One-particle irreducible density matrix for the spin disordered infinite $U$ Hubbard chain

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In this Letter we present a calculation of the one-particle irreducible density matrix $\rho(x)$ for the one-dimensional (1D) Hubbard model in the infinite $U$ limit. We consider the zero temperature spin disordered regime, which is obtained by first taking the limit $U \to \infty$ and then the limit $T \to 0$. Using the determinant representation for $\rho(x)$ we derive analytical expressions for both large and small $x$ at an arbitrary filling factor $0 < \varrho < 1/2$. The large $x$ asymptotics of $\rho(x)$ is found to be remarkably accurate starting from $x \sin(2\pi \varrho) \sim 1$. We find that the one-particle momentum distribution function $\rho(k)$ is a smooth function of $k$ peaked at $k = 2k_F$, thus violating the Luttinger theorem.

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Recently, we reported results on the one-particle correlation functions of the continuous 1D system of impenetrable spin 1/2 fermions in the spin disordered regime [1, 2]. It was found that the infrared asymptotic behavior of the correlation functions, although consistent with the assumption of spin-charge separation, is not adequately described by the Luttinger model. This is to be contrasted with the asymptotic behavior of the previously studied correlation functions of the infinite $U$ Hubbard model in the “antiferromagnetic” ground state, understood as a limit of the ground state of the Hubbard model as $U \to \infty$. In the latter case the Luttinger model gives correct predictions [3, 4, 5].

In this paper we explore the 1D Hubbard model (6) in the spin disordered regime obtained [7]. For the equal time correlation function [8] the determinant representation, given in Ref [7], can be written in the following form:

$$\rho(x) = \frac{1}{8\pi i} \oint_{|z|=1} \frac{dz}{z} F(z) B_{--}(z) \det(\hat{I} + \hat{V})(z).$$ (4)

Here the function $F(z)$ is

$$F(z) = 1 + \frac{z}{2-z} + \frac{1}{2z-1}. \quad (5)$$

The determinant

$$\det(\hat{I} + \hat{V}) = \prod_{N=0}^{\infty} \frac{1}{N!} \int_{-K}^{K} dk_1 \cdots \int_{-K}^{K} dk_N$$

$$\times \det \left[ V(k_1, k_1) \cdots V(k_1, k_N) \right] \cdots \det \left[ V(k_N, k_1) \cdots V(k_N, k_N) \right]$$

is the Fredholm determinant of a linear integral operator $\hat{V}$ with the kernel

$$V(k, p) = \frac{e_+(k)e_-(p) - e_+(p)e_-(k)}{2 \tan \left[ \frac{1}{2}(k-p) \right]}$$

defined on $[-K, K] \times [-K, K]$. Here

$$K = 2\pi \varrho$$

is twice the Fermi momentum. The functions $e_{\pm}$ entering Eq. (7) are defined as follows

$$e_-(k) = \frac{1}{\sqrt{\pi}} e^{-ikx/2},$$

$$e_+(k) = \frac{i}{2\sqrt{\pi}} e^{ikx/2}(1 - z).$$

We find that the one-particle momentum distribution function $\rho(k)$ is a smooth function of $k$ peaked at $k = 2k_F$, thus violating the Luttinger theorem.
The function $B_{-}(z)$ is

$$B_{-}(z) = \int_{-K}^{K} dke_{-}(k)(\hat{I} + \hat{V})^{-1}e_{-}(k)$$  \hspace{1cm} (11)$$

Consider the contour integral in Eq. (4). According to definitions Eqs. (7) and (10) the Fredholm operator $\hat{V}$ is linear in $z$. This implies that the product $B_{-}(z) \det(\hat{I} - \hat{V})(z)$ is analytic in the complex $z$-plane. Therefore, the integral is given by the residue of the integrand at the pole $z = 1/2$ of the function $F(z)$

$$\rho(x) = \frac{1}{4}B_{-}(1/2) \det(\hat{I} + \hat{V})(1/2).$$  \hspace{1cm} (12)$$

Consider the short distance behavior of $\rho(x)$ first. For any $x$ the kernel (7) can be written as a sum of $2x$ separable kernels (recall that $x$ is a discrete variable, $x = 0, 1, 2, \ldots$)

$$V(k, p) = \frac{z - 1}{4\pi} \sum_{m=1}^{2x} u_{m}(k)u_{m}(p),$$  \hspace{1cm} (13)$$

where

$$u_{m}(k) = \begin{cases} e^{i(m - \frac{x}{2})k}, & m = 1, \ldots, x \\ e^{-i(m + \frac{x}{2})k}, & m = x + 1, \ldots, 2x \end{cases}.$$  \hspace{1cm} (14)$$

Therefore, $\det(\hat{I} + \hat{V})$ can be expressed in terms of the determinant

$$\det(\hat{I} + \hat{V}) = \det_{2x}(I + V)$$  \hspace{1cm} (15)$$

of an $2x \times 2x$ matrix $V$:

$$V = \frac{z - 1}{2\pi} \left( \begin{array}{cc} Q & I \\ P & \frac{1}{Q} \end{array} \right).$$  \hspace{1cm} (16)$$

Here $Q$ and $P$ are $x \times x$ matrices with the entries defined by

$$Q_{mn} = \sin[K(m - n)], \quad n, m = 1, \ldots, x$$  \hspace{1cm} (17)$$

$$P_{mn} = \sin[K(m + n - x)], \quad n, m = 1, \ldots, x$$  \hspace{1cm} (18)$$

where

$$Q_{nn} = P_{(x-n)n} = K.$$  \hspace{1cm} (19)$$

For $B_{-}(z)$ one has

$$B_{-} = \frac{2\sin Kx}{\pi x} - \frac{z - 1}{4\pi} a^{T}(I + V)^{-1} b,$$  \hspace{1cm} (20)$$

where the $2x$-dimensional vectors $a$ and $b$ are defined by

$$a_{n} = \begin{cases} \frac{2\sin Kn}{\sqrt{\pi n}}, & n = 1, \ldots, x \\ \frac{2\sin K(n - 2x)}{\sqrt{\pi(n - 2x)}}, & n = x + 1, \ldots, 2x \end{cases}$$  \hspace{1cm} (21)$$

and

$$b_{n} = \frac{2\sin Kn(n - x)}{\sqrt{\pi(n - x)}}, \quad n = 1, \ldots, 2x.$$  \hspace{1cm} (22)$$

Eqs. (15) through (22) combined with (12) are convenient for the calculation of $\rho(x)$ at small enough $x$. For example,

$$\rho(0) = \frac{K}{2\pi},$$  \hspace{1cm} (23)$$

$$\rho(1) = \frac{\sin K}{2\pi},$$  \hspace{1cm} (24)$$

$$\rho(2) = \frac{\sin^{2} K}{4\pi^{2}} + \frac{2\pi - K}{8\pi^{2}}.$$  \hspace{1cm} (25)$$

With increasing $x$ the complexity of the exact expression for $\rho(x)$ grows rapidly.

Next, we calculate the long distance asymptotics of the density matrix (2) using the determinant representation (4). Technically, the asymptotic analysis will be similar to that carried out for the continuous limit of the model in Ref. [2].

To calculate $\det(\hat{I} + \hat{V})$ write the difference equation for the kernel (7):

$$V(k, p; x + 1) = e^{\frac{i}{2}(k-p)} V(k, p; x) + ie_{-}(k; x)e_{+}(p; x) \cos \frac{k - p}{2}.$$  \hspace{1cm} (26)$$

From this equation it follows that

$$\det(\hat{I} + \hat{V})(x + 1; z) = \det(\hat{I} + \hat{V})(x; z) W(x; z),$$  \hspace{1cm} (27)$$

where

$$W(x) = \det \begin{bmatrix} 1 + \frac{1}{2} B_{+}(x) & \frac{1}{2} B_{-}(x) \\ \frac{1}{2} C_{+}(x) & 1 + \frac{1}{2} A_{+}(x) \end{bmatrix}.$$  \hspace{1cm} (28)$$

and

$$A_{ab} = \int_{-K}^{K} dke_{a}(k)e^{-ik(\hat{I} + \hat{V})^{-1}[e^{ik}e_{b}(k)]},$$  \hspace{1cm} (29)$$

$$B_{ab} = \int_{-K}^{K} dke_{a}(k)(\hat{I} + \hat{V})^{-1}e_{b}(k),$$  \hspace{1cm} (30)$$

$$C_{ab} = \int_{-K}^{K} dke_{a}(k)e^{ik(\hat{I} + \hat{V})^{-1}e_{b}(k)},$$  \hspace{1cm} (31)$$

$$D_{ab} = \int_{-K}^{K} dke_{a}(k)e^{-ik(\hat{I} + \hat{V})^{-1}e_{b}(k)}.$$  \hspace{1cm} (32)$$

The indices $a$ and $b$ run through two values: $a, b = \pm$.

The resolvent operator $(\hat{I} + \hat{V})^{-1}$ and, therefore, the functions $B_{ab}$ can be found from the solution of the corresponding matrix Riemann-Hilbert problem [8]. The scheme of the asymptotic solution of the matrix Riemann-Hilbert problem associated with the kernel (7) is very similar to the one given in [2]. It is based on the
non-linear steepest-descend method. The main results of the asymptotic analysis are as follows. For \( z = 1/2 \)

\[
W(x; z = 1/2) = 2^{-K/\pi} \left[ 1 + \frac{\nu^2}{2x} \right] + \delta W(x), \tag{33}
\]

where

\[
\nu = \frac{\ln 2}{\pi}. \tag{34}
\]

The error term \( \delta W(x) \) decays as \( x^{-2} \) for \( x \sin K > 1 \). Solving Eq. (27) with \( W \) given by Eq. (33) one gets in the large \( x \) limit

\[
\det(\hat{I} + \hat{V})(x) = e^{C(K)(\sin K)\frac{x^2}{\pi} - \frac{4K}{\pi}x \frac{x^2}{\pi}}, \tag{35}
\]

where \( C(K) \) is independent of \( x \). Numerically, \( \exp[C(K)] \) is close to unity for all \( K \), as can be seen in Fig. 1. The exact expression for \( C(0) \) is given in Ref. [2] and is, numerically, equal to 0.0550839\ldots. This agrees perfectly with Fig. 1.

The asymptotic formula for the one particle density matrix reads

\[
\rho(x) = \frac{i\pi 2 \sqrt{2} e^{C(K)(\sin K)\frac{x^2}{\pi}} e^{-\nu K x} x^{\nu}}{\cosh^2(\nu K/2)} \times \left[ \frac{(2 \sin K)^{-i\nu} e^{iKx}}{\Gamma(-i\nu/2)^2 x^{1+i\nu}} - \frac{(2 \sin K)^{i\nu} e^{-iKx}}{\Gamma(i\nu/2)^2 x^{1-i\nu}} \right], \tag{36}
\]

with the relative correction of the order of \( x^{-1} \). The formula (36) is the main result of the paper.

Let us discuss Eq. (36). The structure of the correlation function is essentially the same as for the impenetrable fermion gas. The correlation function contains the exponentially decaying factor \( \exp(-\nu K x) \), and factors obeying the power law scaling. The complex-valued anomalous exponents do not depend on \( K \) or, equivalently, on the filling factor \( \rho \). A similar situation takes place for the infinite \( U \) Hubbard model in the Luttinger regime: the Luttinger scaling exponents do not depend on the filling factor [3]. The results for the continuous model, impenetrable fermion gas [1, 2, 10], can be recovered by taking the limit \( K \to 0 \) in Eq. (36) at a fixed \( Kx \).

Formally, the asymptotic formula given in Eq. (36) is valid for \( x \sin K \gg 1 \). Nevertheless, it is remarkably good even for \( x \sin K \sim 1 \) as can be seen from Fig. 2 where the exact expression obtained from Eqs. (15) through (22) is compared with the asymptotics Eq. (36).

Finally, consider the momentum distribution function

\[
\rho(k) = \sum_{x=-\infty}^{\infty} e^{-ikx} \rho(x). \tag{37}
\]

Due to the exponentially decaying term in the asymptotic expression Eq. (36), the function \( \rho(k) \) is continuous with all its derivatives for all \( k \). Combining the short distance representation Eqs. (15)-(22) and the long distance expansion (36) we plot \( \rho(k) \) for \( 0 \leq k \leq \pi \) at different filling factors \( \rho \) in Fig. 3. Note that the smoothness of \( \rho(k) \) in the spin disordered regime, considered here, is in contrast with the Luttinger regime considered in Ref. [3], where \( d\rho(k)/dk \) is singular at the Fermi momentum \( k_F = K/2 \), in accordance with the Luttinger theorem [11]. Another peculiarity of the spin disordered regime is that \( d\rho(k)/dk \) is peaked around \( k = 2k_F \) as it can be seen in Fig. 3. This can be viewed as a mild violation of the Luttinger theorem for this system.

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FIG. 3: Momentum distribution function $\rho(k)$ (thick line) and its derivative $-d\rho(k)/dk$ (dotted line) for different filling factors $\rho$: (a) $\rho = 1/8$ (b) $\rho = 1/4$ (c) $\rho = 0.45$ (d) $\rho = 0.49$. The Fermi-Dirac distribution (thin line) corresponding to these filling factors is shown for comparison. The function $\rho(k)$ satisfies $\rho(k) = \rho(-k)$.

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