1D half–filled paramagnetic Hubbard model.
The Luttinger critical exponents

N. I. Chashchin*

Ural State Forestry University
Ekaterinburg, Sibirskii trakt 37, 620100 Russia

Abstract

The electronic system of the 1D Hubbard model is not stable due to Peierls instability; the correlations are strong even for the weak Coulomb interaction. The resulting strongly correlated state without Landau quasi–particle excitations is known as the Luttinger liquid. Critical exponents of a power–law dependence of correlation functions at low energies differ substantially for the Luttinger and Fermi liquids. In this paper we evaluate two critical exponents that define non–trivial behavior of the density of electronic states at low frequencies and the momentum distribution of the occupation number nearby $k_F$.

**Keywords:** 1D Hubbard model, Luttinger liquid, electronic spectrum, momentum distribution, critical exponents.

1.Introduction

Originally, the Hubbard model (HM) was introduced for describing electron’s correlations in narrow energy bands of transition metals. In particular, a first theoretical picture of the Mott metal–insulator transition due to one–site Coulomb electron–electron interaction had been presented. Subsequently it turned out to be very useful and convenient model for

*E–mail: nik.iv.chaschin@mail.ru
studying strongly correlated systems, their transport properties, band collapsing and mass enhancement at the Fermi level (heavy fermions) and so on.

In last decades numerous materials appeared with a quasi one-dimensional structure such as carbon nanotubes (graphene) and organic one-dimensional conductors, where an electron’s motion over the lattice is limited by their self-interaction, i.e., correlations. The physics of interacting electrons in 1D is significantly different from that in higher dimensions. The correspondence between interacting electrons and correlated fermionic quasiparticles, which is the core of Fermi liquid (FL) theory, breaks down in 1D. The resulting strongly correlated state without Landau quasiparticle excitations known as the Luttinger liquid (LL) cannot be treated by conventional FL methods. Charge and spin excitations of the bosonic type become a determinant factor and specify the behavior of the system at low energies.

In 1968 Lieb and Wu (LW) published the rigorous solution of the problem based on the Bethe ansatz [1]. They showed that half-filled HM has an antiferromagnetic ground state without Mott transition for any values of the one-site Coulomb electron–electron interaction. However, in this approach not all important physical parameters can be calculated, e.g., structure factors, magnetic and charge susceptibilities, and other correlation functions. In particular, an important question that cannot be answered by LW solution: if HM is the Fermi liquid or the Luttinger liquid?

All solutions of the 1D HM can be roughly divided in two main groups. The first group represents rigorous results, based on the Bethe ansatz approach, but they give almost no informations of correlation functions. The second group represents solutions that were found by numerical simulations, renormalization group approach, bosonization method. All of them allow to get some useful information about correlation functions, but those approaches are not quite rigorous.

Most impressive results were achieved by the bosonization method [2, 3, 4, 5, 6]. The gist of the method consists in rewriting an initial Hamiltonian with a linearized fermion dispersion into pair of uncoupled oscillators of collective charge and spin modes, and then the subsequent procedure of diagonalizing. It was showed that the system has power-law–dependence of the correlation functions with certain critical exponents. In the spinless limit only the one dimensionless constant K serves as an effective strength’s measure of the interaction between correlated electrons: K=1 corresponds to a non–interacting Fermi gas, K<1 to repulsion, and K>1 to attraction. The Luttinger parameter K and critical
exponents are closely connected. In the spinless Tomonaga–Luttinger (TL) model [2] the
momentum distribution function and the density of one–particle states (DOS) have the
following asymptotic forms: \( n(k) \propto (k_F - k)^{2\alpha} \) \( (k \approx k_F) \), \( \rho(\omega) \propto |\omega|^{2\alpha} \) \( (\omega \approx 0) \) with the
same critical exponents

\[
\alpha = (K + K^{-1} - 2)/4
\]

for both of them. In real 1D structures the constant \( K \) is the key parameter characterizing
the behaviour of any system under consideration, and it is a quite difficult problem to get the
parameter analytically [7], numerically, and experimentally [8, 9]. That is because constant
\( K \) is hidden in power–law–dependencies of observable theory’s functions.

The purpose of our work is to get the LL solution of 1D paramagnetic HM without the
bosonization scheme and the linearization of free electronic spectra; to calculate the critical
exponents for the momentum distribution \( n(k) \) and DOS \( \rho(\omega) \), and then to estimate the
Luttinger constant \( K \) for different generic Coulomb interactions.

We have at our disposal an alternative vigorous instrument, namely the set of integral
equations derived in our previous works [10, 11] by the method of the generating functional
of Green’s functions with the subsequent Legendre transformation. This technique was
successfully applied to the single–impurity Anderson model and the HM [12, 13]. As was
shown, the results well agreed with the solutions obtained by other methods, and that verify
the scheme.

2. Model and Method

In the simplest form – half–filled and symmetrical – the Hamiltonian of the Hubbard
model is written as

\[
\mathcal{H} = -t \sum_{\langle i,j \rangle} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow},
\]

where \( U \) is the parameter of the Coulomb interaction at a site; \( c_{i\sigma} \) (\( c^\dagger_{i\sigma} \)) annihilates (creates)
an electron with spin up and down \( \sigma = \uparrow, \downarrow \); \( n_{i\sigma} \) is the one–site density operator; \( t \) is the
parameter of hopping of electrons from site to site; in the designation \( \langle i, j \rangle \) sites are adjacent.

In our earlier articles [10, 11] we developed the detailed procedure of the deriving of
equations for partition functions. A closed system of equations in variational derivatives
determine the partition function as a functional of the inverse of free Green’s functions:
\[ Z = Z[G_{\sigma}^{-1}, G_{\sigma}^{-1}] \]. Each multiparticle GF can be obtained as an multiple variational derivative of \( Z \) with respect to the corresponding \( G^{-1}_{\sigma} \), therefore the functional \( Z \) or better \( \Phi = \ln Z \) is viewed as the generating functional of GFs.

The simple iteration solution with respect to \( U \) gives well–known Feynman diagrams; the identical procedure with respect to the hopping parameter \( t \) gives the series, where the atomic GF is the leading element. The follow–on Legendre transformation of those equations \[12, 13\] brings us to coupled nonlinear integral equations for propagators \( N = G_{\uparrow} + G_{\downarrow} \) and \( M = G_{\uparrow} - G_{\downarrow} \). Here we have adapted them to the problem under consideration: the paramagnetic half–filled HM with one sub–lattice and the free electronic energy spectrum as \( \varepsilon_k = -2t \cos(k) \) (henceforth we will suppose \( 2t = 1 \)). The momentum \( k \) lies within the limits \( k \in [-\pi, \pi] \), \( k_F = \pi/2 \), and the space symmetry of the model allows to make an obvious suggestion \( f(k) = f(-k) \) for each function of the theory. In this case we have

\[
\frac{1}{N_{\text{at}}} \sum_k f(k) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(k) \, dk = \frac{1}{\pi} \int_{0}^{\pi} f(k) \, dk . \tag{2.2}
\]

Thus, we arrive at two coupled sets of equations which are controlling correlated fermions and bosons in the system.

The system of equations below describes fermions:

\[
\begin{align*}
\Im N(k, \omega) &= \frac{2 \Im \Sigma(k, \omega)}{\omega - \varepsilon_k - \Re \Sigma(k, \omega)} + \frac{\Im \Sigma(k, \omega)}{\omega - \varepsilon_k - \Re \Sigma(k, \omega)} , \\
\Im \Sigma(k, \omega) &= -\frac{U}{2\pi} \int_{0}^{\pi} \left[ 1 - \tanh\left(\frac{\varepsilon_q}{2T}\right) \tanh\left(\frac{\varepsilon_q - \omega}{2T}\right) \right] \Im Q(q - k, \varepsilon_q - \omega) \, dq , \\
\Re \Sigma(k, \omega) &= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\Im \Sigma(k, \omega')}{\omega' - \omega} \, d\omega' ; \\
\Im \Sigma(k + \pi, -\omega) &= \Im \Sigma(k, \omega) , \\
\Re \Sigma(k + \pi, -\omega) &= -\Re \Sigma(k, \omega) , \\
\Im N(k + \pi, -\omega) &= \Im N(k, \omega) .
\end{align*}
\tag{2.3}
\]

In Eqs. \[2.3\] the imaginary \( \Im \Sigma \) and real \( \Re \Sigma \) parts of the electronic self–energy, related by means of the Kramers–Krönig relation, directly determine the analytical expression of the
particle’s number propagator $\Im N$. The last relations in the set show the useful symmetrical properties of the functions with respects to the $k$ and $\omega$.

The bosonic charge excitations are determined by the following equations:

\[
\begin{align*}
\Im Q(q, \Omega) &= \frac{-U^2 \Im \Pi(q, \Omega)}{\left[1 + \frac{U^2}{2} \Re \Pi(q, \Omega) \right]^2 + \left[\frac{U^2}{2} \Im \Pi(q, \Omega) \tanh\left(-\frac{\Omega}{2T}\right)\right]^2}, \\
\Im \Pi(q, \Omega) &= \frac{1}{4\pi} \int_0^\pi \left[1 - \tanh\left(\frac{\epsilon_k}{2T}\right) \tanh\left(\frac{\epsilon_k - \omega}{2T}\right)\right] \Im N(k - q, \epsilon_k - \Omega) \, dk, \\
\Re \Pi(q, \Omega) &= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\tanh\left(\frac{\Omega'}{2T}\right) \Im \Pi(q, \Omega')}{\Omega' - \Omega} \, d\Omega'; \\
\Im \Pi(q + \pi, -\Omega) &= \Im \Pi(q, \Omega), \quad \Re \Pi(q + \pi, -\Omega) = \Re \Pi(q, \Omega), \\
\Im Q(q + \pi, -\Omega) &= \Im Q(q, \Omega).
\end{align*}
\]

(2.4)

In Eqs. (2.4) singular functions $\Pi(q, \Omega)$ and $Q(q, \Omega)$ are the charge bosonic self-energy and excitation’s propagator correspondingly. Note that both coupled sets of Eqs. (2.3, 2.4) have the same structure; they are mathematically identical within the obvious substitutions: $\Im N \leftrightarrow \Im Q$, $\Re \Sigma \leftrightarrow \Re \Pi$, and $\Im \Sigma \leftrightarrow \Im \Pi$.

3. Results and Discussion

An elaborated computer program allows to calculate the imaginary parts of the GFs — $\Im N(k, \omega)$, $Q(q, \Omega)$, and the real parts we recieve from the Kramers–Krönig relations.

Taking into account (2.2), we write the DOS at one spin direction in a standard form:

\[
\rho(\omega) = -\frac{1}{2\pi N_{\text{at}}} \sum_k \Im N(k; \omega) = -\frac{1}{2\pi^2} \int_0^\pi \Im N(k; \omega) \, dk.
\]

(3.1)

Graphics of the $\rho$s for $U = 0, 0.5, 1.0, 2.0$ are shown in Fig.1; the vestiges of van Hove singularities at $\omega \approx 2t (= 1)$ are noticeable even for $U > 0$. A critical exponent $\gamma$ of the function $\rho(\omega) \approx |\omega|^{2\gamma}$ nearby $\omega = 0$ can be estimated as

\[
2\gamma = \frac{\ln \rho(\omega)}{\ln |\omega|} \bigg|_{\omega \to 0}.
\]

(3.2)
Figure 1: Densities of one-electron states $\rho(\omega)$ for different $U$. When $U$ increases, the energy width of states is smoothly extended, but for $U > 0$ the dependence of functions at $\omega \approx 0$ is almost unchanged, and here $\rho(0) \simeq 0$.

The calculated function $\gamma = \gamma(U)$ is depicted in Fig.4.

The energy spectra express a distribution of single-particle fermionic excitations in the $k$-space, $E_k = E(k)$. For strongly correlated system they display a number of visible features which distinguish the correlated electrons from the free ones. The electronic band spectrum $E(k)$ is determined from the following dispersion equation:

$$E_k - \varepsilon_k - \Re \Sigma(k, E_k) = 0.$$  \hspace{1cm} (3.3)

The results of calculations we observe in Fig.2. On increasing $U$ the band width is decreasing, and the inset exhibits the distinct jump at $k_F$ due to Peierls instability, as it should be in the theory.

The analytical expression of the momentum distribution functions $n(k)$ is:

$$n(k) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} f_F\left(\frac{\omega}{2T}\right) \Im N(k, \omega) \, d\omega,$$  \hspace{1cm} (3.4)

where $f_F$ is the Fermi function.

Graphics of functions $n(k)$ for the different values $U$: 0, 0.5, 1.0, 2.0 are presented in Fig.3. The unbroken continuity of the functions $n(k)$ at $k_F$ explicitly illustrates the absence of fermionic quasi-particles; in the FL $n(k)$ has a jump at $T=0$ with an amplitude
Figure 2: Correlated electronic band spectra $E(k)$ for different $U$. As expected, on increasing $U$ the band width is decreasing. The inset exhibits the distinct jump at $k_F$ due to Peierls instability.

$$Z = n(k_F - 0) - n(k_F + 0) \neq 0.$$ The critical exponent $\alpha$ of the function $|n_{k_F} - n_{k}| \approx |k_F - k|^{2\alpha}$ nearby $k = k_F$ can be estimated as:

$$2\alpha = \frac{\ln[n(k) - n(k_F)]}{\ln|k - k_F|} \bigg|_{k \sim k_F}.$$ (3.5)

The calculated function $\alpha = \alpha(U)$ is depicted in Fig.4. We see that the $\alpha$- and $\gamma$-critical exponents practically coincide only for very small $U \leq 0.2$. Further on, their values are decreasing to $\alpha \approx 0.44$ and $\gamma \approx 0.48$. Unlike the TL solution, there is a persistent difference between them, though quite small one: $< 0.05$. In accordance with (1.1) we get the Luttinger constant in the form

$$K = 1 + 2\alpha - 2\sqrt{\alpha + \alpha^2}.$$ (3.6)

Thus, we have the LL solution for all admissible Coulomb interactions, and what is more, for very small $U < 0.1$ the difference from the FL behaviour is more perceptible: $K \sim 0.26$ ($U < 0.1$), $K \sim 0.30$ ($U > 1.0$). Only the required paramagnetic solution $\langle (n_{\uparrow} - n_{\downarrow})^2 \rangle \geq 0$ stipulates the range of variability of Coulomb interaction $U \leq 3.0$. 

7
Due to Peierls instability there is a visible unsmoothness for $k \leq k_F$. In contrast to the FL we have $Z = n(k_F - 0) - n(k_F + 0) = 0$ for $U>0$. The jump is reduced to a power law functions $|n_{k_F} - n_k| \approx |k_F - k|^{2\alpha}$, which implies the LL behaviour.

Figure 4: Critical exponents versus Coulomb interaction U. Graphics $\alpha$ and $\gamma$ represent critical exponents for the functions $n(k \sim k_F)$ and $\rho(\omega \sim 0)$ correspondingly. Unlike the TL solution there is a difference between them for $U>0.25$. 

Figure 3: The momentum distribution in the occupation number for different U and T=0.
References

[1] Lieb E.H., Wu F.Y.: The one–dimensional Hubbard model. Phys.Rev.Lett. 1968, vol.20, pp.1445–1448.

[2] J.M.Luttinger: An exact soluable model of many fermion system. J.Math.Phys., 1963, vol.4, No.9.

[3] F.D.M. Haldane: Luttinger liquid theory of one-dimensional quantum fluids: I. properties of the Luttinger model and their extension to the general 1D interacting spinless Fermi gas. J. Phys. C, 14:2585–2609, 1981.

[4] J.Voit: A brief introduction to Luttinger liquids. arXiv:1212.1632v1 [cond-mat.str-el], 5 May 2000.

[5] J. von Delft and H. Schoeller: Bosonization for Beginners – Refermionization for Experts. Ann. Phys. (Leipzig) vol.7, p.225, 1998.

[6] Götz S.Uhrig: Correlated fermionic systems: Fermi Liquid and Luttinger liquid. Universität zu Köln, Koeln, Germany. Wintersemester 2004/2005.

[7] G. Benfatto and V. Mastropietro: On the density-density critical indices in interacting Fermi systems. Comm. Math. Phys., 231:97–134, 2002.

[8] J.K.Kühne, I.V.Protopopov, Y.oreg, and A.D.Mirlin: Measuring the Luttinger liquid parameter with shot noise. arXiv:1506.07553v1 [cond-mat.str-el], 24 Jun 2015.

[9] T.Müller, R.Thomale, B.Trauzettel, E.Bocquillon, and O.Kashuba: Dynamical transport measurement of the Luttinger parameter.... arXiv:1701.03050v1 [cond-mat.str-el], 11 Jun 2017.

[10] N.I.Chaschin: Variational derivative equations for the partition functions of the Hubbard and Anderson models. The Physics of Metals and Metallography, 2011, vol.111, No.3, p.221;

[11] N.I.Chaschin: Legendre transformation in Hubbard and Anderson models. The Physics of Metals and Metallography, 2011, vol.111, No.4, p.329;
[12] *N.I.Chaschin*: Symmetrical Hubbard model in the $D = \infty$ limit. Low-temperature paramagnetic solution. The Physics of Metals and Metallography, 2012, vol.112, No.6, p.533;

[13] *N.I.Chaschin*: Ground state of the one-dimensional half-filled Hubbard model. The Physics of Metals and Metallography, 2016, vol.117, No.7, p.663