Breakdown of the Luttinger sum rule within the Mott-Hubbard insulator

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(Received 31 March 2008; revised manuscript received 29 July 2008; published 9 October 2008)

The validity of the Luttinger sum rule is investigated within the prototype tight-binding model of interacting fermions in one dimension, i.e., the t-V model including the next-nearest-neighbor hopping t', in order to break the particle-hole symmetry. Scaling analysis of finite-system results at half filling reveals evident breakdown of the sum rule in the large gap regime at $V \gg t$ while the sum rule appears to recover together with vanishing of the Mott-Hubbard gap.

DOI: 10.1103/PhysRevB.78.153103 PACS number(s): 71.10.−w, 71.27.+a

The Luttinger theorem[1,2] is the essential building block supporting the concept of the Fermi liquid (FL) as formulated by Landau.[3] The Luttinger sum rule (LSR) in a homogeneous system relates the Fermi volume to the density of fermions irrespective of the presence of the electron-electron interactions. Stimulated by experiments on electronic materials with strongly correlated electrons which indicate possible deviations from the FL scenario and from LSR,[4] theoretical studies of the validity of the LSR and its limitations have intensified.

In a metal at $T=0$ the Fermi surface is located by the poles of the Green's function (GF) $G(\mathbf{k},\omega=0)$ and the LSR shows that the Fermi volume being equal to the density of electrons n is unchanged by the interaction. It has been pointed out[5,6] that the original derivation[1] and the LSR can be generalized as well to insulators where the corresponding "Luttinger surface" (LS) is defined by zeros $G(\mathbf{k},0)=0$. Such LSR concept becomes of interest as well as easier to test in strongly interacting electrons and in Mott-Hubbard (MH) insulators in particular. It has been recently applied to spin ladders.[7] On the other hand, there are several indications that LSR might be violated within the MH insulators in general.[8–10] The argument is based on the observation that the LSR is satisfied only for a particular value of chemical potential μ within the MH gap. It has been shown that, for models with the particle-hole (p-h) symmetry, the latter is the case and the LSR is fulfilled.[8] At the same time, it has been realized that the LSR should also apply to finite systems.[11,12] This allows us to test the validity of LSR in nontrivial models of correlated electrons.[13] Based on analytical expansion for $U/t \gg 1$, it has been shown on small systems that within the Hubbard model on a planar triangular lattice (without the p-h symmetry) LSR is indeed violated for a range of parameters.[13]

In this Brief Report, we present results of the numerical study within the prototype model of interacting fermions in one dimension (1D), i.e., the generalized t-V model. The advantage of such a 1D model is that it allows for the finite-size scaling to the thermodynamic limit. Our results show clear violation of the LSR for $V \gg t$ within the MH insulating phase which appears to persist down to critical $V > V_c$ where the MH gap opens.

In the following we study the extended t-V model,

$$H = -t\sum_i (c_{i+1}^\dagger c_i + \text{H.c.}) - t'\sum_i (c_{i+2}^\dagger c_i + \text{H.c.}) + V\sum_i n_i n_{i+1}, \tag{1}$$

where t and t' are nearest-neighbor (n.n.) and next-nearest-neighbor (n.n.n.) hoppings, respectively, and V is the n.n. repulsive interaction between fermions. We are interested in the MH insulator state which appears at half filling with the electron density $n=1/2$. It is well known that the model with $t'=0$ is equivalent to the anisotropic Heisenberg model, which can be solved exactly via Bethe ansatz.[14] The model shows the transition from the metallic state $V < V_c$ to a MH insulator for $V > V_c$ with $V_c = 2t$. Our study is focused on systems with nonzero t', for which there is no exact solution. We choose such a system due to the lack of p-h symmetry since for $t'=0$ the LSR is automatically satisfied for $n=1/2$.[8] In the following we study $t'/t=0.4$ and 0.2 in order to have substantial deviation from the p-h symmetry but at the same time to maintain the simple momentum distribution for noninteracting fermions.

Let us first consider the opening of the MH gap Δ_0 at $n=1/2$. It is well known[14] that within the t-V model the gap opens at $V=2t$ being exponentially small for $V > 2t+$ and nearly linear in V for $V > 4t$ (see Fig. 1). We analyze the effect of t' on Δ_0 by performing the exact diagonalization of chains with $N=14$, 18, 22, 26, and 30 sites using the Lanczos technique. Chains (with periodic boundary conditions) were chosen to have an odd number of electrons $N_e = N/2$ since this leads to a nondegenerate ground state. The MH gap is then determined via

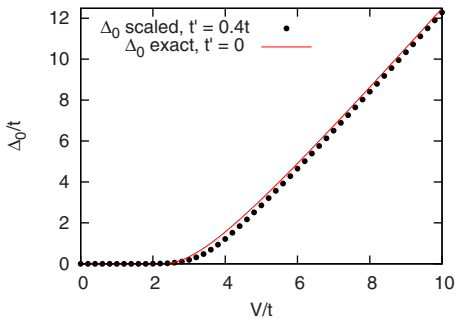

FIG. 1. (Color online) Scaled gap Δ_0 for nonsymmetric case $t'=0.4t$ (points), and exact Bethe ansatz results for $t'=0$ (line).

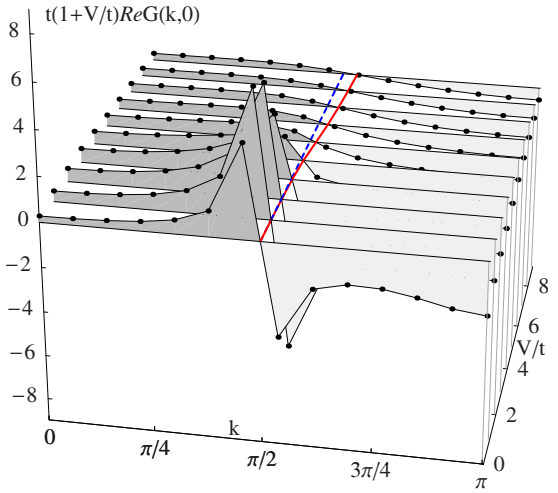

FIG. 2. (Color online) Evolution of Re $G(k,0)$ with increasing interaction V for $t'/t=0.4$ and for half-filled system of $N=26$ sites with allowed wave vectors (points), and indications of $k_F=\pi/2$ (dashed line) and k_L (full line). Points are connected with straight lines.

$$\Delta(N) = (E_0^{N_e+1} - E_0^{N_e}) - (E_0^{N_e} - E_0^{N_e-1}). \tag{2}$$

To obtain the gap in thermodynamic limit as $\Delta_0 = \lim_{N\to\infty} \Delta(N)$, we perform the finite-size scaling for $N=14-30$ using $\Delta(N)=a+b/N+c/N^2$. In the metallic regime, $V<2t$, the gap scales expectedly with $a\sim 0$ and at large $V \gg 2t$ with $b\sim 0$. In general parameters a, b, and c were obtained from least-squares fit. Scaled gap $\Delta_0=a$ for $t'=0.4t$ is shown in Fig. 1 together with the exact Bethe ansatz[14] result for $t'=0$. The result reveals that the gap for a nonsymmetric case deviates only slightly from the exact result for a symmetric case.

The (retarded) Green's function $G(k,\omega)$ at $T=0$ is defined as

$$G(k,\omega) = -i\int_0^\infty dt e^{i(\omega+\mu)t}\langle 0|\{c_k^\dagger, c_k(t)\}_+|0\rangle,$$

where μ is the chemical potential. We are studying finite systems at a fixed number of electrons, $N_e=N/2$. Clearly, the position of μ within the MH gap is crucial for further discussion of LSR.[8,9] Within this approach the correct choice is[15,16]

$$\mu(N) = (E_0^{N_e+1} - E_0^{N_e-1})/2. \tag{3}$$

For LSR Re $G(k,0)$ is important. In order to start with a general perspective, we present in Fig. 2 the evolution of $G(k,0)$ with increasing V. For noninteracting system Re $G(k,0)$ has a singularity at $k_F=\pi/2$ persisting apparently within the metallic state, $V<2t$. This is the normal Fermi-liquid (in 1D Luttinger-liquid) behavior connected with the poles (singularities) of the spectral function $A(k,\omega) = -\mathrm{Im}\, G(k,\omega)/\pi$ approaching $\omega=0$ for $k\to k_F$. With increasing V/t and the opening of the MH gap, the behavior changes qualitatively. Within the gap, $A(k,\omega)=0$; hence $G(k,0)$ has no singularity and goes through zero smoothly at $k\sim\pi/2$. Moreover, for $V>4t$, $G(k,0)$ becomes small for all k. This happens because, at $V\gg t$, $A(k,\omega)$ consists of two nearly equal weights at approximately $\pm V$ and their contributions to the real part of GF almost cancel each other at the chemical potential; therefore $G(k,0)\sim 1/V^2$.[13]

Let us now focus on the LSR and its breakdown. The content of LSR is the precise locus of $k=k_L$, where $G(k,0)$ changes sign[1,2] and k_L is called Luttinger wave vectors.[5] According to the LSR, for the spinless model at $n=1/2$ one should generally have $k_L=\pi/2$ if the topology of the electronic band is not changed qualitatively (which could happen, e.g., for $t'>0.5t$). From Fig. 2 we note that k_L is indeed near $\pi/2$; however, even without finite-size scaling a small deviation $k_L\neq\pi/2$ may be observed for $V>4t$. More accurate analysis with the finite-size scaling is presented below.

To determine k_L in the thermodynamic limit $N\to\infty$, we perform the finite-size scaling of results at various N. Our procedure is as follows. Due to periodic boundary conditions, $k=2\pi l/N$ are allowed. Since we work with the nondegenerate case with odd $N_e=N/2$, $k=\pi/2$ does not appear directly for any system. The closest are, however, $k^-(N) = \pi/2-\pi/N$ and $k^+(N)=\pi/2+\pi/N$. Next we determine μ using Eq. (3) for given N. Then, the GF is evaluated via ED using the Lanczos algorithm for $T=0$ dynamical quantities,[17] i.e., from Eq. (3), we have $G=G^c+G^a$,

$$G^c(k,\omega) = \langle 0|c_k^\dagger(\omega+\mu+E_N^0-H)^{-1}c_k|0\rangle, \tag{4}$$

and analogously to G^a. In particular, we calculate values of GF at $k^\pm(N)$,

$$G^\pm(N) = G_N(k^\pm(N),0), \tag{5}$$

where $G_N(k,\omega)$ stands for the GF of a system size N. These values are used to calculate k_L in the following manner. For each N, we evaluate the mean value $\bar{G}(N)=[G^+(N)+G^-(N)]/2$ and the difference $\Delta G(N)=G^+(N)-G^-(N)$, which later on serve for the evaluation of the derivative $\partial G(k,0)/\partial k$. Next, we perform scaling of both $\bar{G}(N)$ and $\Delta G(N)$ to obtain their values in the limit $N\to\infty$.

Finite-size scaling of $\bar{G}(N)$ is performed by assuming

$$\bar{G}(N) = a_1 + b_1\frac{1}{N} + c_1\frac{1}{N^2}. \tag{6}$$

The quadratic term $c_1\frac{1}{N^2}$ is included in analogy with $\Delta(N)$. For $V\sim 4t$ the linear term $1/N$ is dominant. But with increasing V, parameter b_1 in Eq. (6) decreases and the c_1 term becomes more important. In Fig. 3 values of $\bar{G}(N)$ and obtained scaling from least-squares fit are shown for $t'/t=0.4$ and for two values $V/t=4,10$. As is seen from Fig. 3, the relevant limiting value is $\bar{G}=\lim_{N\to\infty}\bar{G}(N)=a_1$. Note that $a_1=G(\pi/2,0)$ should be zero according to the LSR. Obviously our finding in Fig. 3 that $a_1\neq 0$ is the indication that the LSR is violated.

For the estimate of k_L also the scaling of $\Delta G(N)$ is needed. $G(k,0)$ within an insulator is a continuous function of k; hence $\Delta G(N)$ goes to zero as $N\to\infty$ so that the proper scaling function is $\Delta G(N)=b_2/N+c_2/N^2$. Least-squares fits for the same parameters as in Fig. 3 are shown in Fig. 4. We

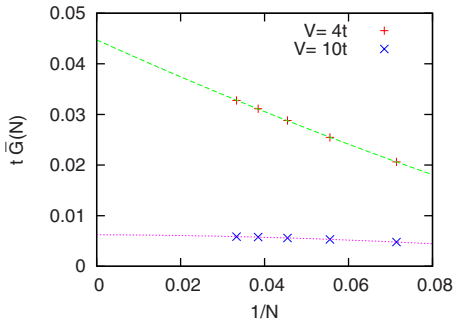

FIG. 3. (Color online) Scaling of $\bar{G}(N)$ for two values of V/t and $t'=0.4t$.

notice that for large $V \gtrsim 10t$ the linear term b_2/N is dominant while for $V \sim 4t$ quadratic correction with c_2 also becomes relevant.

For further analysis the derivative of GF at $\pi/2$ is relevant,

$$\left.\frac{\partial G(k,0)}{\partial k}\right|_{k=\pi/2} = \lim_{N\to\infty} \frac{\Delta G(N)}{2\pi/N} = \frac{b_2}{2\pi}. \tag{7}$$

To calculate the Luttinger momentum k_L for which GF changes sign, we use linear approximation of GF near $\pi/2$ assuming that k_L does not deviate appreciably from $\pi/2$, being indeed the case. The result for k_L may, in our approximation, be written as

$$k_L = \frac{\pi}{2} - \frac{G(\pi/2,0)}{\partial G(k,0)/\partial k|_{k=\pi/2}} = \frac{\pi}{2} - 2\pi\frac{a_1}{b_2}. \tag{8}$$

Final results for two values $t'/t=0.2,0.4$, and within the whole range of parameters V/t are shown in Fig. 5 with corresponding error bars. Presented values of k_L in regime $V>3.6t$ are calculated as described above via Eq. (8). In a window $2<V/t<3.6$ results are not shown since finite-chain calculations become unreliable due to limited wave-vector resolution and deviations from the simple finite-size scaling behavior. On the other hand, within the metallic regime $V<2t$, $G(k,0)$ has singularity near $\pi/2$. Therefore it makes more sense to apply instead a similar scaling analysis to the inverse values of GF, $[\mathrm{Re}\, G(k,0)]^{-1}$, and to locate in this way k_L. Results obtained in this way are shown in Fig. 5 for regime $V<2t$. Our estimate of the error bar in Fig. 5 is given

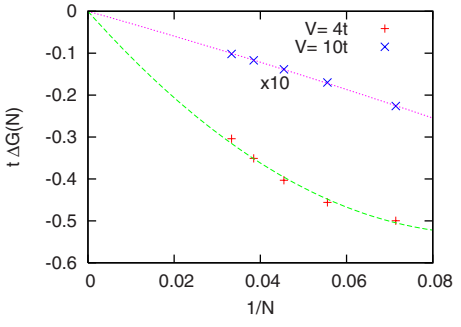

FIG. 4. (Color online) Scaling of $\Delta G(N)$ for two values of V/t and $t'=0.4t$.

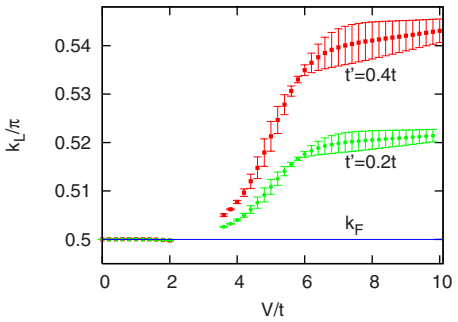

FIG. 5. (Color online) Calculated Luttinger momentum k_L vs V/t for two values of t'/t.

as the larger value obtained either from standard deviations of parameters a_1 and b_2 or from the difference of the scaled value without taking into account the smallest system.

From Fig. 5 it is evident that, at large $V/t>6$, k_L substantially deviates from the LSR prediction $k_F=\pi/2$. The deviation $\Delta k_L = k_L - \pi/2$ from LSR saturates at large $V \gg t$ whereby its value scales with the asymmetry given by t'/t. At the same time, with the decreasing $V/t \to 2$ and with vanishing of the MH gap Δ_0, also Δk_L appears to vanish. In fact, in the regime $2<V/t<6$ the LSR deviation Δk_L seems qualitatively to follow the variation in Δ_0. This is in accordance with our observation that inverse derivative $(-1/b_2)$ has a similar behavior to Δ_0 as a function of V. For large $V>6t$, both b_2 and a_2 behave as $\propto 1/V^2$; hence Δk_L approaches a constant value which could be evaluated via the method of moment expansion.[13] On the other hand, the analysis of data within the metallic phase for $V<2t$ does not show (within our accuracy) any deviation from the LSR $k_F=\pi/2$. Hence, our results are consistent with previous confirmations of the LSR in the metallic phase away from half filling.[18,19]

In conclusion, our results clearly show that the LSR is violated in the Mott-Hubbard insulator within the 1D generalized t-V model where the p-h symmetry is broken via the introduction of the n.n.n. hopping $t' \neq 0$. Although we concentrated only on two values of $t'/t=0.2,0.4$, the behavior is quite generic whereby the violation Δk_L seems to scale with the p-h asymmetry, at least for modest parameter t'/t. It should be stressed that substantially larger t'/t can perturb qualitatively the topology of the noninteracting band and n_k which makes the interpretation more difficult. An important finding is that the violation Δk_L scales as the MH gap Δ_0 on approaching the metallic transition at $V=V_c$ while within the gapless (metallic) phase we do not find any evidence for the LSR violation.

Discussing possible generality of our finding, we first stress several advantages of the extended 1D t-V model analyzed above. Being a spinless model it allows for an accurate enough study of largest systems using the ED (compared, e.g., to the Hubbard model or multiband models), in our case up to $N=30$ sites. A large span of sizes then allows for a reliable finite-size scaling and extrapolation to $N \to \infty$.

Another important ingredient is the absence of a phase with a long-range order in the phase diagram at $n \sim 1/2$. The latter is due to the 1D character of the model and supported by the exact solution at $t'=0$,[14] which is not strongly per-

turbed by moderate t'. Thus we are dealing solely with the MH metal-insulator transition at $V=V_c$ and with its influence on the LSR. Note that in analogous $D>1$ models studied so far, e.g., the two-dimensional (2D) Hubbard model on a square lattice[8,11] or triangular lattice[13] as well as more general MH insulators,[9] the MH insulator is mostly accompanied with an onset of a long-range magnetic ordering while doped MH insulators can show ferromagnetic order, etc. An appearance of the long-range order clearly spoils the translational invariance and thus the validity of the LSR (Ref. 6) or at least requires the reformulation of the latter.

In view of the above discussion, the studied model is just the prototype example of a model with the MH transition and one can expect that in analogy the LSR would be generally violated within the MH insulators without the p-h symmetry, even more if the MH transition is followed with an ordered state breaking the translational or some other symmetry.

A quite open question is, however, the origin of the breakdown of the LSR or more precisely which part of the original proof[1,2,5] becomes invalid within the MH insulator. The basic argument[1] invokes the existence of the functional constructed via the perturbation expansion in the interaction strength. The required adiabatic connectivity[6,8,9] to noninteracting fermions can be clearly questioned at the metal-insulator transition which at least represents a nonanalytic point at $n=1/2$ in the extended t-V model, even at $t'=0$.[14] Moreover, it is evident that zeros $G(k,0)=0$ in the MH gap at the same time require divergent self-energy $\Sigma(k,0)\rightarrow\infty$,[5,8] which enhances doubts on the existence of an appropriate functional. The question is important in connection with the emerging conserving approximations for strongly correlated systems based on a construction of such a functional but also on dynamical-mean-field methods based on approximations for $\Sigma(k,\omega)$.[20,21] In any case, a deeper understanding of the limitations of the validity of LSR is still missing and can provide new insight in the physics of strongly correlated electrons.

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