Topological Approach to Luttinger's Theorem and the Fermi Surface of a Kondo Lattice

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A nonperturbative proof of Luttinger's theorem, based on a topological argument, is given for Fermi liquids in arbitrary dimensions. Application to the Kondo lattice shows that even completely localized spins contribute to the Fermi sea volume as electrons, whenever the system can be described as a Fermi liquid.

PACS numbers: 71.10.Ay, 05.30.Fk, 75.30.Mb

Landau's Fermi liquid theory is among the most important theories in the quantum many-body problem. At zero temperature, a Fermi liquid has a Fermi surface, similar to the noninteracting fermions. One of the most fundamental results on the Fermi liquid is Luttinger's theorem, which states that the volume inside the Fermi surface is invariant by the interaction, if the number of particles is held fixed. Luttinger argued, in his 1960 paper [1], the correction to the volume vanishes order by order in the perturbation expansion.

Recently, there has been renewed interest in Luttinger's theorem. Since Luttinger's original proof was based on the perturbation theory, Luttinger's theorem could be violated by nonperturbative effects. In fact, several claims of possible breakdown of Luttinger's theorem have been reported recently [2-6]. On the other hand, such nonperturbative effects can violate the Fermi liquid theory itself. In fact, the Fermi liquid theory is known to be invalid generally in one dimension, where Tomonaga-Luttinger (TL) liquid is the generic behavior. Although not being a Fermi liquid, a TL liquid in one dimension has a well-defined Fermi surface (actually Fermi points in one dimension). Thus the question of the validity of Luttinger's "theorem" still exists in this case, where Luttinger's original proof certainly does not apply. This question was answered recently by a perturbative proof [7] and a more general nonperturbative proof [8], which can be applied to one-dimensional TL liquids. However, the question on higher (especially two) dimensions remains unanswered. In fact, it is not clear whether a Fermi liquid which violates Luttinger's theorem can exist.

Another interesting problem, which is not answered by the Luttinger's perturbative proof, is the Fermi surface of the Kondo lattice. The Kondo lattice contains a periodic array of localized spins which are coupled to conduction electrons. The Kondo lattice is believed to belong to the Fermi liquid (or TL liquid, in one dimension) in some region of the phase diagram. Even if we assume Luttinger's theorem to be valid, there is a problem in how to count the number of particles. It is rather difficult, by conventional methods, to clarify whether a localized spin should be counted as an electron ("large Fermi surface" picture) or not ("small Fermi surface" picture). In one dimension, the nonperturbative proof of the Luttinger's theorem was also applied to the Kondo lattice [8], to show that the localized spins do participate in the Fermi sea. (See also [9,10] for numerical evidence.) On the other hand, there has been no definite answer for higher dimensions, although there are several results [11,12] supporting the large Fermi surface picture.

The argument in Ref. [8] is a generalization of the Lieb-Schultz-Mattis (LSM) theorem [13], which was given at about the same time as the apparently unrelated Luttinger's theorem [1]. Since the LSM argument itself cannot be applied to higher dimensions, the discussion in Ref. [8] was restricted to one dimension. However, very recently the LSM argument was combined with Laughlin's gauge invariance argument [14] on the quantum Hall effect (QHE) and extended to higher dimensions [15]. Inspired by this observation, we will extend the nonperturbative proof of the Luttinger's theorem to arbitrary dimensions in the present Letter.

We consider an interacting fermion system on a Ddimensional lattice with periodic boundary conditions. We start from a finite system of size $L_x \times L_y \times \cdots \times L_D$, where the length is defined so that the unit cell has the size $1 \times 1 \times \cdots \times 1$. The number of fermions is assumed to be conserved. If the system satisfies a commensurability condition, it can have a finite excitation gap [15]. In this Letter, we will rather focus on the gapless case, which is expected for general incommensurate particle density. For simplicity, let us first start with the case of spinless fermion of single species. We introduce a fictitious electric charge e for each particle, and a coupling to an externally controlled fictitious electromagnetic field. Because of the periodic boundary condition, the system is topologically equivalent to torus. Following Refs. [14,15], we consider an adiabatic increase of a (fictitious) magnetic flux Φ piercing through the "hole" of the torus so that the uniform electric field is induced, say, in the x direction.

While in general the Hamiltonian of the system $H(\Phi)$ depends on the flux Φ reflecting the Aharonov-Bohm (AB) effect, the AB effect is absent when the flux reaches the unit flux quantum $\Phi_0 = hc/e$. We consider the adiabatic increase of the flux from $\Phi = 0$ to $\Phi = \Phi_0$. In the following, we will consider how the total momentum of the

system is changed during the adiabatic process in two different ways, and compare those results. In the remainder of this Letter, we take the units in which $\hbar = 1$, for simplicity.

First, we analyze the momentum change in a system of interacting fermions for general. We remind the reader that the momentum itself is a *gauge dependent* quantity in the presence of the gauge field; a meaningful comparison between momenta can be made only under the same gauge choice. In a simplest gauge choice, the AB flux Φ is represented by the uniform vector potential $A_x = \Phi/L_x$ in the x direction. In this gauge, the Hamiltonian always commutes with the translation operator T_x to the x direction. We further assume that the translation symmetry is not spontaneously broken, as it should not be in a Fermi liquid. Thus the ground state is an eigenstate of the total momentum P_x : $P_x |\Psi_0\rangle = P_x^0 |\Psi_0\rangle$ with the eigenvalue P_x^0 . The x component of the total momentum P_x is related to T_x as $T_x = e^{iP_x}$. After the adiabatic process, the original ground state $|\Psi_0\rangle$ evolves into some state $|\Psi'_0\rangle$. While the state $|\Psi_0\rangle$ could be different from $|\Psi_0\rangle$, it belongs to the same eigenvalue P_x^0 of P_x , because the Hamiltonian always commutes with T_x (and thus P_x) in the uniform gauge [15] during the adiabatic process. Although it naively means that the momentum is unchanged after the adiabatic process, it is not true. The Hamiltonian $H(\Phi_0)$ with the unit flux quantum in the uniform gauge is different from the original one H(0), although the spectrum should be identical. Namely, they correspond to different choices of the gauge for the same physics. In order to get back to the original gauge, we must perform a large gauge transformation [15]

$$U = \exp\left[\frac{2\pi i}{L_x}\sum_{\vec{r}} xn_{\vec{r}}\right],\tag{1}$$

where $n_{\vec{r}}$ is the particle number operator at site \vec{r} , and x is the x coordinate of \vec{r} . This transforms the Hamiltonian $H(\Phi_0)$ back to the original one: $UH(\Phi_0)U^{-1} = H(0)$. After this gauge transformation, the adiabatic evolution of the ground state becomes $U|\Psi'_0\rangle$.

Now we can examine the total momentum P_x of this state, and compare it with the original one P_x^0 . Here we can employ the arguments used in the LSM theorem and its generalizations [8,13]. By using the identity

$$U^{-1}T_{x}U = T_{x}\exp\left[2\pi i\sum_{\vec{r}}\frac{n_{\vec{r}}}{L_{x}}\right],$$
(2)

we see that $U|\Psi'_0\rangle$ is an eigenstate of P_x with

$$P_x = P_x^0 + 2\pi\nu L_y L_z \cdots L_D, \qquad (3)$$

where ν is the particle density (number of particles per unit cell). This result is valid regardless of the interaction strength.

Next, we analyze the momentum change assuming that the system is a Fermi liquid. The Fermi liquid is described in terms of quasiparticles, which are almost noninteracting. More precisely, the low-energy effective Hamiltonian of a Fermi liquid is given by

$$\mathcal{H} \sim \sum_{\vec{k}} \epsilon(\vec{k}) \tilde{n}_{\vec{k}} + \sum_{\vec{k},\vec{k}'} f(\vec{k},\vec{k}') \tilde{n}_{\vec{k}} \tilde{n}_{\vec{k}'}, \qquad (4)$$

where $\tilde{n}_{\vec{k}}$ is the *quasiparticle* number operator of momentum k. Namely, there is an interaction energy due to the second term but no scattering between the quasiparticles. Thus the eigenstates of $\tilde{n}_{\vec{k}}$ are also eigenstates of Hamiltonian. In the ground state, the Fermi sea (region inside the Fermi surface) is completely filled with quasiparticles, while the outside is empty in terms of quasiparticles. Excitations on the ground state are given by quasiparticles outside the Fermi sea and/or quasiholes inside the Fermi sea. In fact, the quasiparticle (or quasiholes) are free from scattering only in the vicinity of the Fermi surface; the very notion of quasiparticle and/or quasihole is useful only in this case. The Fermi liquid theory is valid for the lowenergy phenomena, in which the relevant excitations consist only of quasiparticles (quasiholes) near the Fermi surface.

Let us define the Fermi sea volume $V_F^{(L)}$ in the finite size system $L_x \times L_y \times \cdots \times L_D$. The quasiparticles are scattering free, and their momenta are discretized as in the case of free particles. Thus we can define the Fermi sea volume $V_F^{(L)}$ by an integer "occupation number" of the quasiparticles $N_F^{(L)}$:

$$V_F^{(L)} = \frac{(2\pi)^D N_F^{(L)}}{L_x L_y \cdots L_D}.$$
 (5)

Although the quasiparticles are not free from scattering (and thus are not meaningful) away from the Fermi surface, this expression is still valid because the Fermi sea volume is uniquely determined by its surface. The $V_F^{(L)}$ should approach the true volume of the Fermi sea V_F , in the thermodynamic limit $L_j \rightarrow \infty$.

The adiabatic evolution is determined by the low-energy effective Hamiltonian (4). In the Fermi liquid theory, the charge of the quasiparticle is identical to that of the original particle e. The coupling of the quasiparticles to the uniform vector potential A_x is thus given by the substitution of the momentum $k_x \rightarrow k_x + eA_x/c$ in the Hamiltonian. After the adiabatic insertion of the unit flux quantum, and getting back to the original Hamiltonian by the gauge transformation, each quasiparticle gets a momentum shift: k_x is increased by $2\pi/L_x$. This produces quasiparticles on one side of the Fermi surface, and quasiholes on the opposite side.

Since the result of the adiabatic process is equivalent to the shift of the whole Fermi sea by $2\pi/L_x$, the change of the *x* component of total momentum P_x of the system during the adiabatic process is given by

$$\Delta P_x = \frac{2\pi}{L_x} N_F^{(L)} \,. \tag{6}$$

We note that the only changes after the adiabatic process involve the quasiparticles and quasiholes near the Fermi surface, so that the Fermi liquid theory is still valid. To violate Eq. (6), the system must break some of the properties of Fermi liquid used in the present argument. For example, if a quasiparticle had a charge e' which is different from the charge e of the original particle, we would obtain a different result.

Now, comparing the two results Eqs. (3) and (6) obtained with different arguments, we obtain $N_F^{(L)}/L_x - \nu L_y L_z \cdots L_D$ = integer, where we have used the fact that each component of momenta is defined modulo 2π . Let us choose the system size so that L_x, L_y, \ldots and L_D are mutually prime with the others. We also assume $L_x = ql_x$ where l_x is an integer. (It should be recalled that system size should be an integral multiple of q, to allow the filling factor $\nu = p/q$.) Then, from Eq. (5) we obtain $N_F^{(L)} - pl_x L_y L_z \cdots L_D = L_x \times (integer)$.

Furthermore, we can consider other adiabatic processes, in which the gauge field is induced in one of the other directions y, z, ..., instead of x. Similar calculations for these cases lead to $N_F^{(L)} = L_{\alpha} \times (\text{integer})$, where $\alpha =$ y, z, ..., D. Because we have chosen the lengths L_j 's mutually prime, we conclude that $N_F^{(L)} - pl_x L_y L_z \cdots L_D =$ $nL_x L_y L_z \cdots L_D$, where n is an integer. Writing this in terms of Fermi sea volume, we arrive at

$$\frac{V_F}{(2\pi)^D} - \nu = n,$$
 (7)

where we have replaced the Fermi sea volume $V_F^{(L)}$ for the finite size system by its thermodynamic limit V_F , because this relation is exact already for the finite system. The thermodynamic limit V_F should be independent of our special (mutually prime) choice of L_j 's, if V_F is well defined.

The relation (7) is nothing but the statement of Luttinger's theorem. The integer *n* corresponds to the number of completely filled bands. It is valid also when the Fermi sea consists of several disjoint regions, if V_F is understood as the sum of volumes of all regions. Our proof is much simpler than the original one [1]. Moreover, in contrast to Ref. [1], our argument is nonperturbative and relies only on some of the basic properties of Fermi liquid.

It is straightforward to extend our argument to spinful electrons. When the numbers of up-spin electrons and down-spin electrons are conserved separately, we consider the fictitious electromagnetic field coupled to only up-spin (or down-spin) electrons. Assuming the spinful Fermi liquids, the volume of the Fermi sea V_F^{σ} for spin σ is given by $V_F^{\sigma} = (2\pi)^D \nu_{\sigma}$, where ν_{σ} is the number of particles with spin σ per unit cell. For the spin-symmetric case $\nu_{\uparrow} = \nu_{\downarrow}$, it reads $V_F = V_F^{\uparrow} = V_F^{\downarrow} = (2\pi)^D \nu/2$ where ν is the total particle density $\nu_{\uparrow} + \nu_{\downarrow}$.

As a nontrivial application, let us consider the Kondo lattice. Luttinger's original perturbative proof does not apply to this case, and the question on the volume of the Fermi sea has remained. For the sake of clarity, we consider the Kondo lattice model given by the Hamiltonian

$$H = -\sum_{j,k} t_{jk} c_{j\sigma}^{\dagger} c_{k\sigma} + \text{H.c.} + \sum_{j} U_{j} c_{j\uparrow}^{\dagger} c_{j\uparrow} c_{j\downarrow}^{\dagger} c_{j\downarrow}$$
$$+ \sum_{l} J_{l} \vec{s}_{l} \cdot \vec{S}_{l}, \qquad (8)$$

where $c_{j\sigma}^{\dagger}$ and $c_{j\sigma}$ are standard fermion creation or annihilation operators at site j with spin σ , $\vec{s}_l = c_{l\alpha}^{\dagger} \vec{\sigma}^{\alpha\beta} c_{l\beta}/2$ is the spin operator of the conduction electron, and \vec{S}_l is the localized spin at site l. As in the previous case, we couple the fictitious electromagnetic field only to the up-spin electrons. After the adiabatic insertion of the AB flux of unit flux quantum, we make the gauge transformation as in the previous cases. However, the naive one $U_{\uparrow}^e = \exp[\frac{2\pi i}{L_x}\sum_{\vec{r}} x n_{\vec{r}\sigma}]$, does not bring the Hamiltonian back to the original one, because it changes the Kondo coupling. In order to recover the original Hamiltonian, we must also twist the localized spins. The transformation

$$U_{\uparrow} = \exp\left[\frac{2\pi i}{L_x} \sum_{\vec{r}} x(n_{\vec{r}\sigma} + S_{\vec{r}}^z)\right]$$
(9)

does the required job. We obtain the total momentum after the adiabatic process as

$$P_{x} = P_{x}^{0} + 2\pi [\nu_{\uparrow} + N_{s}(S + m)]L_{y}L_{z}\cdots L_{D}, \quad (10)$$

where N_s is the number of localized spins per unit cell and m is the magnetization per single localized spin. The special contribution proportional to S comes from the boundary term $\exp(2\pi i N_s S_1^z)$ appearing in $U_{\uparrow}^{-1} T_x U_{\uparrow}$, similar to the one-dimensional case [8,13,16].

Thus, provided that the system belongs to a spinful Fermi liquid, the volume of the Fermi sea is given by $V_F^{\sigma} = (2\pi)^D [\nu_{\sigma} + N_s(S \pm m)]$, where \pm takes + for $\sigma = \uparrow$ and - for $\sigma = \downarrow$. For the spin-symmetric case $\nu_{\uparrow} = \nu_{\downarrow}$ and m = 0, we obtain

$$V_F = V_F^{\dagger} = V_F^{\downarrow} = \frac{(2\pi)^D}{2} [\nu + 2N_s S], \quad (11)$$

for the total particle density $\nu = \nu_{\uparrow} + \nu_{\downarrow} = 2\nu_{\uparrow}$. This is exactly what we obtain if we apply the Luttinger's theorem to the Anderson-type model in which the localized spins are represented by electrons. It means that the localized spin *S* does contribute to the Fermi sea volume as 2*S* electrons, even though it is completely immobile. This is the picture conventionally called the large Fermi surface.

It should be noted that we did *not* answer the nontrivial question whether (or when) the Kondo lattice belongs to the Fermi liquid. We have proved only that, if the Kondo lattice is a Fermi liquid (as it is believed to be true in some region of the phase diagram), the localized spins participate in the Fermi sea.

Finally, let us comment on claims [2-6] of the violation of the Luttinger's theorem. There are several possibilities

regarding the apparent contradiction to our nonperturbative proof. Of course, it should be checked whether our argument applies to the model under consideration. However, our argument does apply to a very wide range of lattice models, including the Hubbard and t-J models, for which the violation of the Luttinger's theorem has also been proposed. A possibility is that the system is not a Fermi liquid in these cases. In other words, a violation of the Luttinger's theorem requires the system to be a non-Fermi liquid. We note that, however, merely not being a Fermi liquid is insufficient, as the TL liquid in one dimension does satisfy the Luttinger's theorem [7,8]. Our approach could be extended to a non-Fermi liquid which has an appropriately defined Fermi surface, if such a liquid does exist. Our argument reveals a rigid relationship between the structure of low-energy excitations and the Fermi sea volume.

Another possibility is that the claimed violation of Luttinger's theorem is actually incorrect. In particular, numerical results are available only for restricted system size and/or temperature, and can miss the possibly small singularity at the true Fermi surface. On the other hand, even if they are incorrect in identifying the true Fermi surface, they might still be of physical relevance because the actual experiments are done also at finite energy scale; the experimentally measured "Fermi surface" could be different from the true Fermi surface defined in the low-energy limit, to which our argument applies. In any case, our definite result on the Fermi surface of the Fermi liquid in the low-energy limit would be useful as a guideline. Claims of the violation of the Luttinger's theorem should be examined in the light of the present result.

During the 40 years after the Luttinger's paper [1], several examples of "quantization" of a physical quantity have been found in many-body physics. Namely, despite the complexity of the interacting many-body states, some physical quantity takes a special value which is stable against various perturbations such as interaction strength. Presumably the most natural understanding of such a quantization is given by a topological argument. Indeed, typical examples of the quantization—QHE and the quantized magnetization plateaus—have been related to topological mechanisms [14–16].

Luttinger's theorem perhaps does not look like a quantization, because the volume of the Fermi sea takes continuous values depending on the particle density. However, the insensitivity to the interaction resembles other quantization phenomena, and may well be regarded as a certain kind of quantization, especially when written as in Eq. (7). In fact, we have revealed a close theoretical relationship among Luttinger's theorem, QHE, and magnetization plateaus. In addition, our argument can be related also to the chiral anomaly in quantum field theory [17]. Luttinger's theorem might be actually the first example of the topological quantization discovered in quantum many-body problem, although the topological understanding has been missing for a long time.

I thank Ian Affleck, Hal Tasaki, and Masanori Yamanaka for stimulating discussions which were essential for the present work. This work is supported by Grant-in-Aid from Ministry of Education, Science, Sports, and Culture of Japan.

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