Tomonaga–Luttinger parameters for doped Mott insulators

Satoshi Ejima\textsuperscript{1}, Florian Gebhard\textsuperscript{1} and Satoshi Nishimoto\textsuperscript{2}

\textsuperscript{1} Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg, Germany
\textsuperscript{2} Institut für Theoretische Physik, Universität Göttingen, D-37077 Göttingen, Germany

PACS. 71.10.Fd – Lattice fermion models (Hubbard model, etc.).
PACS. 71.30.+h – Metal-insulator transitions and other electronic transitions.
PACS. 71.10.Hf – Non-Fermi-liquid ground states, electron phase diagrams and phase transitions in model systems.

Abstract. – The Tomonaga–Luttinger parameter $K_{\rho}$ determines the critical behavior in quasi one-dimensional correlated electron systems, e.g., the exponent $\alpha$ for the density of states near the Fermi energy. We use the numerical density-matrix renormalization group method to calculate $K_{\rho}$ from the slope of the density-density correlation function in momentum space at zero wave vector. We check the accuracy of our new approach against exact results for the Hubbard and XXZ Heisenberg models. We determine $K_{\rho}$ in the phase diagram of the extended Hubbard model at quarter filling, $n_c = 1/2$, and confirm the bosonization results $K_{\rho} = n_c^2 = 1/4$ on the critical line and $K_{\rho}^{\text{CDW}} = n_c^2/2 = 1/8$ at infinitesimal doping of the charge-density-wave (CDW) insulator for all interaction strengths. The doped CDW insulator exhibits exponents $\alpha > 1$ only for small doping and strong correlations.

Quasi one-dimensional correlated electronic systems offer the unique opportunity of a detailed comparison between theory and experiment. Some models for correlated lattice electrons can be solved exactly, e.g., the XXZ Heisenberg chain and the Hubbard model, and many of the physical properties of Hubbard-type models are known from analytical and numerical studies. Moreover, their low-energy properties turn out to be universal, i.e., they belong to the generic class of Tomonaga–Luttinger liquids (TLL). It has been a challenge to detect the signatures of TLL in experiments on metallic single-walled carbon nanotubes \cite{1}, anisotropic transition-metal oxides like PrBa\textsubscript{2}Cu\textsubscript{4}O\textsubscript{8} \cite{2}, Bechgaard salts like (TMTSF)\textsubscript{2}ClO\textsubscript{4} \cite{3}, and TTF-TCNQ \cite{4}.

The low-energy properties of TLL are characterized by few quantities, most notably the TL parameter $K_{\rho}$ which determines the long-range behavior of the density-density correlation function and the exponent $\alpha$ for the density of states $D(\omega)$ near the Fermi energy \cite{5},

$$D(\omega \rightarrow 0) \sim |\omega|^\alpha \ , \ \alpha = (K_{\rho} + K_{\rho}^{-1} - 2)/4 .$$

A value $\alpha \gtrsim 1$ was estimated for TTF-TCNQ \cite{4} and in early works on (TMTSF)\textsubscript{2}ClO\textsubscript{4} \cite{3} which would imply $K_{\rho} \lesssim 3 - 2\sqrt{2} \approx 0.17$. More recent measurements report $K_{\rho} = 0.23$ for (TMTSF)\textsubscript{2}ClO\textsubscript{4} \cite{6} and $K_{\rho} = 0.24$ for PrBa\textsubscript{2}Cu\textsubscript{4}O\textsubscript{8} \cite{2}. In the Hubbard model, $K_{\rho}^H \geq 1/2$ so that $\alpha^H \leq 1/8$. Therefore, if electronic correlations are indeed responsible for the algebraic
behavior of the density of states near the Fermi energy, $\alpha > 1/8$ is only possible when the long-range parts of the Coulomb interaction are taken seriously. Unfortunately, the calculation of $K_\rho$ for correlated-electron models is very difficult.

In this work we employ the density-matrix renormalization group (DMRG) method for a reliable numerical calculation of the TL parameter. In order to demonstrate our approach we consider $N$ interacting spin-1/2 electrons on a chain with an even number $L$ sites. The electron density is $n_\uparrow = n_\downarrow = n/2 = N/(2L)$. In the absence of a Peierls dimerization, the extended Hubbard model provides an appropriate description for correlated electron systems in one dimension,

$$\hat{H} = -t \sum_{l,\sigma} \left( \hat{c}_{l,\sigma}^\dagger \hat{c}_{l+1,\sigma} + \hat{c}_{l+1,\sigma}^\dagger \hat{c}_{l,\sigma} \right) + U \sum_l \hat{n}_{l,\uparrow} \hat{n}_{l,\downarrow} + V \sum_l (\hat{n}_l - n)(\hat{n}_{l+1} - n) ,$$

(2)

where $\hat{c}_{l,\sigma}^\dagger$ ($\hat{c}_{l,\sigma}$) is the creation (annihilation) operator of an electron with spin $\sigma$ on site $l$, $\hat{n}_{l,\sigma} = \hat{c}_{l,\sigma}^\dagger \hat{c}_{l,\sigma}$ is the number operator, and $\hat{n}_l = \hat{n}_{l,\uparrow} + \hat{n}_{l,\downarrow}$. Moreover, $t$ is the electron transfer integral between neighboring sites, $U$ is the strength of the Hubbard interaction, and the nearest-neighbor interaction $V$ models the long-range part of the electrons' Coulomb repulsion.

The density-density correlation function is defined by the ground-state expectation value

$$C^{NN}(r) = \frac{1}{L} \sum_{l=1}^L \langle \hat{n}_{l+r} \rangle - \langle \hat{n}_{l+r} \rangle \langle \hat{n}_l \rangle ,$$

(3)

where $\hat{n}_{l} = \sum_{\sigma} \hat{n}_{l,\sigma}$ counts the electrons on site $l$. We have $C^{NN}(r) = C^{NN}(-r)$ due to inversion symmetry, and periodic boundary conditions apply.

Using conformal field theory it can be shown [7,8] that the asymptotic behavior for $1 \ll r \ll L$ is given by

$$C^{NN}(r) \sim -\frac{K_\rho}{(\pi r)^2} + \frac{A \cos(2k_F r)}{r^{1+K_\rho}} \ln^{-3/2}(r) + \cdots ,$$

(4)

where $k_F = n\pi/2$ is the Fermi wave number, and $A$ is a constant. For spinless Fermions, the first term should be multiplied by 1/2. Field theory further predicts [9] $K_\rho(V_c(U); n_c) = n_c^2/2$ for an interaction-driven metal-insulator transition. For example, we have $K_\rho(V_c(U); 1/2) = 1/4$ for the CDW transition in the quarter-filled extended Hubbard model. In contrast, for the density-driven metal-insulator transition the value from field theory is $K_\rho(V > V_c(U), n_c^-) = n_c^2/2$, e.g., for the extended Hubbard model field theory predicts $K_\rho(V > V_c(U), 1/2^-) = 1/8$ in the infinitesimally doped CDW phase at quarter filling.

As seen from the exactly solvable cases discussed below, we expect that $K_\rho(U,V; n_c - \delta)$ can be expanded in a Taylor series in the doping $\delta = n_c - n \ll 1$,

$$K_\rho(U,V; n_c - \delta) = \frac{n_c^2}{2} + \frac{\delta}{h(U,V)} + \cdots .$$

(5)

Moreover, since the critical line is a line of Kosterlitz–Thouless transitions, we expect that the prefactor diverges exponentially in the vicinity of the critical line,

$$h(V \to V_c(U)^+) \sim \exp \left( \frac{C}{(V - V_c(U))^2} \right) .$$

(6)
Therefore, close to the critical line the value $K_\rho = n_c^2/2$ of the CDW insulator cannot be observed for finite doping.

Field theory does not quantify the convergence radius of (5) or the region in which (6) holds. To answer this question, the TL parameter must be calculated for the extended Hubbard model with accurate numerical methods. We can extract $K_\rho$ via Fourier transformation,

$$\tilde{C}^{NN}(q) = \sum_{r=1}^{L} e^{-iqr} C^{NN}(r),$$

with $0 \leq q < 2\pi$. By construction, $\tilde{C}^{NN}(q = 0) = 0$. For the derivative at $q = 0$ one finds in the thermodynamic limit $[10, 11]$

$$K_\rho = \pi \lim_{q \to 0} \frac{\tilde{C}^{NN}(q)}{q}.$$  (8)

In numerical simulations we treat finite systems. There, Eq. (8) translates into

$$K_\rho = \lim_{L \to \infty} \frac{L}{2} \tilde{C}^{NN}\left(\frac{2\pi}{L}\right).$$  (9)

Several groups have calculated the density-density correlation function in position space for Hubbard-type models. After Fourier transformation they obtained $K_\rho$ from (9), see, e.g., $[10–13]$. The main problem of this approach lies in the accurate calculation of $C^{NN}(r)$ from (3) for large distances. The accuracy of the correlation function becomes worse as the distance $r$ increases which severely limits the precision of the Fourier transform $\tilde{C}^{NN}(q)$, especially for small $q$.

In this work we calculate $\tilde{C}^{NN}(2\pi/L)$ directly in momentum space. To this end we define

$$N(q) = \frac{1}{L} \langle \Psi_0 | \hat{n}(q) \hat{n}(-q) | \Psi_0 \rangle$$  (10)

for $q = 2\pi m/L$ ($m \geq 1$), where $\hat{n}(q)$ is given by

$$\hat{n}(q) = \hat{n}^+(-q) = \sum_{l,\sigma} e^{-iqlr_c} \hat{c}_{l,\sigma} \hat{c}_{l,\sigma}.$$

Here, $r_c = (L + 1)/2$ denotes the central position of the chain. Note that $N(q)$ and $\tilde{C}^{NN}(q)$ are different. It is only in the thermodynamic limit, when boundary effects are absent, that they become identical. Therefore,

$$K_\rho(L) = \frac{L}{2} N\left(\frac{2\pi}{L}\right), \quad K_\rho = \lim_{L \to \infty} K_\rho(L).$$  (12)

The important idea is to target not only the ground state in the DMRG procedure but also the state $|\Psi_q\rangle = \hat{n}(-q) |\Psi_0\rangle$. In this way, a precise DMRG calculation of $N(q)$ and of $K_\rho$ from (12) becomes possible.

We illustrate the accuracy of our method for the Hubbard model $[V = 0$ in (2)], for which $K_\rho(U; n)$ is known from the Bethe Ansatz solution [8]. We investigate systems with $L \leq 128$ and open boundary conditions. The number of density matrix states kept is $m = 1500$, so that the maximum truncation error is $3 \times 10^{-6}$.
In Fig. 1, we show $K_{\rho}(L)$ as a function of the inverse system size for several values of $U/t$. The band filling is fixed at $n = 0.1$, which, apart from the limit $n \to 1$, is the most difficult parameter region in this model because $K_{\rho}$ changes significantly as a function of the interaction strength. For all values $U > 0$, $K_{\rho}(L)$ is found to decrease monotonically as a function of inverse system size, so that we can extrapolate $K_{\rho}$ to the thermodynamic limit systematically by performing a least squares fit of $K_{\rho}$ to a polynomial in $1/L$.

In Fig. 1b we compare our results for $K_{\rho}^{\text{DMRG}}$ with those from Bethe Ansatz for various fillings and interaction strengths. The relative error $|K_{\rho}^{\text{DMRG}} - K_{\rho}^{\text{exact}}| / K_{\rho}^{\text{exact}}$ is below 0.3% for all DMRG data shown. We reproduce the exact results with a much better accuracy than exact diagonalization [8], the DMRG method [11] based on the Fourier transformation formula (8), and the calculation of $K_{\rho}$ from the compressibility and the charge velocity [14].

For the Mott–Hubbard transition at $U_{c} = 0^+ \pm \frac{\pi}{L}$ the Taylor expansion (6) applies [15] $(n_{c} = 1, f(U) = h(U, 0))$

$$f(U) = \frac{4}{\ln 2} \int_{1}^{\infty} \frac{dx}{\sqrt{x^2 - 1} \sinh(2 \pi x / U)} , \quad f(U \to 0) \sim \exp\left(-\frac{2 \pi t}{U}\right) . \quad (13)$$

Fig. 2 shows our results for the infinitesimally doped Mott–Hubbard insulator, $n_{h} = 2/L$, for various values of the interaction strength. The approach is valid because we calculate $N(2\pi/L)$ so that the momentum $q = 2\pi / L$ transferred from the ground state $|\Psi_{0}\rangle$ to $|\Psi_{q}\rangle$ is of the same order of magnitude as the phase shifts induced by the introduction of two holes. For $U \geq 2t$ our systems are larger than the correlation length of the system, and we reproduce $K_{\rho}(U > 0, n \to 1) = 1/2$ numerically. Finite-size effects become prominent for $U \to 0$, and it is difficult to recover the exact value from numerical calculations in that limit.

As our second test we study the extended Hubbard model at quarter filling, $n = 1/2$, for $U = \infty$, which can be mapped onto the exactly solvable Heisenberg XXZ chain. The parameter $K_{\rho}$ for the Hubbard model at $U = \infty$ from the Bethe Ansatz is $(V \leq V_{c} = 2t)$

$$K_{\rho} = \frac{\pi}{4 \arccos[-V/(2t)]} . \quad (14)$$
Figure 2 – $K_\rho(L)$ as a function of the inverse system size for the infinitesimally doped Mott–Hubbard insulator, $n = 1 - 2/L$, for various interaction strengths. It extrapolates to the exact value $K_\rho = 1/2$ for all $U/t$.

In Fig. 3, we show $K_\rho$ as a function of $V$ for $U = \infty$ together with the exact result. For this system we use periodic boundary conditions because $m = 2000$ density-matrix eigenstates are enough to calculate $K_\rho(L)$ with high precision, and finite-size effects are much smaller.

Figure 3 – Left: TL parameter $K_\rho$ for the extended Hubbard model at $U/t = \infty$, $V \leq 2t$ from DMRG (stars) and exact Bethe Ansatz (full line). Inset: $K_\rho(L)$ as a function of inverse system size for periodic boundary conditions.

Right: Contour map for the TL parameter $K_\rho$ in the $U$-$V$ plane of the extended Hubbard model at quarter filling. The bold line represents the boundary of the metal-insulator transition. The infinitesimally doped charge-density-wave insulator (CDW) has $K_\rho = 1/8$. The shaded area indicates the region with an exponentially small gap.
for periodic than for open boundary conditions, see the inset in Fig. 3a. Relative errors $|K_{\rho}^{\text{DMRG}} - K_{\rho}^{\text{exact}}|/K_{\rho}^{\text{exact}}$ are below 0.5%, even for $V = 1.95t$ where the system is close to the CDW insulator. Again, the predictions (13), (14) of field theory apply. Here, the Bethe Ansatz solution [16, 17] gives $n_c = 1/2$, $2g(V) = h(\infty, V)$, $\cosh(\gamma) = V/V_c$

$$g(V) = \frac{1 + 2\sum_{n=1}^{\infty}(-1)^n / \cosh(n\gamma)}{1 + 2\sum_{n=1}[1 - \tanh(n\gamma)]},$$

(15)

$$g(V \to V_c) = \frac{2\pi}{\ln 2} \exp \left( -\frac{\pi^2}{2\sqrt{2(V/V_c - 1)}} \right).$$

(16)

As an application, we study the extended Hubbard model at quarter filling. In Fig. 3b, we show the phase diagram together with the contour lines for the TL parameter $K_{\rho}$. Three different phases are found, namely, a ‘superconducting phase’ ($K_{\rho} > 1$), a metallic phase ($1/4 \leq K_{\rho} \leq 1$), and a $4k_F$-CDW insulator beyond the critical line. The results are in good agreement with previous works [18, 19].

On the CDW transition line we find $K_{\rho} = 1/4$, and $K_{\rho}^{\text{CDW}} = 1/8$ for the infinitesimally doped CDW insulator, in agreement with field theory [9]. The parameter region where finite-size effects are prominent due to an exponentially small gap is shaded in Fig. 3b. Outside this region we can determine the TL parameter reliably.

The results for $\delta = 1/24 \approx 4\%$ are shown in Fig. 4 as a function of $V/t$ for $U/t = 6, 10, \infty$ at filling $n = 11/24$ (from top to bottom). The full line is the result (13). The dashed horizontal line marks $K_{\rho} = 3 - 2\sqrt{2} \approx 0.17$. Inset: $U/t = \infty$ for fillings $n = 21/48, 22/48, 23/48$ (from top to bottom).

The results for $\delta = 1/24 \approx 4\%$ are shown in Fig. 4 as a function of $V/t$ for $U/t = 6, 10, \infty$. Deep in the CDW phase ($U/t \gtrsim 5$, $V/t \gtrsim 6$) neither $U$ nor $V$ have a large influence on $K_{\rho}$. Fig. 4 also shows, however, that $K_{\rho} < 0.17$ and thus $\alpha > 1$ requires very large interaction strengths, or very small doping, $\delta \lesssim 2\%$.

In conclusion, we developed an accurate numerical DMRG method to obtain the TL parameter $K_{\rho}$ for Hubbard-type models. We demonstrated its accuracy for the Hubbard model and the XXZ Heisenberg chain (spinless fermions). We presented an accurate phase diagram
of the $t$-$U$-$V$ model at quarter filling and verified the field-theoretical predictions for $K_{\rho}$. We also showed that a critical exponent $\alpha > 1$ is only possible for a lightly doped CDW insulator with a sizable gap.

***

We thank E. Jeckelmann, R.M. Noack, and F.H.L. Essler for useful discussions. S.E. is supported by the Honjo International Scholarship Foundation.

References

[1] Lee J., Eggert S., Kim H., Kahng S.-J., Shinohara H. and Kuk Y., Phys. Rev. Lett., 93 (2004) 166403.
[2] Takenaka K., Nakada K., Osuka A., Hori S., Ikuta H., Hirabayashi I., Sugai S. and Mizutani U., Phys. Rev. Lett., 85 (2000) 5428.
[3] Bourbonnais C., Creuzet F., Jérôme D., Bechgaard K. and Moradpour A., J. Phys. (Paris) Lett., 45 (1984) L755; Wzierek P., Creuzet F., Bourbonnais C., Jérôme D. and Moradpour A., J. Phys. (Paris) I, 3 (1993) 171.
[4] Sing M., Schwingenschlögl U., Claessen R., Blaha P., Carmelo J.M.P., Martelo L.M., Sacramento P.D., Dressel M. and Jacobsen C.S., Phys. Rev. B, 68 (2003) 125111.
[5] For a review, see Voit J., Rep. Prog. Phys., 58 (1995) 977.
[6] Vescoli V., Deiorgi L., Henderson W., Grüner G., Starkey K.P. and Montgomery L.K., Science, 281 (1998) 1181, and references therein.
[7] Frahm H. and Korepin V.E., Phys. Rev. B, 42 (1990) 10553.
[8] Schulz H.J., Phys. Rev. Lett., 64 (1990) 2831.
[9] Giamarchi T., Physica B, 230-232 (1997) 975; Giamarchi T. and Millis A.J., Phys. Rev. B, 46 (1992) 9325; Schulz H.J., Strongly Correlated Electronic Materials, edited by K.S. Bedell et al. (Addison–Wesley, Reading) 1994, p. 187.
[10] Dzierzawa M., The Hubbard Model, edited by Baeriswyl D., Campbell D.K., Carmelo J.M.P., Guinea F. and Louis E., Vol. NATO ASI Series B 343 (Plenum Press, New York) 1995, p. 327.
[11] Noack R.M., Daul S. and Kneer S., Density-Matrix Renormalization, edited by Peschel I., Wang X., Kaulke M. and Hallberg K. (Springer, Berlin) 1999, p. 197.
[12] Daul S. and Noack R.M., Phys. Rev. B, 58 (1998) 2635.
[13] Clay R.T., Sandvik A.W. and Campbell D.K., Phys. Rev. B, 59 (1999) 4665.
[14] Ejima S., Gebhard F., Nishimoto S. and Ohta Y., cond-mat/0411151.
[15] Kawakami N. and Yang S.-K., Phys. Lett. A, 148 (1990) 359; Phys. Rev. B, 44 (1991) 7844.
[16] Des Cloizeaux J. and Gaudin M., J. Math. Phys., 7 (1966) 1384.
[17] Yang C.N. and Yang C.P., Phys. Rev., 150 (1966) 327.
[18] Mila F. and Zotos X., Europhys. Lett., 24 (1993) 133.
[19] Sano K. and Ôno Y., Phys. Rev. B, 70 (2004) 155102.