Violation of the Luttinger sum rule within the Hubbard model on a triangular lattice

J. Kokalj\(^1\) and P. Prelovšek\(^{1,2}\)

\(^{1}\) J. Stefan Institute, SI-1000 Ljubljana, Slovenia
\(^{2}\) Faculty of Mathematics and Physics, University of Ljubljana, SI-1000 Ljubljana, Slovenia

Received: July 11, 2008/ Revised version: date

Abstract The frequency-moment expansion method is developed to analyze the validity of the Luttinger sum rule within the Mott-Hubbard insulator, as represented by the generalized Hubbard model at half filling and large \(U\). For the particular case of the Hubbard model with nearest-neighbor hopping on a triangular lattice lacking the particle-hole symmetry results reveal substantial violation of the sum rule.

PACS. 71.10.-w Theories and models of many-electron systems – 71.27.+a Strongly correlated electron systems; heavy fermions – 71.18.+y Fermi surface: calculations and measurements; effective mass, \(g\) factor

1 Introduction

The concept of a Fermi liquid (FL) is the basic one for the understanding of electrons in solid state. The central pillar of the FL theory is the existence of a Fermi surface with a volume unchanged by electron-electron interactions, having the firm support in the Luttinger sum rule (LSR) \(^{1,2,3}\). In last two decades experiments on novel materials with strongly correlated electrons, in particular superconducting cuprates \(^4\), and theoretical analyzes of corresponding microscopic electronic models revived the question of the possible limitations and the breakdown of the LSR.

The LSR within a paramagnetic metal relates the density of electrons to the Fermi surface (k space) volume defined by poles of the Green’s function (GF) \(G(k, \omega = 0)\). Only recently it has been recognized that the concept can be generalized to insulators \(^5,6\) whereby the corresponding ‘Luttinger’ surface is defined by the zeros of \(G(k, 0) = 0\). It has been shown that the LSR is indeed satisfied for models with a particle-hole symmetry at half filling, and in particular for the frequently invoked Hubbard model on a one-dimensional (1D) chain and on a 2D square lattice \(^7\). There are several indications that in the absence of particle-hole symmetry the LSR can be generally violated \(^7,8\) although no explicit example emerging from a microscopic model with a repulsive Coulomb interaction term and within the canonical ensemble (assuming fixed particle density) has been presented so far. On the other hand, such cases seem to be found for a Hubbard model on an inhomogeneous lattice and on a homogeneous lattice with odd number of sites close to half filling \(^9\). Recently, the present authors pointed out on the generalization of the LSR to finite systems of interacting electrons \(^10\). Since the original proof \(^2,11\) of the LSR remain valid even for small systems, this allows an alternative way to show and understand a possible breakdown of LSR. So far, results confirm cases of violation in restricted (nonperturbative) models as the \(t-J\) model, whereas reachable systems and discussed model regimes did not provide a clearcut violation within the translationally symmetric Hubbard model \(^10\).

In this paper we analyze in more detail the validity of the LSR within the insulating state emerging from a single-band metal via the Mott-Hubbard mechanism of strong electron-electron repulsion. As the prototype model we use the Hubbard model on triangular lattice with the large onsite repulsion \(U \gg t\). We develop an approach employing the expansion of frequency moments in powers of \(t/U\) to determine the value of the \(G(k, 0)\) leading to the location of the Luttinger surface \(G(k_L, 0) = 0\). The method is valid in the thermodynamic limit (for an infinite system) but can be tested as well on small systems, which can provide also required static quantities as input. While the method confirms the validity of LSR in Hubbard models with a particle-hole symmetry \(^7\), we further concentrate on the Hubbard model on a triangular lattice as the case without the latter symmetry. Results show that the LSR is violated substantially for large \(U/t\), being an indication for analogous violation in more general Mott-Hubbard insulators without particle-hole symmetry.

For simplicity we restrict in the following our discussion to the single-band Hubbard model on a general lattice

\[
H = - \sum_{i \neq j} t_{ij} c_{i \sigma}^\dagger c_{j \sigma} + U \sum_{i} n_{i \uparrow} n_{i \downarrow},
\]

where \(U\) is the local Coulomb repulsion, while as the inter-site hopping \(t_{ij}\) we can consider besides the nearest neighbor (n.n.) term \(t_{ij} = t\) also extended model, e.g., with the next-nearest neighbor (n.n.n.) hopping \(t_{ij} = t’\). We are interested in the regime of large enough \(U \gg t_{ij}\) and half filling \(n = 1\), where the ground state is insulating with a Mott-Hubbard gap separating both Hubbard bands. Reduced models, such as the
2 Large $U$ expansion

The central quantity for the LSR is the GF at temperature $T = 0$, given by

$$G(k, \omega) = -i \int_{-\infty}^{\infty} dt e^{i(\omega + \nu)t} \langle 0| c_{k} c_{k}^{\dagger}(t)|0 \rangle$$

$$+ i \int_{0}^{\infty} dt e^{i(\omega + \nu)t} \langle 0| c_{k}(t) c_{k}^{\dagger}|0 \rangle,$$

(2)

where $\nu$ is the chemical potential. Representing the GF in terms of the spectral function

$$G(k, \omega) = \int_{-\infty}^{\infty} A(k, \omega') d\omega',$$

(3)

We deal with the insulator with real $G(k, \omega \sim 0)$ and a large gap $\Delta \sim U$ separating regions of nonzero spectral functions $A(k, \omega)$. In order to evaluate the relevant $G(k, 0)$ we separate contributions

$$G(k, 0) = G^{-}(k, 0) + G^{+}(k, 0) =$$

$$= \int_{-\infty}^{\mu} A(k, \omega') d\omega' + \int_{\mu}^{\infty} A(k, \omega') d\omega'$$

(4)

Since $\mu \sim U/2$ it is reasonable to expand both $G^{-}(k, 0)$ and $G^{+}(k, 0)$ in powers of $(t_{ij}/U)^n$.

Let us first consider $G^{-}$,

$$G^{-}(k, 0) = \sum_{n=0}^{\infty} \left( \frac{2}{U} \right)^{n+1} \int_{-\infty}^{\mu} A(k, \omega') (\omega' - \tilde{\mu})^n d\omega' =$$

$$= \sum_{n=0}^{\infty} \left( \frac{2}{U} \right)^{n+1} \sum_{m=0}^{n} M^{-n-m}_m(k) \left( \frac{n}{m} \right) (-\tilde{\mu})^m,$$

(5)

where $\tilde{\mu} = \mu - U/2$. Note that $M^{-}_m(k)$ are frequency moments which can be directly expressed in terms of the equal-time expectation values within the half-filled ground state $|0\rangle$ involving $l$ commutators with $H$,

$$M^{-}_l(k) = \langle [H, \ldots [H, c_{k}^{\dagger}]] c_{k} \rangle.$$

(6)

Analogous procedure can be repeated for $G^{+}$ with the result

$$G^{+}(k, 0) = \sum_{n=0}^{\infty} \left( \frac{2}{U} \right)^{n+1} \sum_{m=0}^{n} M^{+n-m}_m(k) \left( \frac{n}{m} \right) (\tilde{\mu})^m,$$

$$M^{+}_m(k) = \langle c_{k} [H', \ldots [H', c_{k}^{\dagger}]] \rangle,$$

(7)

where $H' = H - U(N_e - N)$, with $N_e$ being electron-number operator and $N$ is the number of sites in the system. $G^{+}$ is also tightly related to $G^{-}$ with the particle-hole transformation, as discussed later.

Let us now present first two moments explicitly,

$$M^{-}_0(k) = \langle c_{k} c_{k}^{\dagger} \rangle = n_{ks},$$

$$M^{-}_1(k) = \langle c_{k} \rangle n_{ks} + \frac{U}{N} \sum_{ij} e^{-i(k(t_{ij}) + \delta)} \langle c_{k}^{\dagger} n_{is} c_{js} \rangle,$$

$$M^{+}_1(k) = \langle c_{k} (1 - n_{ks}) + \frac{U}{N} \sum_{ij} e^{-i(k(t_{ij}) + \delta)} \langle c_{k}^{\dagger} (n_{is} - 1) c_{js} \rangle,$$

(8)

where $\delta(k)$ is the free band $(U = 0)$ dispersion as determined by hopping parameters $t_{ij}$.

One expects that for large $U \gg t_{ij}$, $M^{-}_1$ is of the order of $t_{ij}^4$, at least for lowest orders $l$, as well as $\mu \propto t_{ij}$. Hence the series Eq. (4) should be well converging. To show that $M^{-}_1 \propto t_{ij}^4$, we employ at this stage the well known canonical transformation of the Hubbard model for large $U$ [11,12,13], with which the number of doubly occupied sites becomes a good quantum number. This leads at half-filling, $n = 1$, to an effective spin model [12] and at finite doping to strong coupling (SC) model for the lowest orders [13].

$$H_{ef} = e^{S} H e^{-S}, \quad a_{is} = e^{S} c_{is} e^{-S}.$$  (9)

Within the lowest order of the $t_{ij}/U$ expansion one gets $S = S^1$.

$$S^1 = -\frac{1}{U} \sum_{t_{ij}s} t_{ij} n_{is} c_{is}^{\dagger} c_{js} (1 - n_{js}) - (1 - n_{is}) c_{is}^{\dagger} c_{js} n_{js}.$$  (10)

Transforming expressions for moments (8) and using Eq. (10), we arrive to explicit expressions at $n = 1$.

$$M^{-}_0(k) = \frac{1}{2} \pm \frac{1}{U} \sum_{\delta} \varepsilon_{\delta}(k)[\langle S_{\delta} \cdot S_{0} \rangle - \frac{1}{4} + O(t_{ij}^2/U),$$

$$M^{+}_1(k) = \frac{\varepsilon(k)}{2} + \frac{1}{U} \sum_{\delta} \varepsilon_{\delta}(k)[\langle S_{\delta} \cdot S_{0} \rangle - \frac{1}{4} + O(t_{ij}^2/U),$$

(11)

where $\varepsilon_{\delta}(k)$ refers to partial 'free' bands corresponding to particular neighbors (n.n., n.n.n. etc.), respectively

$$\varepsilon_{\delta}(k) = -t_{\delta} \sum_{t_{js}} e^{i(kr_{js})}.$$  (12)

We note that spin correlations $\langle S_{\delta} \cdot S_{0} \rangle$ in Eq. (11) are to be evaluated in the ground state of $H_{ef}$ and that such state does not contain doubly occupied sites.
2.1 Particle-hole symmetry

Let us now return to $G^+$. In order to show that its moments are closely related to $M_i^-$, it is very instructive to realize that $G^+$ can be obtained from $G^-$ with particle-hole transformation, which changes $c_i \rightarrow c_i^\dagger$ and vice versa. Applying the transformation to $G^+$ in Eq. (2) we note that also the ground state $|0\rangle$ changes to $|\bar{0}\rangle$, corresponding to transformed $H$. $H$ is obtained from $H$ by replacing $t_{ij} \rightarrow -t_{ij}$ and adding the extra potential term $U(N - N_e)$. We therefore arrive to the following expression for $G^+$,

$$G^+(k, 0) = i \int_{-\infty}^{\infty} d\epsilon e^{i(U-\mu)\epsilon} \langle \bar{0}| c_{k\downarrow}^\dagger e^{iHt} c_{k\uparrow} e^{-iHt}|0\rangle. \quad (13)$$

which is analogous to $G^-$ in Eq. (2). One can then continue by analogy to $G^-$ using the unitary transformation with $\bar{S}$, which is the same form as $S$ with $-t_{ij}$ instead of $t_{ij}$. State, for which expectation value must be calculated, is now the ground state of $\bar{H}_{ef}$. Moreover, for half filling at $n = 1$, $H_{ef}$ contains only spin operators, whereby odd spin terms (also odd terms of $t_{ij}$) are forbidden by the isotropy of original Hamiltonian, and $\bar{H}_{ef} = H_{ef} [12]$, and therefore also ground states of them are the same. Finally we can relate

$$G^+(k, 0) = -\bar{G}^-(k, 0) \bar{\mu} \rightarrow -\bar{\mu}, \quad (14)$$

where $\bar{G}^-$ stands for $G^-$ with $t_{ij}$ changed to $-t_{ij}$ and $\bar{\mu} \rightarrow -\bar{\mu}$. Eq. (14) confirms that $M_i^+$ are simply related to $M_i^-$ as already seen from relations (11).

Expressions are so far valid for general hopping $t_{ij}$, with the only assumptions that we are dealing with the paramagnetic state with total spin $S = 0$ and without broken translational symmetry.

2.2 Chemical potential

We are interested in the case of Mott-Hubbard insulator at half filling, $n=1$ and within the canonical ensemble the chemical potential $\mu$ should be determined from the grand partition function by first fixing the number of particles in the system and then taking the limit $T \rightarrow 0$. Such a procedure gives an unique value for $\mu$ in the middle of the gap [8][14][15], and works as well for finite systems [10]. Different limits with $\mu$ being anywhere within the Mott-Hubbard gap have been also recently considered [8][9]. Our procedure simply locates $\mu$ (as well as in any finite system with $N_e$ particles [10]) with the ground state energies of systems with one electron more and less, respectively [8][14][15],

$$\mu = \frac{(E_0^{N_e+1} - E_0^{N_e-1})}{2} \quad (15)$$

where for half-filling $N_e = N$. Since the ground state of one hole for $H_{ef}$ does not contain doubly occupied sites, we get $E_0^{N_e-1} = O(t_{ij})$. On the other hand, ground state with one added electron more contains one doubly occupied site and therefore $E_0^{N_e+1} = U + O(t_{ij})$. $\mu$ is therefore within the gap and approximately $\mu \sim U/2$. Energies $E_0^{N_e+1}$, $E_0^{N_e-1}$ as well as $\mu$ might be expanded analytically in terms of $t_{ij}/U$, however we use furtheron numerical results instead.

3 Results

Using expanded moments (11) in $G^-$ (5) and Eq. (14) for $G^+$, we finally get for the total GF (4),

$$G(k, 0) = \frac{4}{U^2} \sum_{\delta} 4\varepsilon_{\delta}(k) \langle S_\delta \cdot S_0 \rangle - \bar{\mu} + O\left(\frac{t_{ij}^2}{U^2}\right), \quad (16)$$

From Eq. (4) and (14) one can also conclude, that for $\bar{\mu} = 0$, GF consists only of odd terms in $t_{ij}$.

It has been already realized [7], that the LSR remains valid for cases with particle-hole symmetry, where $H = \bar{H}$. This follows also from our analysis. If we assume in Eq. (16) only nearest neighbors and put $\bar{\mu} = 0$, which is the consequence of the particle-hole symmetry, GF changes sign at same k as $\varepsilon(k)$. Within the lowest order in $t_{ij}/U^2$, this leads to the same Luttinger volume as for noninteracting fermions.

In order to find cases where the LSR might be violated, we turn to systems without the particle-hole symmetry. Here, in general $\bar{\mu} \neq 0$ and also $\varepsilon(k)$ is not negative for exactly half of the Brillouin zone. Then, Eq. (16) seem to suggest that the LSR must be violated in most cases, since the perfect cancellation of two quite different terms in Eq. (16) looks quite improbable. In the following, we show that such compensation indeed does not occur for one of simplest non-symmetric cases, i.e. within the Hubbard model with only n.n. hopping on the triangular lattice.

3.1 Hubbard model on a triangular lattice

Furtheron we consider the model with n.n. hopping only, $t_{ij} = t$. To check the LSR on triangular lattice at least to lowest order in $t/U$, some quantities are needed. Free band dispersion $\varepsilon(k)$ is given with Eq. (12) and equals $\varepsilon_1(k)$. Spin correlations $C_\delta = \langle S_\delta \cdot S_0 \rangle$ should be evaluated in the ground state of $H_{ef}$ at half-filling. Within the first order in $t^2/U$ this corresponds just to the Heisenberg model on a triangular lattice. The value for n.n. spin correlations in Heisenberg model has been evaluated by a number of authors [16][17][18] and $C_1 \approx -0.182$. This value is quite insensitive to finite $t^2/U$, e.g. we obtain within the Hubbard model on $N = 15$ sites $-C_1 \approx 0.183 - 0.189$ for $t^2/U = 0.05 t \rightarrow 0.02 t$.

The chemical potential $\bar{\mu}$ is more delicate quantity. Here, we estimate $\bar{\mu}$ as accurate as possible by calculating $E_0^{N_e+1}$ and $E_0^{N_e-1}$, performing the exact diagonalization of finite clusters using the Lanczos algorithm. Lattices with periodic boundary conditions are chosen in such way, that they allow three-sublattice order [16] and have a minimal imperfection [19], that is zero for all chosen lattices, except for $N=18$ it is 2. The maximum size for the Hubbard model is $N = 15$, for which we present $\bar{\mu}$ in Fig. 1. Fortunately, for larger $U/t$ the Hubbard model can be well represented by the SC model (equivalent to the $t-J$ model additionally including three-site correlated hopping term of the order $t^2/U$) [13]. As seen in Fig. 1 $\bar{\mu}$ calculated from the Hubbard model and from the SC model for $N = 15$ match well for small $t^2/U < 0.05$. This gives support to the values obtained for $\bar{\mu}$ within the SC model, as presented in Fig. 1 for systems up to $N = 24$.

In considering $\bar{\mu}$ one should take into account that at large $U/t$ the Nagaoka ferromagnetic state is possible, i.e., $E_0^{N_e+1}$
corresponds to $S = N/2$ or at least not to $S = 0, 1/2$. In Fig.1 we therefore present results only within the regimes of lowest $S$. In finite systems the onset of Nagaoka state shows a size dependence and moves to lower values $t^2/U$ with increasing sizes. From our analysis we can estimate, that the paramagnetic state with $S = 0$ (for even $N + 1$) remains stable at least for $t^2/U > 0.025t$. Taking mentioned limitations into account, we can analyse results in Fig.1 which give $\tilde{\mu} \sim -0.19t + 6.8t^2/U \pm 0.1t$ for $0.025t < t^2/U < 0.05t$. Unfortunately, the proper finite size scaling cannot be performed since lattice shapes as well as $S$ are not the same for different $N$ therefore the uncertainty is an estimate.

Before presenting the final result, we comment on the higher order corrections to Eq. (16) on a triangular lattice. With the use of particle-hole transformation we can show that for $\tilde{\mu} = 0$ there is no correction of order $t^2/U^3$ and the next correction of order $t^3/U^4$ can be presented as

$$G(k, 0)_{\tilde{\mu}=0} = \frac{16}{U^2} \epsilon(k) |S_\delta \cdot S_0| + B(k) \frac{t^3}{U^4}. \quad (17)$$

We evaluate $B(k)$ for some $k$ with the use of numerical calculations on $N = 12$ site Hubbard cluster. $B(k)$ is obtained by the expansion of numerically calculated GF for the range $U = 60t - 120t$. Results are presented in Table 1. A relevant observation is that the higher order correction is small in vicinity of the Luttinger surface for large enough $U > 20t$. Moreover, the correction is negative and suggests (even) smaller Luttinger volume, which is the tendency towards larger LSR violation.

### Table 1. Numerically obtained expansion coefficients.

| $k$          | $B(k)$     |
|--------------|------------|
| $(0, 0)$     | $-2320 \pm 40$ |
| $(2\pi/3, 0)$ | $-167 \pm 3$  |
| $(\pi, \pi/\sqrt{3})$ | $200 \pm 5$  |
| $(4\pi/3, 0)$ | $1810 \pm 40$ |

In conclusion, we presented evidence that the LSR is violated on triangular lattice for half-filled Hubbard band in regime of large $U/t$. Clearly we should stress again limitations to our analysis and results. First, $U/t$ must be large enough so that the ground state corresponds to an insulator with a Mott-Hubbard gap which is the case for the Hubbard model on triangular lattice at $U \sim 12t$ [20]. On the other side, at very large $U/t$ the onset of Nagaoka instability appears for the $N+1$ ground state. In absence of other studies we estimate that this can happen only for $U > 40t$.

Finally, let us speculate on the origin of the violation of the LSR. A frequent mechanism for the latter is related to the breakdown of the paramagnetic state or the loss of translational symmetry, in a microscopic system connected with a phase transition and the onset of the corresponding long-range order. Besides discussed Nagaoka instabilities possible at very large $U/t$, within the triangular lattice another possibility is the
long-range antiferromagnetic order which has been established within the Heisenberg model \[16\] but so far not within the Hubbard model at half filling \[21\]. The onset of such order would limit the relevant \( U/t \) parameter window of the paramagnetic insulating state. On the other hand, any breaking of translational symmetry is expected to change entirely the Fermi surface topology and not to partially reduce its volume as found in our study.

More radical conclusion would be that the LSR is generally violated within the Mott-Hubbard insulators without the particle-hole symmetry \[7,8\], and in particular within the insulating state of the Hubbard model on a triangular lattice. We note that the main formal requirement for the validity of the LSR \[1\] is the adiabatic development of the ground state (i.e. of the free energy in the limit \( T \to 0 \), where the LSR becomes applicable) with the increasing electron-electron repulsion. Hubbard model is perturbative in \( U \) and adiabatically connected to the noninteracting fermion system at least for weak \( U/t \). On the other hand, the metal-insulator transition at \( U = U_c \) seems to represent a point, where the perturbation theory as well as LSR breaks down. Such scenario is still far from obvious so further studies in this direction are needed.

References

1. J.M. Luttinger, J.C. Ward, Phys. Rev. \textbf{118}(5), 1417 (1960)
2. J.M. Luttinger, Phys. Rev. \textbf{119}(4), 1153 (1960)
3. A.A. Abrikosov, L.P. Gorkov, I.E. Dzyaloshinski, \textit{Methods of quantum field theory in statistical physics} (Dover Publ, NY, 1975)
4. T. Yoshida et al., Phys. Rev. B \textbf{74}(22), 224510 (2006)
5. I. Dzyaloshinskii, Phys. Rev. B \textbf{68}(8), 085113 (2003)
6. R.M. Konik, T.M. Rice, A.M. Tsvelik, Phys. Rev. Lett. \textbf{96}(8), 086407 (2006)
7. T.D. Stanescu, P. Phillips, T.P. Choy, Phys. Rev. B \textbf{75}, 104503 (2007)
8. A. Rosch, Eur. Phys. J. B \textbf{59}(4), 495 (2007)
9. J. Ortollof, M. Balzer, M. Potthoff, Eur. Phys. J. B \textbf{58}, 37 (2007)
10. J. Kokalj, P. Prelovsek, Phys. Rev.B \textbf{75}(4), 045111 (2007)
11. A.B. Harris, R.V. Lange, Phys. Rev. \textbf{157}(2), 295 (1967)
12. A.H. MacDonald, S.M. Girvin, D. Yoshioka, Phys. Rev. B \textbf{37}(16), 9753 (1988)
13. H. Eskes, A.M. Oleš, M.B.J. Meinders, W. Stephan, Phys. Rev. B \textbf{50}(24), 17980 (1994)
14. J.P. Perdew, R.G. Parr, M. Levy, J.L. Balduz, Phys. Rev. Lett. \textbf{49}(23), 1691 (1982)
15. T. Kaplan, J. Stat. Phys. \textbf{122}, 1237 (2006)
16. B. Bernu, C. Lhuillier, L. Pierre, Phys. Rev. Lett. \textbf{69}(17), 2590 (1992)
17. L. Capriotti, A.E. Trumper, S. Sorella, Phys. Rev. Lett. \textbf{82}(19), 3899 (1999)
18. T. Koretsune, M. Ogata, Phys. Rev. Lett. \textbf{89}(11), 116401 (2002)
19. P.R.C. Kent, M. Jarrell, T.A. Maier, T. Pruschke, Physical Review B \textbf{72}(6), 060411 (2005)
20. K. Aryanpour, W.E. Pickett, R.T. Scalettar, Phys. Rev. B \textbf{74}(8), 085117 (2006)
21. N. Bulut, W. Koshibae, S. Maekawa, Phys. Rev. Lett. \textbf{95}(3), 037001 (2005)