

According to this hypothesis the momentum-distribution exponent is exactly given by $\theta = \frac{1}{8}$. The nonvanishing value of θ indicates that the 1D HM remains, for $U \to \infty$, a marginal conductor, which cannot be described by standard Fermi-liquid theory.

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