Luttinger's theorem in the presence of Luttinger surfaces

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Breakdown of Landau's hypothesis of adiabatic continuation from noninteracting to fully interacting electrons is commonly believed to bring about a violation of Luttinger's theorem. Here, we elucidate what may go wrong in the proof of Luttinger's theorem. The analysis provides a simple way to correct Luttinger's expression of the electron number in single-band models where perturbation theory breaks down through the birth of a Luttinger surface without symmetry breaking. In those cases, we find that the Fermi volume only accounts for the doping away from half-filling. In the hypothetical circumstance of a non-symmetry-breaking Mott insulator with a Luttinger surface, our analysis predicts the noteworthy existence of quasiparticles whose Fermi surface is just the Luttinger one. Therefore, those quasiparticles can be legitimately regarded as spinons, and the Mott insulator with a Luttinger surface as realization of a spin-liquid insulator.

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I. INTRODUCTION

Landau originally derived his celebrated theory of Fermi liquids [1] assuming that the noninteracting many-body excited states evolve adiabatically into the fully interacting ones upon gradually turning on interaction. The theory was later microscopically derived [2] by means of the just-developed diagrammatic many-body perturbation theory [3,4]. A famous byproduct of the diagrammatic formalism is the so-called Luttinger theorem [5], which, in conventional Landau's Fermi liquids, predicts that the volume fraction enclosed by the quasiparticles' Fermi surface is just the electron filling fraction. Over the years, Landau's adiabatic hypothesis and Luttinger's theorem have become almost synonyms, in the sense that if one is violated, so is the other. Such belief has been mostly triggered by the anomalous properties of many strongly correlated materials, especially underdoped cooper-oxide superconductors.

However, the traditional derivation [5–8] of Luttinger's theorem simply relies on the existence of a Luttinger-Ward functional [3], which can be constructed nonperturbatively [9]. Therefore, it is not at all evident why Luttinger's theorem should be violated at the breakdown of perturbation theory, as it is likewise not true that Landau's Fermi liquid theory applies only in the perturbative regime [10,11].

The topological arguments by Oshikawa [12] in periodic models clarify Luttinger's theorem violation in nontrivial examples that host fractionalized excitations [13,14] or topological order [15,16], but does not allow identifying at which point the traditional proof may go wrong. Moreover, it is not instructive in nonmagnetic Mott insulators at integer number of electrons per site, like the model discussed by Rosh [17], where Luttinger's theorem does not yield the correct electron number, nor in models that lack translation symmetry, like quantum impurity models, where Luttinger's theorem is still applicable and can be violated [18].

The detailed analysis of Heath and Bedell [19] highlights which properties the self-energy must possess for Luttinger's theorem to hold true, even in nonperiodic models. However, it leaves open the question how to count the number of particles when Luttinger's theorem is violated.

Indeed, there are by now several examples of Luttinger's theorem violation, see, e.g., Refs. [13–15,17,18,20–22]. In addition, there is numerical evidence that Luttinger's theorem fails in models of doped Mott insulators below a critical doping [23–28] that seems to be associated with the birth of a Luttinger surface [29], which, according to Ref. [19], does violates the requirements for Luttinger's theorem validity.

In this paper, we try to shed further light on such a fundamental issue, beyond the great progress that have been already accomplished [13,15,19,30,31]. We do that paying particular attention to the role of Luttinger surfaces or, more generally, to the zeros of the single-particle Green's function at zero imaginary frequency, a concept that does not require translation invariance.

II. LUTTINGER'S THEOREM

We start by deriving Luttinger's theorem in a slightly different way as conventionally done [5,6], somehow closer to Refs. [7,8], which better highlights under which circumstances that theorem may fail. Moreover, the derivation below, though based on old-fashioned many-body theory, naturally brings us to the concept of quasiparticles and their Fermi or Luttinger surfaces [11].

We consider a system of interacting electrons with annihilation operators c_α corresponding to a complete basis of single-particle wave functions labeled by $\alpha = 1, \ldots, K$, with $K \to \infty$ in the thermodynamic limit. The Hamiltonian admits a set of conserved quantities Q, represented by Hermitian matrices $\hat{Q}$ with components $Q_{\alpha\beta}$ defined in such a way that

the eigenvalues are integers. $Q_{\alpha\beta} = \delta_{\alpha\beta}$ corresponds to the total number N of electrons, while all other independent Q's are represented by traceless matrices $\hat{Q}$. We hereafter consider the evolution of the operators in imaginary time and use the Matsubara formalism, which is more convenient [29] since on the imaginary frequency axis the single-particle Green's function and self-energy cannot have singularities but, eventually, at the origin. Moreover, to avoid any issue related to the discontinuity at zero imaginary time of the Green's functions, we use instead of N the deviation $N - K/2$ of the electron number with respect to half-filling, so we can write the expectation value of any conserved quantity as

$$\begin{aligned} Q &= \frac{1}{2} \sum_{\alpha\beta} Q_{\beta\alpha} \left(\langle\, c^\dagger_\beta \, c_\alpha \,\rangle - \langle\, c_\alpha \, c^\dagger_\beta \,\rangle \right) \\ &= T \sum_n \mathrm{Tr}(\hat{G}(i\epsilon_n)\, \hat{Q}), \end{aligned} \tag{1}$$

where $\hat{G}(i\epsilon_n) = \hat{G}(-i\epsilon_n)^\dagger$ is the Green's function matrix in Matsubara frequencies $\epsilon_n = (2n+1)\,\pi T$. According to Dyson's equation,

$$\hat{G}^{-1}(i\epsilon_n) = i\epsilon_n\, \hat{I} - \hat{H}_0 - \hat{\Sigma}(i\epsilon_n), \tag{2}$$

with $\hat{I}$ the identity matrix, and $\hat{H}_0$ the noninteracting Hamiltonian, including the chemical potential term, represented in the chosen basis. $\hat{\Sigma}(i\epsilon_n) = \hat{\Sigma}(-i\epsilon_n)^\dagger$ is the self-energy matrix that accounts for all interaction effects. We can equivalently write Eq. (1) as

$$Q = -T \sum_n \frac{\partial}{\partial i\epsilon_n} \mathrm{Tr}(\ln \hat{G}(i\epsilon_n)\, \hat{Q}) + I_L(Q), \tag{3}$$

where

$$I_L(Q) = T \sum_n \mathrm{Tr}\left(\hat{G}(i\epsilon_n) \frac{\partial \hat{\Sigma}(i\epsilon_n)}{\partial i\epsilon_n}\, \hat{Q} \right). \tag{4}$$

Hereafter, we denote Eq. (4) as the Luttinger integral for the conserved quantity Q and use simply I_L for the case $\hat{Q} = \hat{I}$.

We just note that at particle-hole symmetry, $I_L(Q)$ vanishes identically for all non-particle-hole invariant Q's, thus also the total electron number, in which case Luttinger's theorem holds trivially. Seemingly, $I_L(Q) = 0$ in absence of interaction, where $\hat{\Sigma}(i\epsilon_n) = 0$.

In more general circumstances, we consider the Luttinger-Ward functional $\Phi[G]$, satisfying [3,9]

$$\delta\Phi[G] = T \sum_n \mathrm{e}^{i\epsilon_n \eta}\, \mathrm{Tr}(\hat{\Sigma}(i\epsilon_n)\, \delta\hat{G}(i\epsilon_n)), \tag{5}$$

with $\eta > 0$ that must be sent to zero after performing the summation. In perturbation theory, the explicit expression of $\Phi[G]$ reads [3]

$$\begin{aligned} \Phi[G] &= T \sum_n \mathrm{e}^{i\epsilon_n \eta} \sum_{m \geqslant 1} \frac{1}{2m} \mathrm{Tr}(\hat{G}(i\epsilon_n)\, \hat{\Sigma}^{(m)}(i\epsilon_n)) \\ &\equiv T \sum_n \mathrm{e}^{i\epsilon_n \eta}\, \Phi(i\epsilon_n), \end{aligned} \tag{6}$$

where $\hat{\Sigma}^{(m)}(i\epsilon_n)$ is the sum of all m th-order skeleton diagrams. We assume that the nonperturbative $\Phi[G]$ [9] can still be written as a series of terms $\Phi(i\epsilon_n)$ as in Eq. (6). Through Eqs. (5) and (6), it readily follows that

$$\begin{aligned} \frac{\delta\Phi[G]}{\delta i\epsilon} &\equiv T \sum_n \mathrm{Tr}\left(\hat{\Sigma}(i\epsilon_n) \frac{\partial \hat{G}(i\epsilon_n)}{\partial i\epsilon_n} \right) \\ &= T \sum_n \frac{\partial \Phi(i\epsilon_n)}{\partial i\epsilon_n}, \end{aligned} \tag{7}$$

where we set $\eta = 0$ before performing the sum since the function decays faster than $1/\epsilon_n$ for $\epsilon_n \to \pm\infty$. Equation (7) allows us to rewrite $I_L(Q)$ of Eq. (4) for $\hat{Q} = \hat{I}$ simply as

$$I_L = T \sum_n \mathrm{Tr}\left(\hat{G}(i\epsilon_n) \frac{\partial \hat{\Sigma}(i\epsilon_n)}{\partial i\epsilon_n} \right) = T \sum_n \frac{\partial I_L(i\epsilon_n)}{\partial i\epsilon_n}, \tag{8}$$

where

$$I_L(i\epsilon_n) = \mathrm{Tr}(\hat{\Sigma}(i\epsilon_n)\, \hat{G}(i\epsilon_n)) - \Phi(i\epsilon_n). \tag{9}$$

In other words, it is always possible to represent the Luttinger integral as a sum over ϵ_n of a derivative. It follows that the total number of electrons can be written as

$$\begin{aligned} N &= \frac{K}{2} - T \sum_n \frac{\partial}{\partial i\epsilon_n} \mathrm{Tr}(\ln \hat{G}(i\epsilon_n)) + T \sum_n \frac{\partial I_L(i\epsilon_n)}{\partial i\epsilon_n} \\ &\xrightarrow[T \to 0]{} \frac{K}{2} - \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \frac{\partial}{\partial i\epsilon} \mathrm{Tr}(\ln \hat{G}(i\epsilon)) \\ &\quad + \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \frac{\partial I_L(i\epsilon)}{\partial i\epsilon}. \end{aligned}$$

Since $\hat{G}(-i\epsilon) = \hat{G}(i\epsilon)^\dagger$ and, similarly, $I_L(-i\epsilon) = I_L(i\epsilon)^*$, if we define, through the polar decomposition of $\hat{G}(i\epsilon)$, the matrix

$$\hat{\delta}(\epsilon) \equiv \arg(\hat{G}(i\epsilon)) = \mathrm{Im}\, \ln\, (\hat{G}(i\epsilon)), \tag{10}$$

then, for $T \to 0$, and noticing that $\mathrm{Im}\, I_L(i\epsilon) \to 0$ while $\hat{\delta}(\epsilon) \to -\pi/2\, \hat{I}$ for $\epsilon \to \infty$,

$$\begin{aligned} N &= \frac{K}{2} + \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \mathrm{Tr}(\hat{G}(i\epsilon)) \\ &= K + \frac{1}{\pi} \mathrm{Tr}(\hat{\delta}(0^+)) - \frac{1}{\pi} \mathrm{Im}\, I_L(i0^+). \end{aligned} \tag{11}$$

This expression is exact. It is still not Luttinger's theorem but a kind of generalization of it, and it is remarkable as it shows that a quantity requiring integration over all frequencies can be alternatively calculated through boundary terms.

In reality, Luttinger's theorem statement is that $\mathrm{Im}\, I_L(i0^+) = 0$ in Eq. (11), which is not to be expected *a priori*. Nonetheless, the proof goes as follows. The Luttinger-Ward functional $\Phi[G]$ is invariant if the Matsubara frequency of each internal Green's function is replaced, see Eq. (2), by $i\epsilon_n\, \hat{I} + i\omega\, \hat{Q}$ for any conserved Q, where $\omega = 2\pi\, T$. Therefore,

$$0 = \frac{\Delta^Q \Phi[G]}{i\omega} = T \sum_n \mathrm{Tr}\left(\hat{\Sigma}(i\epsilon_n) \frac{\Delta^Q \hat{G}(i\epsilon)}{i\omega} \right), \tag{12}$$

with

$$\frac{\Delta^Q \hat{G}(i\epsilon)}{i\omega} \equiv \frac{\hat{G}(i\epsilon_n + i\omega\, \hat{Q}) - \hat{G}(i\epsilon_n)}{i\omega}, \tag{13}$$

the finite difference of $\hat{G}(i\epsilon)$. For $\hat{Q} = \hat{I}$, that implies

$$\begin{aligned} 0 &= T\sum_n \mathrm{Tr}\left(\hat{\Sigma}(i\epsilon_n)\,\frac{\hat{G}(i\epsilon_n+i\omega)-\hat{G}(i\epsilon_n)}{i\omega}\right) \\ &= -T\sum_n \mathrm{Tr}\left(\hat{G}(i\epsilon_n)\,\frac{\hat{\Sigma}(i\epsilon_n+i\omega)-\hat{\Sigma}(i\epsilon_n)}{i\omega}\right) \\ &\equiv -T\sum_n \frac{I_L(i\epsilon_n+i\omega)-I_L(i\epsilon_n)}{i\omega} \equiv -I_L^{\Delta}, \end{aligned} \tag{14}$$

which just means that the convergence of the series allows the change of variable $i\epsilon_n + i\omega \to i\epsilon_n$ that makes I_L^{Δ} trivially vanish. It is tempting to assume that I_L^{Δ}, i.e., the sum over ϵ_n of the finite difference, coincides with I_L in Eq. (8), i.e., the sum over ϵ_n of the derivative, in the limit $T \to 0$, thus $\omega \to 0$. That is actually what is commonly assumed in the proof of Luttinger's theorem, in which case $I_L = 0$ follows, and thus $\mathrm{Im}\, I_L(i0^+) = 0$ in Eq. (11). However, that apparently reasonable assumption is not at all guaranteed, as we now discuss.

In the Supplemental Notes of Ref. [11] it has been shown that, at leading order in T,

$$I_L = -\frac{1}{\pi}\,\mathrm{Im}\, I_L(i0^+) = I_L - I_L^{\Delta} \simeq -\frac{1}{4\pi i}\lim_{\epsilon\to 0^+} S(i\epsilon). \tag{15}$$

where

$$S(i\epsilon) \equiv \mathrm{Tr}[(\hat{G}(i\epsilon)+\hat{G}(i\epsilon)^\dagger)\,(\hat{\Sigma}(i\epsilon)-\hat{\Sigma}(i\epsilon)^\dagger)]. \tag{16}$$

It follows that, if $S(i\epsilon)$ is finite for $\epsilon \to 0^+$, then Luttinger's theorem is definitely violated. That happens, e.g., in the Sachdev-Ye-Kitaev model [32,33]. On the contrary, one can readily prove that $S(i\epsilon \to 0^+) = 0$ when perturbation theory holds. Indeed, if we define the quasiparticle residue,

$$\sqrt{\hat{Z}(i\epsilon)^{\dagger-1}\,\hat{Z}(i\epsilon)^{-1}} \equiv \hat{I} - \frac{\hat{\Sigma}(i\epsilon)-\hat{\Sigma}(i\epsilon)^\dagger}{2i\epsilon}, \tag{17}$$

where $\hat{Z}(i\epsilon) = \hat{Z}(-i\epsilon)$, we do know that perturbatively $\hat{Z}(0) = \hat{Z}(0)^\dagger$ is positive definite, so

$$\hat{\Sigma}(i\epsilon)-\hat{\Sigma}(i\epsilon)^\dagger \underset{\epsilon\to 0}{\longrightarrow} 2\,(\hat{I}-\hat{Z}(0)^{-1})\,i\epsilon,$$

and thus $S(i\epsilon)$ vanishes as $\epsilon \to 0^+$. However, $S(i\epsilon \to 0^+) = 0$, though necessary for $I_L = 0$, is not a sufficient condition. The reason is that the right-hand side of Eq. (15) is just the leading term of an expansion in T. Its vanishing means that each term of the series expansion goes to zero as $T \to 0$, which does not guarantee that the whole series vanishes [11]. In other words, while we can safely state that, in the regime where perturbation theory is valid, $S(i\epsilon \to 0^+) = 0$ does imply that $I_L = 0$, and thus that Luttinger's theorem holds true, we cannot exclude that the theorem is violated when perturbation theory breaks down.

However, let us assume the necessary condition $S(i\epsilon \to i0^+) = 0$ and draw its consequences. By definition, the single-particle density of states (DOS) A at the chemical potential is

$$A = -\lim_{\epsilon\to 0^+}\frac{1}{2\pi i}\,\mathrm{Tr}(\hat{G}(i\epsilon)-\hat{G}(i\epsilon)^\dagger) \equiv \lim_{\epsilon\to 0^+}\mathrm{Tr}(\hat{A}(i\epsilon)),$$

where $\hat{A}(i\epsilon) = \hat{A}(i\epsilon)^\dagger = -\hat{A}(-i\epsilon)$. Through $\hat{A}(i\epsilon)$, we can write

$$\hat{\Sigma}(i\epsilon)-\hat{\Sigma}(i\epsilon)^\dagger = 2i\epsilon - 2\pi i\,\hat{G}(i\epsilon)^{-1}\,\hat{A}(i\epsilon)\,\hat{G}(i\epsilon)^{\dagger-1},$$

and thus $S(i\epsilon)$ in Eq. (16) becomes

$$\begin{aligned} S(i\epsilon) &= 2i\epsilon\,\mathrm{Tr}(\hat{G}(i\epsilon)+\hat{G}(-i\epsilon)) \\ &\quad - 2\pi i\,\mathrm{Tr}[(\hat{G}(i\epsilon)^{-1}+\hat{G}(i\epsilon)^{\dagger-1})\,\hat{A}(i\epsilon)]. \end{aligned}$$

We now formally filter out the quasiparticle Green's function through the quasiparticle residue Eq. (17),

$$\hat{G}_{\mathrm{qp}}(i\epsilon)^{-1} \equiv \sqrt{\hat{Z}(i\epsilon)^\dagger}\;\hat{G}(i\epsilon)^{-1}\sqrt{\hat{Z}(i\epsilon)} = i\epsilon\,\hat{I} - \hat{\Xi}(i\epsilon), \tag{18}$$

where

$$\hat{\Xi}(i\epsilon) \equiv \sqrt{\hat{Z}(i\epsilon)^\dagger}\;(\hat{H}_0 + \mathrm{Re}\,\hat{\Sigma}(i\epsilon))\sqrt{\hat{Z}(i\epsilon)} \tag{19}$$

is a $K \times K$ Hermitian matrix and thus has real eigenvalues $\epsilon_{*\ell}(\epsilon) = \epsilon_{*\ell}(-\epsilon)$, $\ell = 1, \ldots, K$. Therefore, if we further define

$$\begin{aligned} \hat{A}_{\mathrm{qp}}(i\epsilon) &\equiv -\frac{1}{2\pi i}\,(\hat{G}_{\mathrm{qp}}(i\epsilon)-\hat{G}_{\mathrm{qp}}(i\epsilon)^\dagger) \\ &= \frac{\epsilon}{\pi}\,\hat{G}_{\mathrm{qp}}(i\epsilon)\,\hat{G}_{\mathrm{qp}}(i\epsilon)^\dagger = \frac{\epsilon}{\pi}\,\frac{1}{\epsilon^2+\hat{\Xi}(i\epsilon)^2} \\ &= \sqrt{\hat{Z}(i\epsilon)^{-1}}\;\hat{A}(i\epsilon)\,\sqrt{\hat{Z}(i\epsilon)^{\dagger-1}}\,, \end{aligned} \tag{20}$$

which is diagonal in the basis that diagonalizes $\hat{\Xi}(i\epsilon)$ with elements

$$A_{\mathrm{qp}\,\ell}(i\epsilon) = \frac{1}{\pi}\,\frac{\epsilon}{\epsilon^2+\epsilon_{*\ell}(\epsilon)^2},$$

then

$$\begin{aligned} S(i\epsilon) &= 2i\epsilon\,\mathrm{Tr}(\hat{G}(i\epsilon)+\hat{G}(-i\epsilon)) + 4\pi i\,\mathrm{Tr}[\,\hat{\Xi}(i\epsilon)\hat{A}_{\mathrm{qp}}(i\epsilon)\,] \\ &= 2i\epsilon\,\mathrm{Tr}(\hat{G}(i\epsilon)+\hat{G}(-i\epsilon)) \\ &\quad + 4\pi i\sum_{\ell=1}^{K}\frac{\epsilon_{*\ell}(\epsilon)}{\pi}\,\frac{\epsilon}{\epsilon^2+\epsilon_{*\ell}(\epsilon)^2}. \end{aligned} \tag{21}$$

Since the first term on the right-hand side of Eq. (21) vanishes for $\epsilon \to 0$, the necessary condition for Luttinger's theorem to hold becomes

$$\begin{aligned} &\lim_{\epsilon\to 0^+}\mathrm{Tr}[\,\hat{\Xi}(i\epsilon)\hat{A}_{\mathrm{qp}}(i\epsilon)\,] \\ &\quad = \lim_{\epsilon\to 0^+}\sum_{\ell=1}^{K}\frac{\epsilon_{*\ell}(\epsilon)}{\pi}\,\frac{\epsilon}{\epsilon^2+\epsilon_{*\ell}(\epsilon)^2} = 0. \end{aligned} \tag{22}$$

In the thermodynamic limit, $K \to \infty$, $\epsilon_{*\ell}(\epsilon)$ defines a continuous spectrum where ℓ runs in a d-dimensional space, with d the spatial dimension of the system times the number of internal degrees of freedom. For instance, in the periodic case, ℓ labels the momentum within the Brillouin zone, the band index, and the spin. Any ℓ such that $\epsilon_{*\ell}(\epsilon \to 0) \neq 0$ yields a contribution to the sum Eq. (22) that trivially vanishes as $\epsilon \to 0$. Let us instead consider the manifold $\ell = \ell_*$ such that $\epsilon_{*\ell_*}(\epsilon \to 0) = 0$. If, for a given ℓ_*, $\epsilon_{*\ell_*}(\epsilon \to 0) \sim c_*\,|\epsilon|^\alpha$,

with $\alpha > 0$, its contribution to the sum Eq. (22) is

$$\frac{\epsilon_{*\ell_*}(\epsilon)}{\pi}\ \frac{\epsilon}{\epsilon^2+\epsilon_{*\ell_*}(\epsilon)^2}\ \xrightarrow[\epsilon\to 0^+]{}\ \frac{c_*\,|\epsilon|^\alpha}{\pi}\ \frac{\epsilon}{\epsilon^2+c_*^2\,|\epsilon|^{2\alpha}},$$

and vanishes only if $\alpha > 1$, which thus becomes the necessary condition for the validity of Luttinger's theorem. We can further distinguish two different cases. For instance, if we assume that

- $\hat{\Xi}(i\epsilon)$is, at leading order, analytic at $\epsilon = 0$, (23)

then $\alpha = 2$ since $\epsilon_{*\ell}(\epsilon)$ is even in ϵ, which automatically satisfies the necessary condition for Luttinger's theorem to hold. In this case, $\epsilon_{*\ell}(\epsilon \to 0) \simeq \epsilon_{*\ell}(0) + O(\epsilon^2)$, where $\epsilon_{*\ell}(0) \equiv \epsilon_{*\ell}$ are the eigenvalues of

$$\hat{H}_* \equiv \sqrt{\hat{Z}(0)^\dagger}\ (\hat{H}_0 + \hat{\Sigma}(0))\sqrt{\hat{Z}(0)}\,. \tag{24}$$

Accordingly, the quasiparticle Green's function and DOS at the chemical potential are

$$\hat{G}_{\rm qp}(i\epsilon) \xrightarrow[\epsilon\to 0]{} \frac{1}{i\epsilon\,\hat{I}-\hat{H}_*}, A_{\rm qp} = \lim_{\epsilon\to 0^+}\ {\rm Tr}(\hat{A}_{\rm qp}(i\epsilon)) = \sum_\ell \delta(\epsilon_{*\ell}), \tag{25}$$

and correspond to those of free particles, thus the quasiparticles, described by the quasiparticle Hamiltonian $\hat{H}_*$ with eigenvalues $\epsilon_{*\ell}$.

On the contrary, if $\hat{\Xi}(i\epsilon)$ is nonanalytic and yet satisfies the necessary condition for Luttinger's theorem, then $1 < \alpha < 2$, since any nonanalyticity yielding noninteger $\alpha > 2$ will be hidden by the ever-present analytical terms. That is precisely what happens for interacting electrons in one dimension. Those systems do not sustain quasiparticles in the sense of Eqs. (25), and yet Luttinger's theorem is valid [34,35]. The same occurs in marginal Fermi liquids [36] or metals with quantum critical behavior [37], which, despite a nonanalytic self-energy, satisfy Luttinger's theorem [19]. Conversely, since $S(i\epsilon \to i0^+) = 0$ is not sufficient for Luttinger's theorem to hold, we must also conclude that quasiparticles may exist even when Luttinger's theorem is violated [11].

We also emphasize that $1 < \alpha < 2$ entails singularities in perturbation theory. Therefore, Eq. (23) must always be verified when perturbation theory is well-defined, which is equivalent to saying that quasiparticles always exist in the perturbative regime, in agreement with Landau's adiabatic hypothesis.

Hereafter, we assume the analyticity condition Eq. (23), thus Eqs. (25). We believe that this choice, though limiting, may be pertinent to doped Mott insulators in dimensions $d > 1$ [23–28]. In that case, $\hat{\delta}(\epsilon)$ is diagonal in the basis that diagonalizes $\hat{H}_*$ with elements $-\pi + \pi\,\theta(-\epsilon_{*\ell})$. It follows that Eq. (11) becomes

$$N = K + \frac{1}{\pi}\,{\rm Tr}(\hat{\delta}(0^+)) - \frac{1}{\pi}\,{\rm Im}\,I_L(i0^+) = \sum_{\ell=1}^{K}\theta(-\epsilon_{*\ell}) - \frac{1}{\pi}\,{\rm Im}\,I_L(i0^+),$$

which represents the general statement Eq. (11) of Luttinger's theorem when quasiparticles exist. We note that N is an integer at $T = 0$ and so is the sum over ℓ, which implies that the Luttinger integral I_L is quantized in integer values when Eq. (23) holds. Therefore,

$$N = \sum_{\ell=1}^{K}\theta(-\epsilon_{*\ell}) + \mathcal{L}, \quad \mathcal{L} \in \mathbb{Z}, \tag{26}$$

where $\mathcal{L} = 0$ in the perturbative regime, in which case conventional Luttinger's theorem holds, while $\mathcal{L}$ may be finite when perturbation theory breaks down.

A. Generalized Luttinger's theorem in presence of quasiparticles and in periodic systems

In a single-band periodic system invariant under spin SU(2) symmetry, we have the possibility to further elaborate on the meaning of quasiparticle. In this case, $\hat{G}(i\epsilon)$ is diagonal in momentum and spin with elements $G(i\epsilon, \mathbf{k})$ independent of spin, and thus $\hat{\Xi}(i\epsilon)$ is diagonal, too, with elements $\epsilon_*(\epsilon, \mathbf{k})$ equal for spin $\sigma = \uparrow$ and $\downarrow$, now defined, see Eq. (19), as

$$\epsilon_*(\epsilon, \mathbf{k}) = |Z(i\epsilon, \mathbf{k})|\ (\epsilon(\mathbf{k}) + {\rm Re}\,\Sigma(i\epsilon, \mathbf{k})). \tag{27}$$

Correspondingly, the quasiparticle, $A_{\rm qp}$, and physical electron, A, DOS at the chemical potential are, in units of the number of sites V, see Eqs. (25),

$$A_{\rm qp} = \frac{1}{V}\sum_{\mathbf{k}\sigma}\delta(\epsilon_*(\mathbf{k})),$$
$$A = \frac{1}{V}\sum_{\mathbf{k}\sigma} Z(i\epsilon \to i0^+, \mathbf{k})\,\delta(\epsilon_*(\mathbf{k})), \tag{28}$$

where $\epsilon_*(\mathbf{k}) = \epsilon_*(\epsilon \to 0, \mathbf{k})$. We already know that Eqs. (22) and (23) imply that, if a manifold $\mathbf{k} = \mathbf{k}_*$ exists such that $\epsilon_*(0, \mathbf{k}_*) = 0$, then $\epsilon_*(\epsilon \to 0, \mathbf{k}_*) \simeq \epsilon^2$. We observe that $\epsilon_*(0, \mathbf{k}_*) = 0$ may occur

(1) **Fermi surface** if $\mathbf{k}_* = \mathbf{k}_F$, with $\mathbf{k}_F$ such that $\epsilon(\mathbf{k}_F) + \Sigma(0, \mathbf{k}_F) = 0$ while $0 < Z(0, \mathbf{k}_F) < 1$, which defines a conventional Fermi surface $\mathbf{k} = \mathbf{k}_F$ through the roots of $G(0, \mathbf{k})^{-1}$ in momentum space. The Fermi surface contribution to the physical electron DOS Eqs. (28) is finite since $Z(0, \mathbf{k}_F) \neq 0$.

(2) **Luttinger surface** if $\mathbf{k}_* = \mathbf{k}_L$, with $\mathbf{k}_L$ such that $\epsilon(\mathbf{k}_L) + \Sigma(0, \mathbf{k}_L) \neq 0$ but

$$\lim_{\epsilon\to 0^+}|Z(i\epsilon, \mathbf{k}_L)| = \lim_{\epsilon\to 0^+}\frac{\epsilon}{\epsilon - {\rm Im}\,\Sigma(i\epsilon, \mathbf{k}_L)} \sim \lim_{\epsilon\to 0}\epsilon^2 = 0, \tag{29}$$

which implies $\Sigma(i\epsilon, \mathbf{k}_L) \sim 1/i\epsilon$ and, correspondingly, $G(i\epsilon, \mathbf{k}_L) \to 0$ as $\epsilon \to 0$. Therefore, Eq. (29) defines the so-called Luttinger surface [29], i.e., the manifold of roots $\mathbf{k} = \mathbf{k}_L$ of $G(0, \mathbf{k})$ in momentum space, whose existence is due to a singular self-energy and thus signals the breakdown of perturbation theory. Remarkably, even though the Luttinger surface contribution to the quasiparticle DOS, $A_{\rm qp}$ in Eqs. (28), is finite, its contribution to the physical electron DOS vanishes [11].

Therefore, under the analyticity assumption Eq. (23), Fermi and Luttinger surfaces are both defined by the one and only equation $\epsilon_*(0, \mathbf{k}_{F/L}) = 0$ [11]. Moreover, as we earlier

mentioned, if perturbation theory is valid there are always quasiparticles, only a Fermi surface may exist within the Brillouin zone and, see Eq. (26) at $\mathcal{L} = 0$,

$$N = \sum_{\mathbf{k}\sigma} \theta(-\epsilon_*(\mathbf{k})), \tag{30}$$

which is the standard perturbative Luttinger's theorem statement that the fraction of the quasiparticle Fermi volume, i.e., the manifold of $\mathbf{k}$: $\epsilon_*(\mathbf{k}) < 0$, with respect to the whole Brillouin zone is equal to the electron filling fraction $\nu = N/2V$.

When perturbation theory breaks down without breaking translational and spin SU(2) symmetries and Luttinger surfaces appear inside the Brillouin zone, we must use the more general formula

$$N = \sum_{\mathbf{k}\sigma} \theta(-\epsilon_*(\mathbf{k})) + \mathcal{L}, \mathcal{L} \in \mathbb{Z}, \tag{31}$$

and thus the quasiparticle Fermi volume fraction no more accounts for the electron filling fraction.

To proceed in this case, we use Oshikawa's topological approach to Luttinger's theorem in periodic systems [12]. We first note that the above quasiparticle derivation holds even when the system is a non-symmetry-breaking Mott insulator provided it has a Luttinger surface within the Brillouin zone. In the single-band model we are discussing, that may occur only at half filling. Following Oshikawa [12], we imagine adiabatically threading in the above Mott insulator a fictitious flux quantum Φ_0 that only couples to one spin species, whose particle number is conserved by charge $U(1)$ and spin SU(2), assuming, e.g., a gauge in which the vector potential has only a finite x component. The final state differs from the initial one by a lattice momentum of π in the x direction [12] and that must be supplied by the quasiparticles at the Luttinger surface [11]. The same result holds true if we couple the flux to the other spin species. On the contrary, if the flux couples to both spin species, the system acquires a momentum $2\pi \equiv 0$, and that suggests that each spin species contributes with momentum π. The conclusion is that the Luttinger surface, whatever its shape and volume are, contributes to the particle count by one electron per site. If that remains true even when, upon doping the Mott insulator, Fermi pockets appear in the Brillouin zone, then Oshikawa's argument implies that the electron filling fraction ν is given by

$$\nu = \frac{1}{2} + v_{\mathrm{EP}} - v_{\mathrm{HP}}, \tag{32}$$

where v_{EP} and v_{HP} are the fraction of electronlike and holelike Fermi pockets with respect to the whole Brillouin zone. This result is consistent with the proposal of Yang and coworkers [38,39] in the pseudogap phase of underdoped cuprates, but also of fractionalized Fermi liquids [13]. Equation (32) is graphically shown in Fig. 1.

To better understand how the situation depicted in Fig. 1 may occur, let us start from the perturbative regime and, upon varying the Hamiltonian parameters λ, like the interaction strength or the doping, reach the point λ_c at which perturbation theory breaks down, i.e., its convergence radius. For convenience, we assume that $\lambda < \lambda_c$ identifies the perturbative regime and $\lambda > \lambda_c$ the nonperturbative one. Therefore, $\lambda = \lambda_c$ corresponds to the birth of a Luttinger surface and

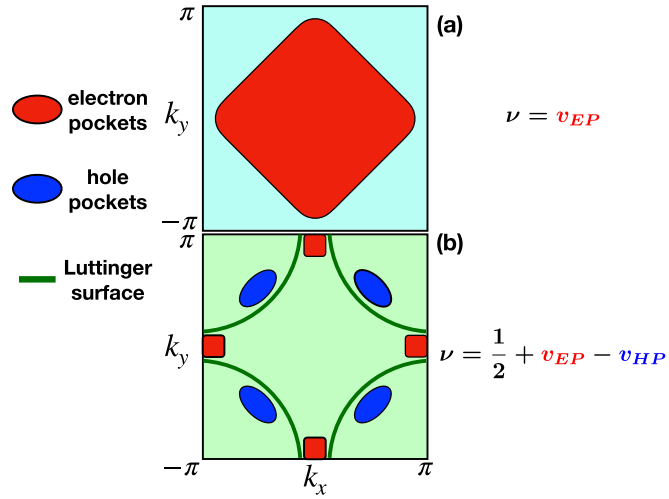

FIG. 1. Graphical representation of electron count when perturbation theory is valid (a), or (b) when it breaks down and a Luttinger surface appears, green line in the figure. Electronlike, i.e., $\epsilon_*(\mathbf{k}) < 0$, and holelike, i.e., $\epsilon_*(\mathbf{k}) > 0$, Fermi pockets are shown, respectively, in red and blue and have volume fraction v_{EP} and v_{HP} with respect to the whole Brillouin zone. When perturbation theory is valid, the electron filling fraction $\nu = N/2V$, where N is the total number of electrons and V the number of sites, is simply given by $\nu = v_{\mathrm{EP}}$, (a). When a Luttinger surface exists, the filling fraction is obtained through $\nu = 1/2 + v_{\mathrm{EP}} - v_{\mathrm{HP}}$, (b).

a concomitant dramatic change within the Brillouin zone: a large Fermi surface either disappears or abruptly turns into small hole and/or electron Fermi pockets, consistently with Eq. (32). Let us try to imagine how that may occur. In general, $\mathrm{Re}\, G(i\epsilon, \mathbf{k}) = \mathrm{Re}\, G(-i\epsilon, \mathbf{k})$ has an even number of roots $2\ell_{\mathbf{k}}$ on the imaginary frequency axis, symmetrically located around $\epsilon = 0$. If we borrow the results obtained in the Hubbard model by single-site dynamical mean field theory (DMFT) [40], see Fig. 2, and translate them in finite dimensions, we expect that at fixed $\epsilon = \epsilon_r > 0$, which is function of λ and vanishes as $\lambda \to \lambda_c$ from below, there is a surface of roots of $\mathrm{Re}\, G(i\epsilon_r, \mathbf{k}_L(\epsilon_r)) = \mathrm{Re}\, G(-i\epsilon_r, \mathbf{k}_L(\epsilon_r))$ or, equivalently, of $\epsilon_*(\epsilon_r, \mathbf{k}_L(\epsilon_r))$, which smoothly evolves into the Luttinger surface as $\lambda \to \lambda_c$. Similarly, we can always define at any small ϵ, thus also at ϵ_r when $\lambda \lesssim \lambda_c$, a surface of zeros of $\epsilon_*(\epsilon, \mathbf{k}_F(\epsilon))$ that are instead smoothly connected to the Fermi surface at $\epsilon = 0$, i.e., the roots of $\epsilon_*(0, \mathbf{k}_F)$. Since $\epsilon_*(\epsilon_r, \mathbf{k})$ are the eigenvalues of a Hermitian operator, if the two surfaces, $\mathbf{k}_L(\epsilon_r)$ and $\mathbf{k}_F(\epsilon_r)$, cross within the Brillouin zone, those are actually avoided crossings. That simply rationalizes the Fermi surface reshaping predicted by Eq. (32), see Fig. 1, as $\lambda \to \lambda_c$, thus $\epsilon_r \to 0$.

In the case of Fig. 2, where the breakdown corresponds to the metal spinodal point, the two zeros at $\epsilon = \pm\epsilon_r$ simply annihilate each other when $\epsilon_r \to 0$ as $\lambda \to \lambda_c$. Beyond single-site DMFT, we cannot exclude that the Luttinger surface survives after the breakdown, thus Eq. (32), changes shape and eventually disappears, as in the case discussed in Ref. [17]. Once that has happened, namely, once the two zeros that had merged at $\epsilon = 0$ finally annihilate each other, it is difficult to ascertain from the behavior at $\epsilon = 0$ whether

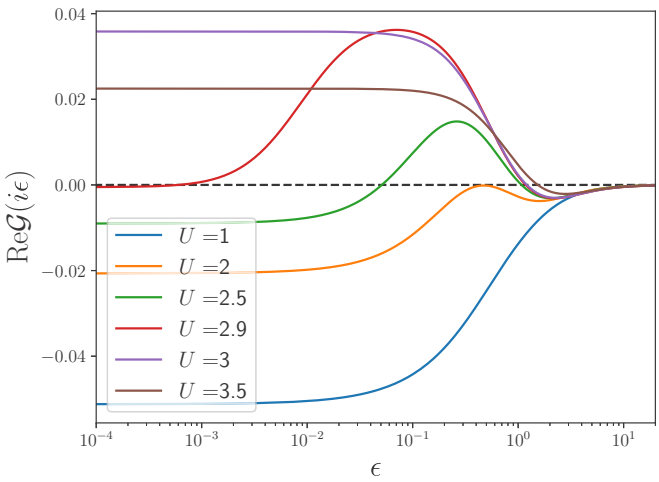

FIG. 2. Real part of the local Green's function as obtained by dynamical mean field theory in the Hubbard model with a very weak chemical potential breaking particle-hole symmetry. Upon increasing the Hubbard U, the model has a transition between a metal and a Mott insulator, which, away from particle-hole symmetry, is first order. In the figure, we show the evolution of $\mathrm{Re}\mathcal{G}(i\epsilon)$ starting from the weak coupling metal and raising U. Note that a double zero first appears in the metal at $U \simeq 2$ at finite ϵ, which signals the birth of the Hubbard bands. Upon further increasing U, that zero splits into two, one moving toward $\epsilon = 0$. The value of $U \simeq 2.9$ at which the root reaches $\epsilon = 0$ corresponds to the metal spinodal point, above which the only stable phase is insulating.

the system is in the perturbative regime, and thus we can use conventional Luttinger's theorem or, instead, perturbation theory has broken down and, in that case, how to count the electron number. There is, however, a circumstance where we can make a firm statement, namely, when the self-energy is local, as in single-site DMFT [40], see Fig. 2, or in impurity models. In that case, the sign of the real part of the impurity Green's function $\mathcal{G}(i\epsilon)$, which is the local Green's function in DMFT, is fixed as $\epsilon \to \infty$, i.e., in the Hartree-Fock regime, and it is negative if the impurity is less than half filled, the case of Fig. 2, and positive otherwise. It follows that, when perturbation theory is valid and Luttinger's theorem holds, then the sign of $\mathrm{Re}\,\mathcal{G}(i\epsilon)$ at $\epsilon = 0$ must be the same as at $\epsilon \to \infty$. When it breaks down, the sign must be opposite, corresponding to the two zeros of $\mathrm{Re}\,\mathcal{G}(i\epsilon)$ that have annihilated each other at $\epsilon = 0$. Therefore, the expectation value of the impurity occupation number close to half filling is

$$n = \sum_\sigma \left(\frac{1}{2} - \int_0^\infty \frac{d\epsilon}{\pi} \frac{\partial \delta(\epsilon)}{\partial \epsilon} \right) - \sum_\sigma \frac{1-(-1)^\ell}{4} \,\mathrm{sign}(\mathrm{Re}\,\mathcal{G}(0)), \tag{33}$$

where now $\delta(\epsilon) = \arg(\mathcal{G}(i\epsilon))$ and ℓ is simply the number of roots of $\mathrm{Re}\,\mathcal{G}(i\epsilon)$ in the semiaxis $0 < \epsilon < \infty$.

In what follows, we discuss a few solvable cases where perturbation theory breaks down and Luttinger's theorem is violated, and test the validity of Eqs. (32) and (33).

III. SDW FLUCTUATION STATE

The first example that we analyze is the model studied in Ref. [20] as representative of a nearly antiferromagnetic Fermi liquids. The model consists of electrons on a V-site cubic or square lattice, with noninteracting dispersion $\epsilon(\mathbf{k})$. The electrons exchange critical longitudinal spin fluctuations, with dynamical susceptibility

$$\chi(i\,\omega, \mathbf{q}) = \frac{\Delta^2}{g} \frac{\delta_{\omega,0}}{T} V\, \delta_{\mathbf{q},\mathbf{Q}}, \tag{34}$$

where $\mathbf{Q} = (\pi, \ldots, \pi)$ and g is the exchange constant. The exact self-energy in the paramagnetic phase reads [20,41]

$$\Sigma(i\epsilon, \mathbf{k}) = \frac{\Delta^2}{i\epsilon - \epsilon(\mathbf{k}+\mathbf{Q})} = \Delta^2\, G_0(i\epsilon, \mathbf{k}+\mathbf{Q}), \tag{35}$$

where $G_0(i\epsilon, \mathbf{k})$ is the no-interacting Green's function, hence

$$G^{-1}(i\epsilon, \mathbf{k}) = G_0^{-1}(i\epsilon, \mathbf{k}) - \Delta^2\, G_0(i\epsilon, \mathbf{k}+\mathbf{Q}). \tag{36}$$

In this case, a Luttinger surface always exists and Luttinger's theorem is violated at any $\Delta \neq 0$ [20]. Through the exact Green's function Eq. (36) one readily finds [20] that, for a single spin species,

$$n(\mathbf{k}) + n(\mathbf{k}+\mathbf{Q}) = \theta(\epsilon_+(\mathbf{k})) + \theta(\epsilon_-(\mathbf{k})), \tag{37}$$

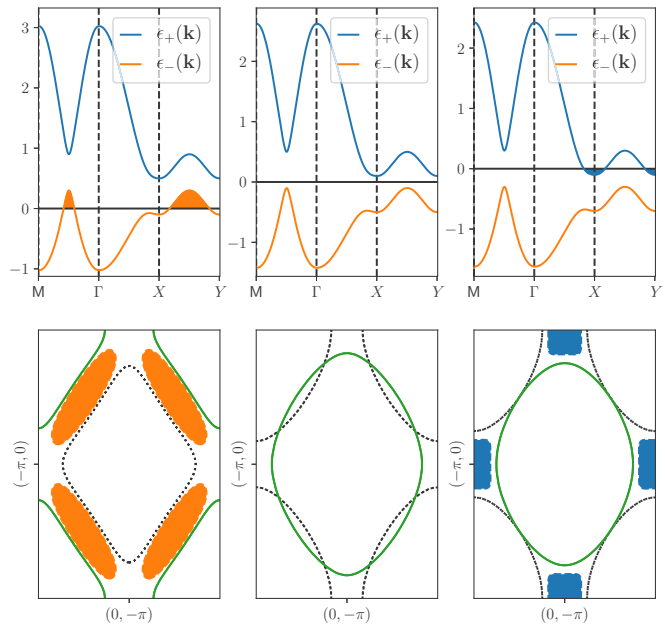

FIG. 3. Top panels: Band structure Eq. (38) on a square lattice with nearest t and next-nearest, $t' = -0.2t$, neighbor hopping, at $\Delta = -0.3$ and different chemical potentials corresponding to hole, left panel, and electron (right panel) doping with respect to half filling (middle panel). Bottom panels: Corresponding Luttinger surface, green line, and Fermi pockets, holelike in orange and electronlike in blue. The noninteracting Fermi surface is also shown, black dotted line. In the present case, our conjecture Eq. (32) predicts that all $\mathbf{k}$ points in the Brillouin zone contribute with one to the total electron number, with the exception of those inside the Fermi pockets, which contribute with zero or with two if the pockets are, respectively, hole- or electronlike.

where

$$\epsilon_{\pm}(\mathbf{k}) = \frac{\epsilon(\mathbf{k}) + \epsilon(\mathbf{k}+\mathbf{Q})}{2} \pm \sqrt{\left(\frac{\epsilon(\mathbf{k}) - \epsilon(\mathbf{k}+\mathbf{Q})}{2}\right)^2 + \Delta^2}, \quad (38)$$

see Fig. 3, so

(1) $n(\mathbf{k}) + n(\mathbf{k}+\mathbf{Q}) = 2\theta(-\epsilon(\mathbf{k}))$ if $\epsilon(\mathbf{k})\epsilon(\mathbf{k}+\mathbf{Q}) > \Delta^2 > 0$,

(2) $n(\mathbf{k}) + n(\mathbf{k}+\mathbf{Q}) = 1$ if $\Delta^2 > \epsilon(\mathbf{k})\epsilon(\mathbf{k}+\mathbf{Q})$.

The quasiparticle residue at $\epsilon = 0$ is now

$$Z(\mathbf{k}) = \frac{\epsilon(\mathbf{k}+\mathbf{Q})^2}{\Delta^2 + \epsilon(\mathbf{k}+\mathbf{Q})^2}, \quad (39)$$

so the Luttinger surface is defined by $\mathbf{k}_L : Z(\mathbf{k}_L) = 0$, i.e., $\mathbf{k}_L : \epsilon(\mathbf{k}_L + \mathbf{Q}) = 0$, while the quasiparticle energy by

$$\epsilon_*(\mathbf{k}) = Z(\mathbf{k}) \frac{1}{\epsilon(\mathbf{k}+\mathbf{Q})} (\epsilon(\mathbf{k})\epsilon(\mathbf{k}+\mathbf{Q}) - \Delta^2), \quad (40)$$

which allows defining the Fermi surface by $\mathbf{k}_F : \epsilon(\mathbf{k}_F)\epsilon(\mathbf{k}_F + \mathbf{Q}) = \Delta^2$. The noninteracting Fermi surface, the interacting Luttinger one, and the interacting Fermi pockets are shown in Fig. 3 for a few exemplary cases. Let us now apply Eq. (32) to calculate the momentum distribution. Through $\epsilon_*(\mathbf{k})$ in Eq. (40), we realize that the Fermi pockets, when they exist, include all $\mathbf{k}$ such that $\epsilon(\mathbf{k})\epsilon(\mathbf{k}+\mathbf{Q}) \geqslant \Delta^2$, and are electronlike if $\epsilon(\mathbf{k}) < 0$ and holelike otherwise. This observation together with Eq. (32) directly yields Eq. (37).

Despite its simplicity, this model is very instructive and yields insights that we believe are rather general. Since the interaction is a δ function in frequency, it is rather easy to express the self-energy as functional of the interacting Green's functions Eq. (36) and of the interaction strength Δ. We find that

$$\Sigma(i\epsilon, \mathbf{k}) = \frac{\sqrt{1 + X(i\epsilon, \mathbf{k}, \mathbf{k}+\mathbf{Q})} - 1}{2G(i\epsilon, \mathbf{k})}, \quad (41)$$

where

$$X(i\epsilon, \mathbf{k}, \mathbf{k}+\mathbf{Q}) \equiv 4\Delta^2 G(i\epsilon, \mathbf{k}) G(i\epsilon, \mathbf{k}+\mathbf{Q}), \quad (42)$$

through which the Luttinger integral can be written as

$$\begin{aligned} I_L(\mathbf{k}, \mathbf{k}+\mathbf{Q}) &= \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \left\{ G(i\epsilon, \mathbf{k}) \frac{\partial \Sigma(i\epsilon, \mathbf{k})}{\partial i\epsilon} + G(i\epsilon, \mathbf{k}+\mathbf{Q}) \frac{\partial \Sigma(i\epsilon, \mathbf{k}+\mathbf{Q})}{\partial i\epsilon} \right\} \\ &= \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \frac{\partial}{\partial i\epsilon} \ln \frac{\sqrt{1 + X(i\epsilon, \mathbf{k}, \mathbf{k}+\mathbf{Q})} + 1}{2} = -\frac{1}{\pi} \operatorname{Im} \ln \frac{\sqrt{1 + X(i0^+, \mathbf{k}, \mathbf{k}+\mathbf{Q})} + 1}{2} \\ &= -\theta(\Delta^2 - \epsilon(\mathbf{k})\epsilon(\mathbf{k}+\mathbf{Q}))\, \theta(\epsilon(\mathbf{k})\epsilon(\mathbf{k}+\mathbf{Q}))\, \operatorname{sign}(\epsilon(\mathbf{k}) + \epsilon(\mathbf{k}+\mathbf{Q})), \end{aligned} \quad (43)$$

consistently with Eq. (8). It is worth noticing that I_L yields an entanglement between the phases $\delta(0, \mathbf{k})$ and $\delta(0, \mathbf{k}+\mathbf{Q})$ of the two Green's functions, which appear as independent quantities in conventional Luttinger's theorem. We believe that is the key role of the Luttinger integral whenever it is finite.

We can take a step further and explicitly build the Luttinger-Ward functional

$$\Phi[G] = \sum_{\mathbf{k}} T \sum_n e^{i\epsilon_n \eta}\, \Phi[G(i\epsilon_n, \mathbf{k}), G(i\epsilon_n, \mathbf{k}+\mathbf{Q})], \quad (44)$$

where the sum over $\mathbf{k}$ is within the reduced Brillouin zone by solving

$$\frac{\delta \Phi[G(i\epsilon, \mathbf{k}), G(i\epsilon, \mathbf{k}+\mathbf{Q})]}{\delta G(i\epsilon, \mathbf{k})} = \Sigma(i\epsilon, \mathbf{k}). \quad (45)$$

We find that $\Phi[G(i\epsilon_n, \mathbf{k}), G(i\epsilon_n, \mathbf{k}+\mathbf{Q})]$ is actually a functional $\Phi[X]$ of X in Eq. (42), specifically

$$\Phi[X] = \sqrt{1+X} - 1 - \ln \frac{\sqrt{1+X}+1}{2}. \quad (46)$$

We end noticing that the square root in the expression Eq. (41) of $\Sigma(i\epsilon, \mathbf{k})$ implies that the inverse of Dyson's equation,

$$G_0(i\epsilon, \mathbf{k})^{-1} = G(i\epsilon, \mathbf{k})^{-1} + \frac{\delta \Phi[G]}{\delta G(i\epsilon, \mathbf{k})}, \quad (47)$$

generally admits two solutions $G_0(i\epsilon, \mathbf{k})$, only one of which is physical. This result agrees with evidence [42–45] that the Luttinger-Ward functional may become multivalued upon increasing the interaction strength.

IV. PSEUDOGAP IMPURITY MODEL

Let us now discuss the failure of Luttinger's theorem in the impurity model studied in Ref. [18] by numerical renormalisation group (NRG). For convenience, we consider a slightly different model with the same physical properties, which was thoroughly investigated in Ref. [46], thus saving us from recalculating the whole phase diagram. The model represents a two-orbital Anderson impurity with inverted Hund's rules. The Hamiltonian is

$$H = H_0 + H_{\text{imp}}, \quad (48)$$

where

$$H_0 = \sum_{i=1}^{2} \sum_{\mathbf{k}\sigma} [\epsilon_{\mathbf{k}}\, c^{\dagger}_{i\mathbf{k}\sigma}\, c_{i\mathbf{k}\sigma} + V_{\mathbf{k}}\, (c^{\dagger}_{i\mathbf{k}\sigma}\, d_{i\sigma} + \text{H.c.})] \quad (49)$$

is the sum of two equivalent resonant level models and

$$H_{\text{imp}} = \epsilon_d\, (n-2) + \frac{U}{2}(n-2)^2 - 2J\, (\boldsymbol{T} \cdot \boldsymbol{T} - T_3^2), \quad (50)$$

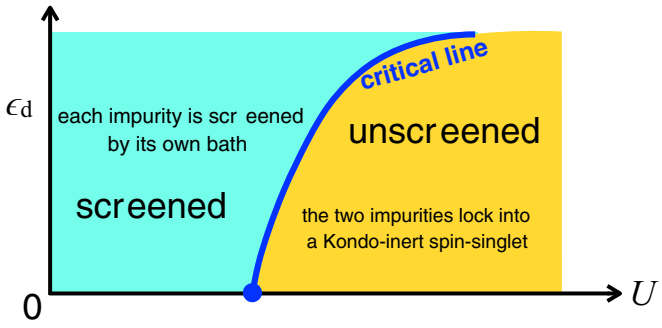

FIG. 4. Phase diagram of the impurity model Eq. (48) at fixed hybridization width Γ and $J \ll \Gamma$, as function of U and $\epsilon_d > 0$. The case $\epsilon_d < 0$ is symmetric.

where $n = \sum_{i\sigma} n_{i\sigma}$, with $n_{i\sigma} = d^\dagger_{i\sigma} d_{i\sigma}$ the occupation number of the impurity orbital $i = 1, 2$ with spin σ, while $\boldsymbol{T} = (T_1, T_2, T_3)$ is a pseudospin operator with

$$T_a = \frac{1}{2} \sum_\sigma \sum_{ij} d^\dagger_{i\sigma} \, (\hat{\tau}_a)_{ij} \, d_{j\sigma}, a = 1, 2, 3, \tag{51}$$

and $\hat{\tau}_a$ the Pauli matrices in the two-orbital space. We assume that H_0 in Eq. (49) is particle-hole (p-h) symmetric, so a finite ϵ_d in Eq. (50) is the only source of p-h symmetry breaking. In the following calculations, we take a hybridization width

$$\Gamma(\epsilon) \equiv \pi \sum_{\mathbf{k}} V^2_{\mathbf{k}} \, \delta(\epsilon - \epsilon_{\mathbf{k}}) = \Gamma \, \theta(1 - |\epsilon|), \tag{52}$$

with $\Gamma = 0.1$, which also defines our unit of energy, and $J = 0.004 \ll \Gamma$.

When U is large, the impurity is occupied by two electrons that can form a spin-triplet orbital-singlet ($S = 1$, $T = 0$) or a spin-singlet orbital-triplet ($S = 0$, $T = 1$). If $J > 0$, as we assume, the lowest energy state,

$$\frac{1}{\sqrt{2}} \, (d^\dagger_{1\uparrow} \, d_{2\downarrow} + d^\dagger_{2\uparrow} \, d_{1\downarrow}) \, |0\rangle \, , \tag{53}$$

has $S = 0$, $T = 1$, and $T_3 = 0$. If we regard the two orbitals as the single orbitals of two impurities, state Eq. (53) simply represents the two impurities coupled into a spin-singlet configuration. In other words, for large U the Hamiltonian Eq. (48) is actually equivalent to two spin-1/2 impurities, each Kondo coupled to its own bath and coupled to each other by an antiferromagnetic exchange, which is the model studied in Ref. [18]. The phase diagram of this model depends on the magnitude of J relative to the Kondo temperature T_K at $J = 0$. If $J \ll T_K$, each impurity is Kondo screened by its bath, leading to a conventional Kondo effect. On the contrary, if $J \gg T_K$, the two impurities lock into a Kondo-inert spin-singlet state. These two regimes, which we denote as screened and unscreened phases, are separated by a quantum critical point [47], actually a whole critical line at $\epsilon_d \neq 0$ [46]. Since we work at constant Γ and $J \ll \Gamma$, and T_K decreases with increasing U, the critical point is reached upon increasing U. Specifically, with the chosen Γ and J, its location is at $U_c \simeq 1.85$ when $\epsilon_d = 0$. In Fig. 4, we sketch the phase diagram as a function of U and $\epsilon_d > 0$.

The screened, $U < U_c$, and unscreened, $U > U_c$, phases are both local Fermi liquids in Nozières sense [48], despite the unscreened phase not being adiabatically connected to the noninteracting limit $U = J = 0$. For instance, at p-h symmetry, $\epsilon_d = 0$, the impurity self-energy in the unscreened phase diverges at the Fermi level [46], the local counterpart of a Luttinger surface, which leads to a pseudogap in the DOS that is gradually filled in when $\epsilon_d \neq 0$ [46]; a totally different behavior from a noninteracting resonant-level model.

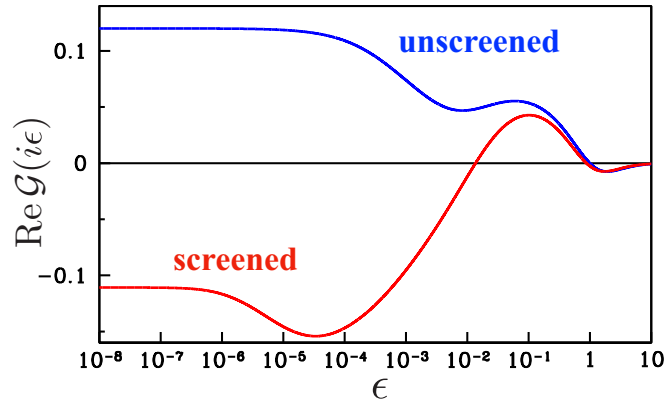

FIG. 5. Re $\mathcal{G}(i\epsilon)$ versus the Matsubara frequency ϵ at $\epsilon_d = 0.1$ in the screened phase, $U = 1.75$ red curve, and in the unscreened one, $U = 2$ blue curve.

A. Fate of Luttinger's theorem in the impurity model

The Hamiltonian Eq. (48) at $\epsilon_d \neq 0$ is invariant under global spin SU(2), separate charge $U(1)$ rotations in each channel $i = 1, 2$, that includes the conduction bath and the corresponding impurity level as well as under the Z_2 symmetry $1 \leftrightarrow 2$. If the conduction bandwidth is large enough, as we assume hereafter, the conserved quantities become effectively those at the impurity site, since the fluctuations in the bath are negligible. The impurity Green's function is

$$\mathcal{G}(i\epsilon) = \frac{1}{i\epsilon - \epsilon_d + i\,\Gamma - \mathrm{Re}\,\Sigma(i\epsilon) - i\,\mathrm{Im}\,\Sigma(i\epsilon)} \tag{54}$$

and, by symmetry, is independent of $i = 1, 2$ and $\sigma = \uparrow, \downarrow$, and therefore Eq. (33) reads

$$n_{i\sigma} = \left(\frac{1}{2} - \frac{\arg(\mathcal{G}(i\infty)) - \arg(\mathcal{G}(0))}{\pi} \right) - \frac{1 - (-1)^\ell}{4} \, \mathrm{sign}(\mathrm{Re}\,\mathcal{G}(0)), \tag{55}$$

where the term in parentheses is just the conventional statement of Luttinger's theorem that was shown in Ref. [18] not to yield the correct result in the unscreened phase at $\epsilon_d \neq 0$. The last term in Eq. (55), which corrects that result when Luttinger's theorem fails, is finite only when the number ℓ of zeros of Re $\mathcal{G}(i\epsilon)$ for $0 < \epsilon < \infty$ is odd. Figure 5 shows Re $\mathcal{G}(i\epsilon)$ in the screened and unscreened phases at $\epsilon_d = 0.1$. Not surprisingly, ℓ is even in the screened phase and odd in the unscreened one, in which case the last term in Eq. (55) is finite and equal to $-1/2$. For $\epsilon_d < 0$, the correction is actually $+1/2$ since the real part of $\mathcal{G}(i\epsilon)$ changes signs after a particle-hole transformation that brings $\epsilon_d \to -\epsilon_d$.

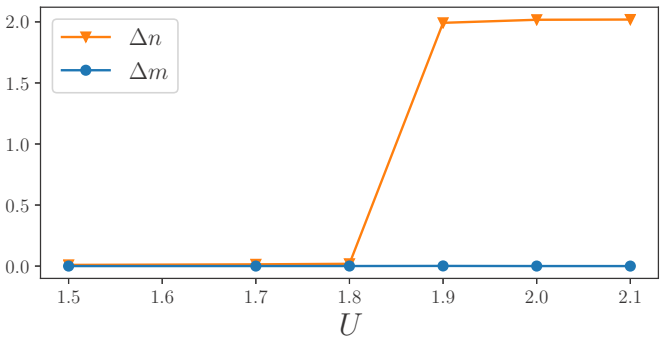

FIG. 6. The behavior of $\Delta n = n_L - n$ and $\Delta m = m_L - m$ as function of U at $\epsilon_d = 0.1$ and $B = 0.0001$. Here, n_L and m_L are, respectively, the electron number and magnetization calculated through Luttinger's theorem, while n and m their actual value.

The $\pm 1/2$ correction is exactly the missing quantized term noticed in Ref. [18], and thus Eq. (55) does reproduce the correct electron number. We note that Fig. 5 explicitly demonstrates that, crossing the point at which perturbation theory breaks down, ℓ changes by one, from $\ell = 2$ in the screened phase to $\ell = 1$ in the unscreened one, as earlier discussed.

Besides the electron number, $n = \sum_{i\sigma} n_{i\sigma}$, the Hamiltonian Eq. (48) admits other conserved quantities, e.g., the magnetization $m = \sum_i (n_{i\uparrow} - n_{i\downarrow})$ and the relative orbital occupancy $n_f = \sum_\sigma (n_{1\sigma} - n_{2\sigma})$. A field that couples to any of those conserved quantities does not spoil the quantum critical point [46]. We may then wonder whether conventional Luttinger's theorem also fails in providing the values of those quantities as it does for the electron number when crossing the critical point. Let us consider, for instance, the magnetization m. According to Luttinger's theorem, we could calculate m through

$$m_L = \sum_{i=1}^{2} \frac{\arg(\mathcal{G}_{i\uparrow}(0)) - \arg(\mathcal{G}_{i\downarrow}(0))}{\pi}. \tag{56}$$

Evidently, both m and m_L vanish when SU(2) symmetry holds. Therefore, we add to the Hamiltonian Eq. (48) with $\epsilon_d = 0.1$ a Zeeman splitting term $-Bm$, with very small $B = 0.0001$ that nonetheless makes $\mathcal{G}_{1\uparrow}(i\epsilon) = \mathcal{G}_{2\uparrow}(i\epsilon) \neq \mathcal{G}_{1\downarrow}(i\epsilon) = \mathcal{G}_{2\downarrow}(i\epsilon)$. In Fig. 6, we show the deviation Δm of m_L in Eq. (56) from the actual value m as function of U. For comparison, we also plot the deviation Δn of the Luttinger's theorem prediction for the number of particles,

$$n_L = 4 + \sum_{i\sigma} \frac{\arg(\mathcal{G}_{i\sigma}(0))}{\pi}, \tag{57}$$

from the correct result n. We observe that while Δn jumps from 0 to 2 crossing the critical point, consistent with the missing contribution from the Luttinger integral, see Eq. (55), Δm remains always zero, showing that the corresponding Luttinger integral vanishes also in the unscreened phase, despite the breakdown of perturbation theory. In reality, if we instead take $B \gg \epsilon_d$, the situation is reversed: Δm jumps from 0 to -2, while Δn remains zero.

More generally, if we add different fields ϵ_d, B, and B_f that couple to n, m, and n_f, respectively, the strongest one identifies the channel where Luttinger's theorem breaks down, whereas the theorem still applies for the other two channels.

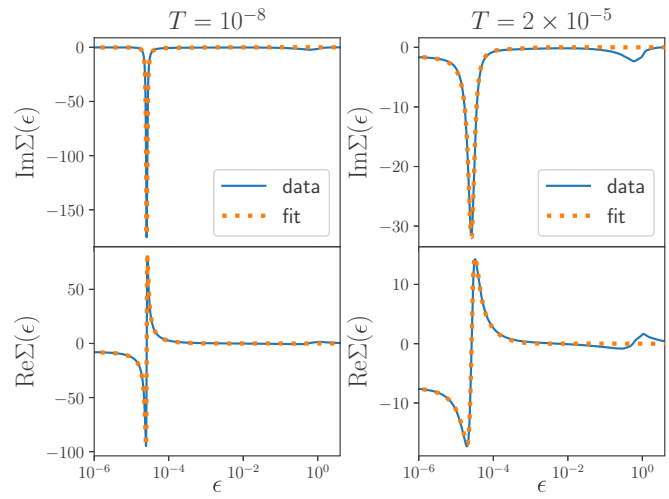

FIG. 7. Real and imaginary parts of the retarded self-energy at $U = 2$, $\epsilon_d = 0.1$, and temperatures $T = 10^{-8}$, left panels, and $T = 2 \times 10^{-5}$, right panels, together with the ansatz Eq. (58) with fitted parameters (dotted lines).

B. The unscreened phase as paradigm of a pseudogapped metal

A lot of effort over the past decades has been put into modeling the self-energy of the pseudogap phase in underdoped cuprates [38,39,49,50], also revealed by cluster extensions of DMFT in the Hubbard model doped away from the half-filled Mott insulator [23,26,27,51]. Since the unscreened phase of the impurity model Eq. (48) is also pseudogapped [46], it is worth modeling its self-energy, which is easily accessible by NRG at and away from p-h symmetry, as well as at zero and finite temperature.

We find that the retarded impurity self-energy $\Sigma_+(\epsilon) \equiv \Sigma(\epsilon + i0^+)$ in the unscreened phase is well fitted at low energy ϵ and temperature T by Refs. [10,11], see Fig. 7,

$$\Sigma_+(\epsilon) = \frac{\Delta^2}{\epsilon - \mu + i\,\gamma\,(\epsilon^2 + \pi^2\,T^2)}, \tag{58}$$

where all real parameters Δ, μ, and γ depend on U, T, and on the strength ϵ_d of the p-h symmetry-breaking term. In particular, Δ^2 and $1/\gamma$ vanish quadratically approaching the critical line $U = U_c$ [46], while, consistently with Fig. 5, μ has the same sign of ϵ_d and vanishes at $\epsilon_d = 0$. In Fig. 8, we show the parameters Δ and γ extracted by the fit as function of T and different $U > U_c$ at $\epsilon_d = 0.1$.

At $T = \epsilon_d = 0$,

$$\Sigma_+(\epsilon) = \frac{\Delta^2}{\epsilon + i\,\gamma\,\epsilon^2} \underset{\epsilon\to 0}{\simeq} \frac{\Delta^2}{\epsilon} - i\,\gamma\,\Delta^2, \tag{59}$$

corresponds to the highly singular expression found in Ref. [46], which, as earlier mentioned, is the local counterpart of a Luttinger surface. On the contrary, at $\epsilon_d \neq 0$ and for $\epsilon, T \ll \mu$,

$$\Sigma_+(\epsilon) \simeq -\frac{\Delta^2}{\mu} - \frac{\Delta^2}{\mu^2}\,\epsilon - i\,\frac{\Delta^2\,\gamma}{\mu^2}\,(\epsilon^2 + \pi^2\,T^2) \tag{60}$$

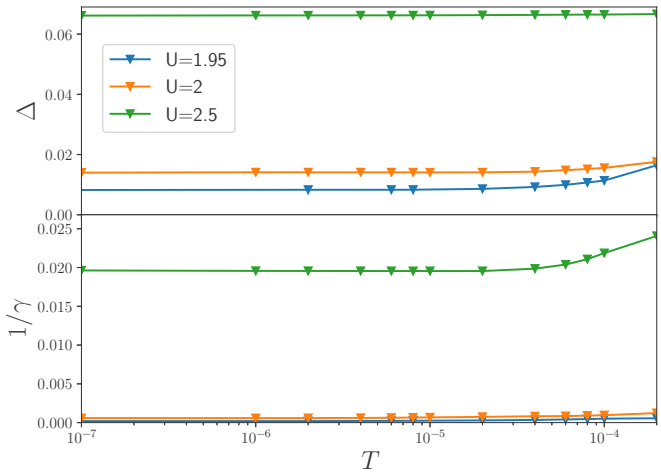

FIG. 8. Temperature dependence of the parameters Δ and γ in Eq. (58) fitted through NRG results at $\epsilon_d = 0.1$ and different $U > U_c$. We note that both Δ^2 and $1/\gamma$ vanish approaching U_c, although $1/\gamma \ll \Delta^2$.

has a conventional Fermi-liquid behavior, despite the spectral function pseudogap, and the Luttinger surface has disappeared.

The quantum critical point entails the existence at finite temperature of a quantum critical region delimited by a crossover temperature T_* that, in the unscreened phase, can be identified with the temperature below which the pseudogap opens, see Fig. 9 where we plot the impurity DOS $\rho(\epsilon)$, at $\epsilon_d = 0.1$, $U = 2$ and different T. The phase diagram Fig. 4 shows that the critical line can be also crossed starting from the unscreened phase at particle-hole symmetry and rising ϵ_d, namely, by doping. In Fig. 10, we show how the parameter μ behaves as function of ϵ_d from 0 up to the critical point $\epsilon_d \simeq 0.26$ at $U = 2$ and almost zero temperature.

We remark that a key feature of the self-energy Eq. (58) is the imaginary part in the denominator, i.e., $\gamma(\epsilon^2 + \pi^2 T^2)$, vanishing quadratically for $\epsilon, T \to 0$, see Fig. 11. This

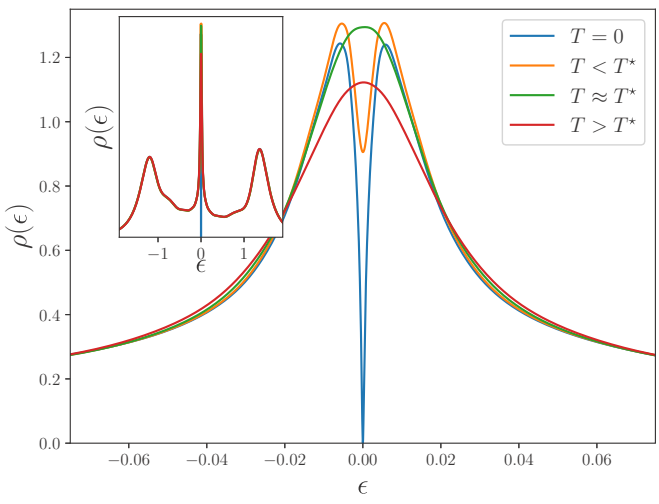

FIG. 9. Impurity density of states at $U = 2$, $\epsilon_d = 0.1$ and different temperatures below and above the pseudogap temperature T_*.

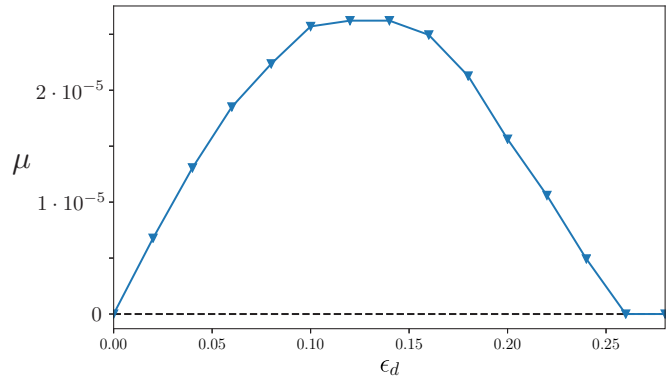

FIG. 10. Parameter μ in Eq. (58) at $T = 10^{-8}$ and $U = 2$ as function of ϵ_d from 0 to above the critical point, see Fig. 4.

guarantees the existence of a well-defined quasiparticle excitation, namely, whose decay rate at $T = 0$,

$$\gamma(\epsilon) \equiv -Z(\epsilon)\,\mathrm{Im}\,\Sigma_+(\epsilon) \propto \epsilon^2, \tag{61}$$

with

$$Z(\epsilon) = \left(1 - \frac{\partial \mathrm{Re}\,\Sigma_+(\epsilon)}{\partial \epsilon}\right), \tag{62}$$

vanishes at zero energy, even in the singular case at p-h symmetry [10,11]. Such a property distinguishes Eq. (58) from all model self-energies introduced to describe the pseudogap phase of underdoped cuprates, where either the imaginary part is missing or assumed to be constant. We believe that Eq. (58), though referring to a specific impurity model, is actually representative of generic pseudogap metal phases and thus can be regarded as paradigmatic of such physical systems.

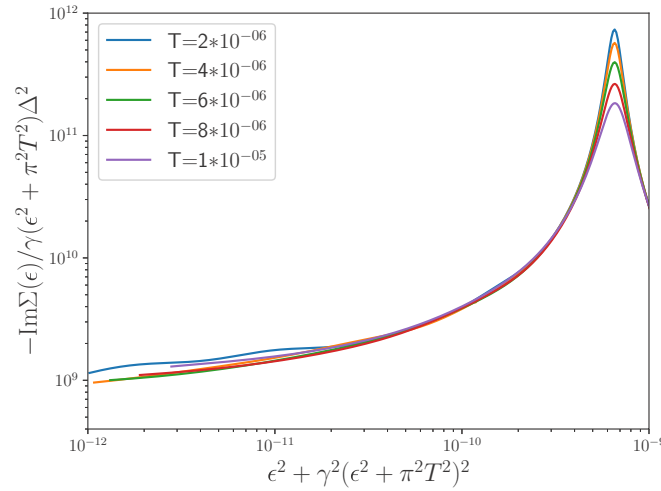

FIG. 11. Imaginary part of the self-energy in Eq. (60) divided by $\Delta^2\,\gamma\,(\epsilon^2 + \pi^2\,T^2)$ as function of $(\epsilon^2 + \pi^2\,T^2)$ for different T at $\epsilon_d = 0.1$ and $U = 2$. Note the collapse of all curves at low Matsubara frequencies.

V. LUTTINGER'S THEOREM IN A NONMAGNETIC MOTT INSULATOR

We now discuss the failure of Luttinger's theorem in the nonmagnetic two-orbital Mott insulator analyzed in Ref. [17]. The model is essentially the bulk generalization of the two-orbital Anderson impurity model Eq. (48), with U and J much larger than width W of the conduction band, whose dispersion is assumed to be $\epsilon_{ij}(\mathbf{k}) = \delta_{ij}\,\epsilon_{\mathbf{k}}$, with $i, j = 1, 2$ the orbital indices. In that limit and for small enough deviation μ from particle-hole symmetry, the ground state of the model represents a nonmagnetic Mott insulator with two electrons per site, each in a different orbital, locked into a spin singlet. The spin and orbital-independent Green's function is

$$G(i\epsilon, \mathbf{k}) = \frac{1}{i\epsilon - \epsilon_{\mathbf{k}} + \mu - \Sigma(i\epsilon, \mathbf{k})}, \tag{63}$$

where, absorbing the Hartree-Fock self-energy in μ, and to leading order in the hopping [17],

$$\Sigma(i\epsilon, \mathbf{k}) \simeq \frac{\Delta^2}{i\epsilon + \mu}, \tag{64}$$

with $2\Delta = U + 6J$ for the Hamiltonian Eq. (48). Rigorously speaking, the expression Eq. (64) is valid if also $|\mu| \gg W$, otherwise additional $\mathbf{k}$-dependent terms appear in the denominator [17]. Therefore, we hereafter assume consistently that

$$U, J, |\mu| \gg W, \tag{65}$$

which also implies that a Luttinger surface is absent. The Green's function Eq. (63) describes an insulator lacking a Fermi surface if

$$\mathrm{Re}\, G(0, \mathbf{k})^{-1} = G(0, \mathbf{k})^{-1} = -\epsilon_{\mathbf{k}} + \mu - \frac{\Delta^2}{\mu} \tag{66}$$

never vanishes within the Brillouin zone. That implies either $0 < \mu < \mu_+$, in which case $G(0, \mathbf{k})^{-1} < 0$, or $\mu_- < \mu < 0$, in which case $G(0, \mathbf{k})^{-1} > 0$, where [17]

$$\mu_+ + \mu_- = \epsilon_{\mathbf{k}}, \quad \mu_+ - \mu_- = \sqrt{\epsilon_{\mathbf{k}}^2 + 4\Delta^2} \simeq 2\Delta. \tag{67}$$

If we use conventional Luttinger's theorem, according to which the number of electrons per site is simply $n = 2 + 2\,\mathrm{sign}(G(0, \mathbf{k})^{-1})$, we obtain the wrong result that $n = 4$ if $\mu_- < \mu < 0$ and $n = 0$ if $0 < \mu < \mu_+$. However, in this case, we can use Eq. (33) to calculate the correct electron number. Indeed, since

$$\lim_{\epsilon \to \infty} \mathrm{Re}\, G(i\epsilon, \mathbf{k})^{-1} = \mu - \epsilon_{\mathbf{k}} \simeq \mu, \tag{68}$$

the $\mathrm{Re}\, G(i\epsilon, \mathbf{k})$ crosses zero an odd number of times from $\epsilon = 0$ to $\epsilon = \infty$. According to Eq. (33), valid for a local self-energy close to halffilling, that implies $n_{1\mathbf{k}\sigma} + n_{2\mathbf{k}\sigma} = 1$, which is indeed correct.

If the condition $|\mu| \gg W$ is not fulfilled, the no more negligible momentum dependent terms in the denominator of the self-energy Eq. (64) yield a true Luttinger surface for a small interval of μ around zero [17], in which case Eq. (32) provides the correct electron number.

A. Atomic limit of the SU(N) Hubbard model

At $J = 0$, the previous model becomes the $N = 4\mathrm{SU}(N)$ Hubbard model at half filling, which admits, for strong enough U, a Mott insulating state at any integer density $n = 1, \ldots, N-1$. In the atomic limit, $W = 0$, this model also strongly violates Luttinger's theorem [22]. However, the ground state in the atomic limit has an extensive degeneracy, $\binom{N}{n}$ per site, and thus divergent susceptibilities. In this situation, one does not expect Luttinger's theorem to apply [9,29].

Nonetheless, to make a connection with the previous discussion, we note that the sum of the N local Green's functions in the atomic limit at $T = 0$ [22],

$$\begin{aligned} N\,G(i\epsilon) &= \frac{n}{i\epsilon + \epsilon_-} + \frac{N-n}{i\epsilon - \epsilon_+} \\ &= \frac{\partial}{\partial i\epsilon} \ln (i\epsilon + \epsilon_-)^n\,(i\epsilon - \epsilon_+)^{N-n} \\ &\equiv -\frac{\partial \ln G_N(i\epsilon)}{\partial i\epsilon}, \end{aligned} \tag{69}$$

where $\epsilon_+ = Un - \mu > 0$ and $\epsilon_- = \mu - U(n-1) > 0$ are, respectively, the energies for adding and removing an electron from the atomic n-particle ground state. Therefore,

$$\begin{aligned} N\,G(i\epsilon)\,\frac{\partial \Sigma(i\epsilon)}{\partial i\epsilon} &= N\,G(i\epsilon) + \frac{\partial \ln G(i\epsilon)^N}{\partial i\epsilon} \\ &= \frac{\partial}{\partial i\epsilon} \ln \frac{G(i\epsilon)^N}{G_N(i\epsilon)} \end{aligned}$$

is consistent with Eq. (8) and quantized. In this case, it trivially follows that the role of the Luttinger integral is to freeze the occupation per orbital at n/N rather than the value predicted by Luttinger's theorem, which is either 0 or 1 [22] depending on μ, in that similar to what we have found close to a half-filled Mott insulator. This suggests a natural extension of our results to multiband models close to a Mott insulator at fractional filling n/N.

We end observing that $G_N(i\epsilon)$ is equivalent to the determinant of the $N \times N$ Green's function matrix corresponding to the same Hamiltonian but in the presence of an infinitesimally small symmetry-breaking field that lowers n orbitals with respect to the other $N - n$ ones. In this case, Luttinger's theorem does hold, as Logan *et al.* have explicitly demonstrated in the simpler SU(2) case [52].

VI. DISCUSSION

We have shown that the Luttinger integral, which provides the missing contribution to the electron count when Luttinger's theorem is violated, is a boundary zero-energy term and is quantized in integer values when the self-energy is analytic at any nonzero imaginary frequency. Specifically, in a periodic single-band model of interacting electrons, Luttinger's theorem is violated when perturbation theory breaks down and a Luttinger surface appears in the Brillouin zone. Taking properly into account the quantized contribution from the Luttinger surface, we have found that the volume fraction of the Fermi pockets only measures the doping frac-

tion away from half-filling rather than the full-filling fraction.

In addition, a byproduct of our derivation of Luttinger's theorem is the prediction that quasiparticles do exist even in half-filled non-symmetry-breaking Mott insulators, provided they possess a Luttinger surface, thus extending the results of Ref. [11] to the case of a hard gap. We emphasize that our formal construction in Sec. II just relies on the assumption Eq. (23), with no reference to a model Hamiltonian. However, the analogy with so-called $U(1)$ spin-liquid insulators [53–57] is self-evident, and suggests that the quasiparticles are actually spinons, and the Luttinger surface their Fermi surface.

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