Absence of Luttinger's Theorem due to Zeros in the Single-Particle Green Function

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Absence of Luttinger's Theorem due to Zeros in the Single-Particle Green Function

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We show exactly with an $SU(N)$ interacting model that even if the ambiguity associated with the placement of the chemical potential, μ, for a $T = 0$ gapped system is removed by using the unique value $\mu(T \to 0)$, Luttinger's sum rule is violated even if the ground-state degeneracy is lifted by an infinitesimal hopping. The failure stems from the non-existence of the Luttinger-Ward functional for a system in which the self-energy diverges. Since it is the existence of the Luttinger-Ward functional that is the basis for Luttinger's theorem which relates the charge density to sign changes of the single-particle Green function, no such theorem exists. Experimental data on the cuprates are presented which show a systematic deviation from the Luttinger count, implying a breakdown of the electron quasiparticle picture in strongly correlated electron matter.

While the charge density remains fixed under renormalization from high (UV) to low (IR) energy, precisely what is carrying the charge can change drastically. For example, in QCD, free quarks at UV scales form bound states in the IR. The key signature of bound quark states is that the pole in the propagator is converted to a zero[1], implying the fields in the UV-complete theory no longer propagate at low energy, hence, a breakdown of the elemental particle picture. The conversion of poles to zeros of the single-particle Green function also obtains in superconductivity. In both QCD and superconductivity, the new strongly coupled ground state in the IR lacks adiabatic continuity with the UV-state: free quarks (QCD) or free electrons (superconductivity). The question of how to compute the number of low-energy charged particle states is then problematic because what was a particle (pole) at high energy is no longer so at low energy. It is not surprising then that the only 'theorem', due to Luttinger[2], on the particle density in a fermionic system, makes no distinction between zeros and poles. The precise mathematical statement of Luttinger's theorem for spin-$\frac{1}{2}$ fermions,

$$n = 2\sum_{\boldsymbol{k}} \Theta(\mathrm{Re}G(\boldsymbol{k}, \omega = 0)), \tag{1}$$

sums all momenta, $\boldsymbol{k}$, where the Heaviside step function, $\Theta(\mathrm{Re}G(\boldsymbol{k}, \omega = 0)$ is non-zero, with $G(\boldsymbol{k}, \omega)$ the time-ordered single-particle Green function. The right-hand side of Eq. (1) requires $\mathrm{Re}G(\boldsymbol{k}, \omega = 0) = 0$ or $\mathrm{Re}G(\boldsymbol{k}, \omega = 0) > 0$. The latter obtains either from a pole or a zero of the single-particle Green function. Hence, as far as the mathematics is concerned, poles and zeros of the Green function enter the particle density on the same footing. We show that any statement of this kind in which zeros and poles are treated on equal footing is in error, hence the title of this paper.

While poles of the single-particle Green function represent quasiparticles, zeros[3] are quite different as they indicate the presence of a gap[1]. Equivalently, the self energy diverges, thereby representing a breakdown of perturbation theory. As a result, purported non-perturbative proofs of Luttinger's theorem which assume gapless phases at the outset[4, 5] bear no relevance to the validity of Eq. (1). Rather, such proofs are relevant only to the physical assertion that the volume of the Fermi surface is independent of the interactions—on some level a tautology, since all renormalizations from short-ranged repulsive interactions[6–8] are towards the Fermi surface.

Naively, for gapped incompressible phases at $T = 0$, the chemical potential can be placed anywhere in the gap with impunity. However, as first pointed out by Rosch[9] for a Mott insulator, the placement of the chemical potential will change the energy at which G vanishes and hence affect the particle density. Nonetheless, Farid[10] has argued that the problem arising from this degree of freedom is entirely spurious because the chemical potential even at $T = 0$ is unique, namely the limiting value of μ as $T \to 0$. For the case of the atomic limit of the SU(2) Hubbard model, this limiting procedure places the chemical potential equally far from both bands, the particle-hole symmetric point, and Eq. (1) reduces exactly to $n = 2\Theta(0) = 1$, a result which

[1] The actual zero condition, $\mathrm{Det}[G] = 0$, ensures that zeros are absent if adiabaticity with a band insulator is presents, e. g. mean-field ordered states, (see Appendix).

holds beyond the atomic limit[11]. Farid's claim is interesting then because it would seem to establish a rigorous relationship between a quantity which has no obvious physical import and a conserved one, the particle density. In fact, Rosch[9, 12] has shown that Farid's argument, at least perturbatively in the hopping, is false for a Mott insulator. What would be advantageous is a proof which does not rely on perturbation theory and a general demonstration of precisely where Luttinger's proof goes awry.

We show here exactly using an $SU(N)$ generalization of the atomic limit of the Hubbard model in which N flavors of "iso-spin" and n fermions reside on each site that Farid's[10] placement of the chemical potential does not salvage Eq. (1). The key result is quite simple. For this model, Eq. (1) reduces to

$$n = N\Theta(2n - N) \tag{2}$$

which is clearly not equal to the particle density unless $n \in \{0, N/2, N\}$. Namely, any partially filled band with N odd leads to a violation of Eq. (1). That Eq. (2) actually reduces to the correct result for the SU(2) case is entirely an accident because the Θ function only takes on values of 0, 1/2, or 1. The crux of the problem is that the Luttinger-Ward (LW) functional strictly does not exist when zeros of the Green function are present. Since Eq. (1) relies explicitly on the construction of the LW functional and it does not exist for zeros of the Green function, Luttinger's theorem (Eq. (1)) does not exist.

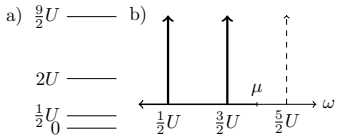

FIG. 1. Schematic of the a) energy levels and b) spectral function for the Hamiltonian $H = \frac{U}{2}(\hat{n})^2$. For $n = 2$, $\epsilon_+ = H(n+1) - H(n) = 5U/2$, $\epsilon_- = H(n) - H(n-1) = 3U/2$, and as a consequence, $\mu = (\epsilon_+ + \epsilon_-)/2 = 2U$.

To illustrate the problem zeros pose for Eq. (1), we consider for simplicity the $SU(N)$ generalization,

$$H = \tfrac{U}{2}(n_1 + n_2 + \cdots + n_N)^2 = \tfrac{U}{2}(\hat{n})^2 \tag{3}$$

of the atomic limit of the Hubbard model. Since our key result hinges only on the existence of zeros, not on the details of a specific model, our conclusion is general. We have not included the site index here as it is superfluous to the many-body physics which is captured entirely by the N-flavors of "iso-spin" that live on a single site. Fig. (1) illustrates the level structure for $N = 3$. We define $K = H(\hat{n}) - \mu\hat{n}$ and write the Green function,

$$G_{\alpha\beta}(\omega) = \frac{1}{Z}\sum_{ab} \mathrm{e}^{-\beta K_a} Q^{ab}_{\alpha\beta}, \tag{4}$$

using the Källén–Lehmann representation, where

$$Q^{ab}_{\alpha\beta} = \frac{\langle a|c_\alpha|b\rangle\,\langle b|c^\dagger_\beta|a\rangle}{\omega - K_b + K_a} + \frac{\langle a|c^\dagger_\beta|b\rangle\,\langle b|c_\alpha|a\rangle}{\omega - K_a + K_b} \tag{5}$$

in which the Green function is a sum of particle addition and removal parts. Here Z is the partition function and $K_a = \langle a|K|a\rangle$. Since K_a is completely determined by the occupancy number $n_a = \sum_\alpha \langle a|c^\dagger_\alpha c_\alpha|a\rangle$ of the SU(N) orbital, we may write $K_a = K(n)$ for $n_a = n$. Noting that there are $\binom{N}{n}$ states of occupancy number n allows us to simplify the Green function to

$$G_{\alpha\beta}(\omega) = \sum_{n=0}^{N} p(n) Q^n_{\alpha\beta} \tag{6}$$

where

$$Q^n_{\alpha\beta} = \frac{x_{+\alpha\beta}(n)}{\omega - K(n+1) + K(n)} + \frac{x_{-\alpha\beta}(n)}{\omega - K(n) + K(n-1)},$$

$$p(n) = \tfrac{1}{Z}\binom{N}{n}\mathrm{e}^{-\beta K(n)}, \quad Z = \sum \binom{N}{n}\mathrm{e}^{-\beta K(n)},$$

and the spectral weights are

$$x_{+\alpha\beta}(n) = \binom{N}{n}^{-1} \textstyle\sum_{n_a=n} \langle a|c_\alpha c^\dagger_\beta|a\rangle \tag{7a}$$

for particle addition and

$$x_{-\alpha\beta}(n) = \binom{N}{n}^{-1} \sum_{n_a=n} \langle a|c^\dagger_\beta c_\alpha|a\rangle \tag{7b}$$

for particle removal.

To simplify the Green function, it suffices to calculate the spectral weights, $x_{\pm\alpha\beta}$. Note that in order for these matrix elements to be nonvanishing, one must have $\alpha = \beta$. In addition, the state a occurring in the summation expression for $x_{+\alpha\beta}$ (resp. $x_{-\alpha\beta}$) must be empty (full) at isospin α. There are $\binom{N-1}{n}$ ($\binom{N-1}{n-1}$) such states, and so the final expressions for $x_{\pm\alpha\beta}$ are

$$x_{+\alpha\beta} = \delta_{\alpha\beta}\binom{N-1}{n} \Big/ \binom{N}{n} = \delta_{\alpha\beta}(1 - \tfrac{n}{N}) \tag{8a}$$

and

$$x_{-\alpha\beta} = \delta_{\alpha\beta}\binom{N-1}{n-1} \Big/ \binom{N}{n} = \delta_{\alpha\beta}\tfrac{n}{N}. \tag{8b}$$

At $T = 0$, $p(n) = 1$ for some fixed n and $p(n) = 0$ otherwise which effectively eliminates the sum over n in the Green function resulting in an expression of the form, $G_{\alpha\beta}(\omega) = \delta_{\alpha\beta} Q^n$, where $Q^n(\omega)$ is $Q^n_{\alpha\beta}(\omega)$ evaluated with Eq. (8). We now come to the issue of the chemical potential. According to Farid[10], the leading $\beta \to \infty$ limit of the Green function is given by evaluating

$$\begin{aligned} & Q^{\,n}(\omega) + \mathrm{e}^{-\beta(K(n+1)-K(n))}(Q^{n+1}(\omega) - Q^n(\omega)) \\ & + \mathrm{e}^{\beta(K(n)-K(n-1))}(Q^{n-1}(\omega) - Q^n(\omega)) \\ & + O(\mathrm{e}^{-\beta(H(n+1)-2H(n)+H(n-1))}). \end{aligned} \tag{9}$$

The chemical potential is fixed by the relationship

$$\frac{n}{N} = \lim_{\beta\to\infty} \int \frac{\mathrm{d}\omega}{\mathrm{e}^{\beta\omega}+1} \left(-\frac{1}{\pi} \Im G(\omega + \mathrm{i}0) \right). \tag{10}$$

Combining the previous two expressions yields

$$\begin{aligned} \frac{n}{N} = & \left(\tfrac{n}{N}\right) (1 - \mathrm{e}^{-\beta(K(n+1)-K(n))}) \\ & + \left(1 - \tfrac{n}{N}\right) e^{\beta(K(n)-K(n-1))} \\ & + O(\mathrm{e}^{-\beta(H(n+1)-2H(n)+H(n-1))}), \end{aligned} \tag{11}$$

which can be solved immediately to yield

$$\mu = \frac{\epsilon_+ + \epsilon_-}{2} + \frac{1}{2\beta} \log \frac{N-n}{n} + o(\beta^{-1}) \tag{12}$$

where $\epsilon_+(n) = H(n+1) - H(n)$ and $\epsilon_-(n) = H(n) - H(n-1)$. Consequently, the chemical potential is equidistant between the poles of $Q^n(\omega)$. Equivalently, this choice for the chemical potential implies that $K(n+1) - K(n) > 0$, $K(n) - K(n-1) < 0$, and $K(n+1) - K(n) = -(K(n) - K(n-1))$. Hence

$$G_{\alpha\beta}(\omega = 0) = \frac{\delta_{\alpha\beta}}{K(n+1) - K(n)} \left(\frac{2n-N}{N} \right) \tag{13}$$

Consequently, Luttinger's theorem for this system, if it is valid, is the statement that

$$n = \sum_\alpha \Theta(G_{\alpha\alpha}(\omega = 0)) = N\Theta(2n - N). \tag{14}$$

This expression clearly fails for any partial filling when N is odd. Also, by making the shift $\omega \to \omega + \epsilon(\boldsymbol{k})$) in Eq. (5), thereby lifting the ground-state degeneracy (see Appendix) cannot change the argument of the Θ-function in Eq. (14). Consider the atomic limit of the Hubbard model for $N = 3$ and two of the iso-spin levels with unit occupancy, that is, $n = 2$ (see Fig. 1). This is the 'half-filled' case. Eq. (2) clearly fails because $\Theta(x)$ can only take on values 1, 0 or 1/2. Hence, no expression of the form of Eq. (2) can ever yield the electron density when N is odd. At play here is the fact that particle-hole symmetry, which is present for N even, is strictly absent for N odd.

Clearly if Eq. (2) fails, there must be an additional term that contributes to the density. The extra term is usually[2] written as an integral involving the self energy. As $\beta \to \infty$, $G(\omega) \equiv G_{\alpha\alpha}(\omega)$ may be rewritten as

$$G(\omega) = \frac{1}{\omega + \mu - \bar{\epsilon} - \Sigma(\omega)} \tag{15}$$

where

$$\bar{\epsilon} = \left(1 - \tfrac{n}{N}\right) \epsilon_+ + \left(\tfrac{n}{N}\right) \epsilon_-, \tag{16}$$

$$\Sigma(\omega) = \tfrac{n(N-n)}{N^2} \tfrac{(\epsilon_+ - \epsilon_-)^2}{\omega + \mu - \epsilon_0} \tag{17}$$

and

$$\epsilon_0 = \left(\tfrac{n}{N}\right) \epsilon_+ + \left(1 - \tfrac{n}{N}\right) \epsilon_-. \tag{18}$$

The expression to be evaluated is

$$I_2 = -N \lim_{\beta\to\infty} \frac{1}{\beta} \sum_\zeta G(\omega) \partial_\omega \Sigma(\omega)|_{\omega = \mathrm{i}\zeta} \tag{19}$$

where the sum is over the fermionic Matsubara frequencies. The explicit calculation yields[10]

$$\begin{aligned} I_2 &= \frac{N}{2} \lim_{\beta\to\infty} \left(\left(\tfrac{n}{N}\right) \tanh \beta(\epsilon_+ - \mu) \right. \\ &\quad \left. + \left(1 - \tfrac{n}{N}\right) \tanh \beta(\epsilon_- - \mu) - \tanh \beta(\epsilon_0 - \mu) \right) \\ &= \frac{1}{2} \left(n \operatorname{sgn}(\epsilon_+ - \mu) + (N-n) \operatorname{sgn}(\epsilon_- - \mu) \right. \\ &\quad \left. - N \operatorname{sgn}(\epsilon_0 - \mu) \right). \end{aligned} \tag{20}$$

Because $\mu = \frac{\epsilon_- + \epsilon_+}{2}$ and $\epsilon_- < \epsilon_+$, we know that $\epsilon_- < \mu$, $\epsilon_+ > \mu$, and $\operatorname{sgn}(\epsilon_0 - \mu) = \operatorname{sgn}(2n - N)$. Thus,

$$\begin{aligned} I_2 &= \frac{1}{2}(2n - N - N \operatorname{sgn}(2n - N)) \\ &= n - N\Theta(2n - N). \end{aligned} \tag{21}$$

Combined with the previous result, $I_1 = N\Theta(2n - N)$, we recover the full particle density,

$$n = I_1 + I_2. \tag{22}$$

The failure of the LW identity, $I_2 = 0$, rests entirely on the form of the self-energy in this problem, Eq. (17). We first note that Σ diverges at $\omega + \mu = \epsilon_0$. Consequently, regardless of what is chosen for H_0, which in this case has been set to zero, Σ cannot be connected to any non-interacting problem as a result of its divergence. Consider the LW functional, defined by

$$\delta I[G] = \int d\omega \Sigma \delta G \tag{23a}$$

$$I[G = G_0] = 0 \tag{23b}$$

which was used by Luttinger[2] to show that the integrand of I_2 is a total derivative. Because Σ diverges for some ω when G is the total Green function, it is not possible to integrate the defining differential expression in the neighborhood of the true Green function, and therefore the LW functional does not exist. Consequently, there is no Luttinger theorem and Eq. (1) does not represent the density of a fermionic system because zeros of the Green function must be strictly excluded, a model-independent conclusion. While zeros are a robust mathematical feature of a Green function, they do not represent a conserved quantity and do not have direct physical meaning. This can be seen from the fact that the zero line is sensitive to the placement of the chemical potential, and there is no observable consequence when the zero crosses μ.

Even in the case where $I_2 = 0$, and our system is gapped, the divergence of the self-energy is still present. Hence, no LW functional exists in this case as well. For N even, particle-hole symmetry is operative and it is this symmetry that results in a vanishing of I_2 not any fact pertaining to the LW functional. For N odd, no such symmetry obtains. In gapless systems, Eq. (1) is still not generally valid. A less general formulation[14, 15] which *assumes* the absence of zeros remains valid. That assumption, means that the interacting system must be perturbatively (adiabatically) connected to non-interacting fermions, which immediately rules out the Mott state which has a divergent self energy. In fact, the work by Hořava[14] provides a promising direction in which the robust features of a Fermi surface admit a K-theoretic formulation.

The key implication the inapplicability of Eq. (1) portends for strongly interacting electron systems is that although the degrees of freedom that give rise to zeros undoubtedly contribute to the current, they have no bearing on the particle density. The particle density is determined by coherence ($\Im\Sigma < \epsilon$) while zeros arise from incoherence ($\Im\Sigma$ diverges[11] signifying that there is no particle to contribute to n). As a result, there exist charged degrees of freedom in strongly correlated electron matter which couple to the current but nonetheless cannot be given an interpretation in terms of elemental fields. Consequently, the particle density will be less than the total number of degrees of freedom that couple to an external gauge field as demonstrated recently[13] when the upper Hubbard band is integrated out exactly. Note the breakdown of Eq. (1) has been demonstrated exactly in a model in which spin and charge are not separated, a purely atomic limit model in which there can be no difference between spin and charge velocities.

Deviations from Eq. (1) are expected then in experimental systems which are strongly correlated as evidenced by either a hard gap or a pseudogap (density of states vanishing at a single energy). Shown in Fig. (2) is a plot of the area enclosed by the locus of k-points for which there is a maximum in the spectral function in $La_{2-x}Sr_xCuO_2$[16] (+ plot symbol) and $Bi_2Sr_2CaCu_2O_{8+\delta}$[17] (× plotting symbol) as a function of the nominal doping level in the pseudogap regime. Although the maxima in the spectral function form an arc as there are zeros present on the opposite side, $x_{\rm FS}$ was extracted by simply closing the arc according to a recent proposal[18] for $Bi_2Sr_2CaCu_2O_{8+\delta}$[17] (Bi-2212) and for $La_{2-x}Sr_xCuO_2$[16] (LSCO) by determining the large Fermi surface $(1-x)$ defined by the k_F measured directly from the momentum-distribution curves and then subtracting unity. Hence, the key assumption that is being tested here in this definition of $x_{\rm FS}$ is that each doped hole corresponds to a single $k-$state. A typical uncertainty in these experiments is ± 0.02. Even when this uncertainty is considered, the deviation from the dashed line persists indicating that one hole does not equal one k-state and hence a fundamental breakdown of the elemental particle picture in the cuprates. For the Hubbard model this systematic deviation has been seen previously[19] and stems from the fundamental fact that since the spectral weight is carried by two non-rigid bands, removing a single k-state is not equivalent to removing a single electron. Another source of deviation from Eq. (1) is the fact

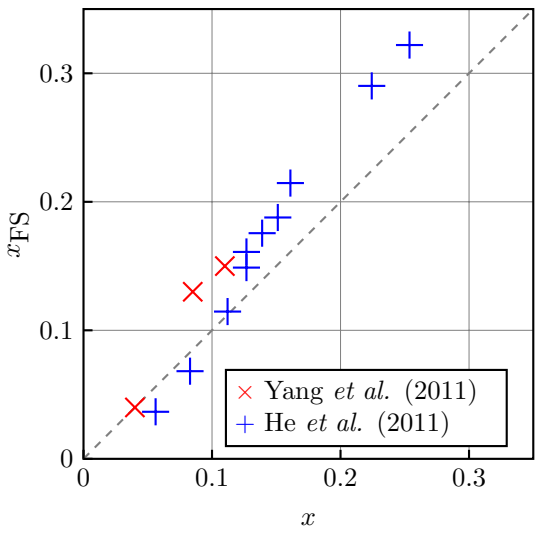

FIG. 2. Apparent doping $x_{\rm FS}$ inferred from the Fermi surface reconstruction as a function of the nominal doping x in LSCO and Bi-2212.

that as x nears optimal doping, the Fermi surface topology must change from scaling with x to $1-x$. Hence, there has to be a deviation $x_{\rm FS} = x$. We hope this work serves to motivate a much more systematic study of deviations from Eq. (1).

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