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Fermi surface volume of interacting systems

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ABSTRACT

Three Fermion sumrules for interacting systems are derived at $T = 0$, involving the number expectation $\bar{N}(\mu)$, canonical chemical potentials $\mu(m)$, a logarithmic time derivative of the Greens function $\gamma_{\vec{k}\sigma}$ and the static Greens function. In essence we establish at zero temperature the sumrules linking:

$$\bar{N}(\mu) \leftrightarrow \sum_{m} \Theta(\mu - \mu(m)) \leftrightarrow \sum_{\vec{k},\sigma} \Theta\left(\gamma_{\vec{k}\sigma}\right) \leftrightarrow \sum_{\vec{k},\sigma} \Theta\left(G_{\sigma}(\vec{k}, 0)\right).$$

Connecting them across leads to the Luttinger and Ward sumrule, originally proved perturbatively for Fermi liquids. Our sumrules are nonperturbative in character and valid in a considerably broader setting that additionally includes non-canonical Fermions and Tomonaga–Luttinger models. Generalizations are given for singlet-paired superconductors, where one of the sumrules requires a testable assumption of particle–hole symmetry at all couplings. The sumrules are found by requiring a continuous evolution from the Fermi gas, and by assuming a monotonic increase of $\mu(m)$ with particle number m. At finite T a pseudo-Fermi surface, accessible to angle resolved photoemission, is defined using the zero crossings of the first frequency moment of a weighted spectral function.

1. Introduction

The Luttinger–Ward (LW) sumrule [1] for interacting electrons expresses the number of electrons in terms of the static limit of the imaginary frequency Greens function [2–4] for $T \to 0$ as

$$\bar{N}(\mu) = \sum_{\vec{k},\sigma} \Theta\left(G_{\sigma}(\vec{k}, \omega = 0|\mu)\right), \tag{1}$$

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with $\Theta(x) = \frac{1}{2}(1 + \mathrm{sgn}(x))$. Since the static Greens function is negative outside the Fermi surface, its volume is fixed by the number of particles [1,4,5], independent of the magnitude of the interaction. This interaction independence is a fundamental result in Landau's theory of the Fermi liquid [6,7]. In condensed matter physics, field theory and statistical mechanics, the origin of this sumrule and its ramifications have been very influential [4,7–11]. It has continued to receive much attention to recent times [12–24], partly motivated by the search for novel phases of matter that might violate this sumrule. The present work provides a physically transparent derivation of the sumrule, and extends it in several directions. The extended version includes non-Fermi liquids, such as the 1-d Tomonaga–Luttinger model (TLM). It is also valid for non-canonical Fermions, such as $U = \infty$ Gutzwiller projected electrons in the t-J model, in treatments where continuity with the Fermi gas is maintained [25], but not otherwise [23,26]. Our extension also includes singlet pairing superconductors. These include the s-wave BCS–Gor'kov–Nambu case and d-wave cuprate superconductors. While analyticity in the coupling is lost in these extensions, they do evolve continuously from the non-interacting limit, which suffices for our purposes. Exotic superconductors, where one hollows out the k-space [27], provide an interesting counter-point where continuity with the gas limit is discarded; we need to exclude them here too.

Since the static Greens function entering Eq. (1) is not directly measurable, one needs to relate it to other directly visible signatures for using it. This work provides a new and experimentally accessible sum-rule Eq. (79), which is equivalent to Eq. (1) at $T = 0$ in the cases considered. It also allows one to define a pseudo Fermi surface at any T. This surface carries useful information on the real part of the on-shell selfenergy.

1.1. Methods used

The technique used here is non-perturbative, it relies on *isothermal* continuity in some parameter λ connecting the interacting and non-interacting systems. Since this type of continuity has not been explicitly discussed in literature, a few words are in order. As some parameter in the Hamiltonian is varied, the variation is required to be isothermal, i.e. at each intermediate value of the parameter, the system is allowed to repopulate energy levels according to the thermal distribution. This is in contrast to adiabatic variations where the population of the energy levels is frozen at their starting values. By continuity we imply that the expectation of the energy and other observables change without discontinuity, i.e. we rule out first order transitions. Illustrating the distinction we note that the change of shape of the Fermi surface for anisotropic systems is allowed by isothermal continuity, but not by adiabatic continuity. Finally our method does not require analyticity in a coupling, isothermal continuity is sufficient for our purpose.

Our other main assumption is that the canonical ensemble (CE) chemical potentials $\mu(m)$ increase monotonically with the particle number m, whereby the canonical free energy is a concave-up function of m. This is tantamount to ruling out phase separation. We argue in Section 2 that such a monotonic behavior could be regarded as a defining feature of repulsive interactions.

In each case covered by our argument, at non-zero T we construct an effective particle density $n_{eff}(T)$, and pseudo-Fermi surface, whose temperature variation reveals lowest lying characteristic energy scales in the system. The pseudo-Fermi surface has the potential to be studied using angle resolved photoemission (ARPES) technique, and hence is discussed in some detail in Section 7

1.2. Organization of the paper

The paper is organized as follows. I first establish in Section 2 a basic thermodynamic number sumrule for electrons with repulsive interactions;

$$\bar{N}(\mu) = \sum_{m=0}^{N_{max}-1} \Theta(\mu - \mu(m)), \tag{2}$$

where the CE chemical potential $\mu(m) = F_{m+1} - F_m$ is the difference of the canonical free energies F with $m+1$ and m particles. We will assume a hard-core set of particles, and therefore the maximum

number of particles is limited by N_{max}. In Section 3 I next introduce γ, the temporal log-derivative of the Greens function:

$$\gamma_{\vec{k}\sigma}(\mu, T) = \lim_{\tau=\beta/2} \partial_\tau \log G_\sigma(\vec{k}, \tau|\mu), \quad \beta = \frac{1}{k_B T}. \tag{3}$$

Setting $\tau = \beta/2$ sandwiches each Fermionic operator of G symmetrically by factors that project all contributing states to the ground state as $T \to 0$. While the study of $G_\sigma(\vec{k}, \frac{\beta}{2}|\mu)$ is popular in quantum Monte-Carlo studies [28], the log-derivative, playing a key role in this work, has not been discussed earlier. Its physical content at low T, as μ minus a $\vec{k}$-weighted average over $\mu(m)$ becomes clear later (see Eq. (32)). In Section 3 we make an important distinction between two ways of taking the zero temperature and thermodynamic limits, in **Limit-I** we take T→0 first and $L \to \infty$ later, while in **Limit-II** we take $L \to \infty$ first and $T \to 0$ later.

In Section 4 the $T = 0$ limit is taken first (i.e. in the limit **Limit-I**), and shown to lead to the sumrule

$$\sum_{\vec{k},\sigma} \Theta\left(\gamma_{\vec{k}\sigma}(\mu, 0)\right) = \sum_m \Theta(\mu - \mu(m)). \tag{4}$$

This is demonstrated for the Fermi liquid and also for the 1-d case of a Tomonaga–Luttinger model.

In Section 5 the $L \to \infty$ limit is taken first (i.e. in the limit **Limit-II**), whereby we obtain a continuous frequency variable in terms of which a spectral function can be defined. Here the sumrule

$$\sum_{\vec{k},\sigma} \Theta\left(\gamma_{\vec{k}\sigma}(\mu, 0^+)\right) = \sum_{\vec{k},\sigma} \Theta\left(G_\sigma(\vec{k}, \omega = 0|\mu)\right), \tag{5}$$

is established for Fermi liquids in Section 5.1 and for 1-d TLL systems in Section 5.2.

Assuming unbroken symmetry, powerful theorems on the uniqueness of the ground state [29,30] are applicable, these allows us to equate the two zero temperature limits

$$\gamma_{\vec{k}\sigma}(\mu, 0) = \gamma_{\vec{k}\sigma}(\mu, 0^+). \tag{6}$$

Upon using Eqs. (2), (7), (4), (5) (or Eqs. (8), (75)) then imply the sumrule Eq. (1). In the infinite volume limit, the $\vec{k}$ sums are replaced by integrals as usual.

In Section 6 a systematic development of the volume theorem for a singlet superconducting state is provided. This broken symmetry state not accessible by the methods of L–W. In Section 6.1 we study the canonical chemical potentials $\mu_e(2m) \equiv \frac{1}{2}(F_{2m+2} - F_{2m})$ constrained to the even particle sector. The $\mu_e(2m)$ are taken to be monotonically increasing in m, reflecting the inherent repulsion between pairs of electrons. In this ensemble we study the effects of adding or removing a particle and thence the Greens function, leading to the sumrule

$$\bar{N}_{SC}(\mu) = 2 \sum_{m=0}^{\frac{1}{2}N_{max}} \Theta(\mu - \mu_e(2m)), \tag{7}$$

which replaces Eq. (2) in the normal state.

In Section 6.2 the Greens function and $\gamma_{\vec{k}}$ are studied at T = 0, (i.e. in the **Limit-I**) in the superconducting state, subject to the assumptions of particle–hole symmetry and of the repulsion between the Cooper pairs of electrons. Here one finds

$$\sum_{\vec{k}\sigma} \Theta(\gamma_{\vec{k}\sigma}(\mu, 0)) = 2 \sum_m \Theta(\mu - \mu_e(2m)) = \bar{N}(\mu), \tag{8}$$

a sumrule corresponding to Eqs. (4).

In Section 6.3 the Greens function and $\gamma_{\vec{k}}$ are studied at L = ∞, (i.e. in the **Limit-II**) in the superconducting state. Here we use the Nambu–Go'rkov [31–35] formalism together with the formally exact quasiparticle representation [34] of the diagonal Greens function. This yields the sumrule Eq. (75), and completes the set of links giving the number sumrule Eq. (1). In summary the

sumrules corresponding to Eqs. (4), (5) for a superconductor are Eqs. (8), (75) in Sections 6.2 and 6.3.

In Section 7 details of the applications of the sumrules at finite T to angle resolved photoemission (ARPES) are given. The main finding is that one can use a first moment of the frequency with respect to the weight function

$$\mathcal{W}(\vec{k},\omega,T) = W_0 \frac{A(\vec{k},\omega)}{\cosh(\frac{1}{2}\beta\omega)} \tag{9}$$

where W_0 is a normalization constant and $A(\vec{k},\omega)$ is the electronic spectral weight measured in experiments. It is denoted in the rest of the paper by the theoreticians favorite symbol $\rho_G(\vec{k},\omega)$. The first moment with respect to $\mathcal{W}$ of the frequency $\langle\omega\rangle_{\vec{k}}$ is found to be equal to $-\gamma_{\vec{k}}(\mu,0^+)$ at T = 0, and in view of the theorems proved here, can be used as a proxy for the inverse static Greens function. It can be found from photoemission at any T, and thereby permits us to define an observable pseudo-Fermi surface (PFS), which becomes the true Fermi surface (FS) at $T \to 0$. Section 7.1 examines the T dependence of the pseudo FS and notes that it can be used to unravel the often sensitive T dependence of the real part of selfenergy. In Section 7.2 the pseudo FS for a singlet superconducting state is discussed in some detail.

In Section 8 I summarize the paper and discuss the results.

1.3. The Hamiltonian

Consider a two component Fermion Hamiltonian

$$\mathcal{H} = \sum_{\vec{k}\sigma} \varepsilon(\vec{k}) C^\dagger_{\vec{k}\sigma} C_{\vec{k}\sigma} + U \times \text{interaction} - \mu\mathcal{N} \tag{10}$$

in the grand canonical ensemble (GCE), where $\mathcal{N}$ is the number operator, μ is the (running i.e. varying) chemical potential, $\varepsilon(\vec{k})$ the energy dispersion. We take the interaction as a short-ranged Hubbard type interaction, possibly with a few further neighbor terms. The initial discussion assumes $U > 0$, and later we allow for pairing i.e. $U < 0$. We assume a finite lattice in d-dimensions with $N_s = L^d$ sites (L the linear dimension) and take the limit of an infinite system at the end.

2. A number sumrule at $T = 0$

We derive a new and useful sumrule Eq. (2) for the electron number at $T = 0$ for electrons with repulsive interactions. It is of thermodynamic origin and is based on an assumption of "good behavior" of the chemical potentials of repulsive finite systems. Let us define the common eigenstates of $\mathcal{N}$, $\mathcal{H}$ as $|m,a\rangle$ with eigenvalues m, $E_a(m) - m\mu$ as the respective eigenvalues. In the canonical ensemble (CE) m particle sector, we will denote $E_0(m)$ and F_m as the ground state energy and free energy $F_m = -k_B T \log Z_m$. We define the CE chemical potentials $\mu(m)$ using

$$\mu(m) = F_{m+1} - F_m, \text{ for } 0 \le m < N_{max}, \tag{11}$$

where T dependence is implied in all variables. The value of N_{max} is twice the number of sites for the prototypical spin-$\frac{1}{2}$ Hubbard model. The set of free energies F_m is conveniently extended by defining F_0 and $F_{N_{max}+1}$ satisfying the conditions $F_0 > 2F_1 - F_2$ and $F_{N_{max}+1} > 2F_{N_{max}} - F_{N_{max}-1}$ but are arbitrary otherwise. By inversion we obtain for $m \ge 1$

$$F_m - F_0 = \mu(m-1) + \mu(m-2) + \cdots + \mu(0). \tag{12}$$

Our essential assumption is that of a positive definite CE compressibility, i.e. a strictly concave-up free energy,

$$F_{m+1} + F_{m-1} - 2F_m > 0,$$
$$\text{or } \mu(m) > \mu(m-1). \tag{13}$$

In a very large system, if we replace differences by derivatives, Eq. (13) becomes the more familiar condition of a positive physical compressibility. We can use it to order the CE chemical potentials as a monotonically increasing set

$$\mu(0) < \cdots < \mu(j) < \cdots < \mu(N_{max}). \tag{14}$$

From the interesting example of the Hubbard model on a buckyball cluster, we learn that this condition can be violated by ostensibly repulsive interactions [36], leading to phase separation and related phenomena. Therefore the ordering in Eq. (14) seem to us to be no more than a robust characterization of truly repulsive interactions.

We introduce a useful set of weight functions

$$\xi_n = e^{\beta\{\mu-\mu(n)\}}. \tag{15}$$

Using these we may write $p_\mu(m)$ the probability of finding m particles in the GCE. With $p_\mu(m) \equiv \exp\beta(m\mu - F_m)/Z(\mu)$, and the grand partition function $Z(\mu) = \sum_m e^{\beta(\mu m - F_m)}$, we obtain

$$p_\mu(m) = Z^{-1}(\mu)\, \xi_0\xi_1 \ldots \xi_{m-1} \tag{16}$$

$$Z(\mu) = 1 + \xi_0 + \xi_0\xi_1 + \xi_0\xi_1\xi_2 + \xi_0\xi_1\xi_2\xi_3 + \cdots \tag{17}$$

The CE chemical potentials $\mu(m)$ are computed at low T from the ground state energies $E_0(m)$.

When $T \ll 2\pi\hbar v/(Lk_B)$ where $v \sim v_F$ the band velocity, the free energies F_m can be replaced by the ground state energies $F_m \to E_0(m)$, and the canonical chemical potentials $\mu(m)$ computed from the ground state energies $E_0(m)$. We note that

$$\lim_{T\to 0} \xi_j \to \begin{cases} \infty, & \text{if } \mu > \mu(j), \\ 1, & \text{if } \mu = \mu(j), \\ 0, & \text{if } \mu < \mu(j). \end{cases} \tag{18}$$

Let us consider the case when μ is in the jth (open) interval $\mathcal{I}_j$ defined as

$$\mathcal{I}_j = \{\mu \mid \mu(j-1) < \mu < \mu(j)\}. \tag{19}$$

When $\mu \in \mathcal{I}_j$ at very low T, the j particle sector is occupied while $j+1$ and higher sectors are unoccupied. To see this, when $T \to 0$ we observe that $\xi_0, \xi_1 \ldots \xi_{j-1}$ grow while $\xi_j, \xi_{j+1} \ldots$ decrease towards zero. Therefore for $\mu \in \mathcal{I}_j$, Z is dominated by a single term

$$\begin{aligned} Z &= \xi_0\xi_1 \ldots \xi_{j-1} \times \mathcal{Y} \\ \mathcal{Y} &= \left(1 + \frac{1}{\xi_{j-1}} + \frac{1}{\xi_{j-1}\xi_{j-2}} + \cdots + \xi_j + \xi_j\xi_{j+1} + \cdots\right) \\ &\to 1, \end{aligned} \tag{20}$$

and therefore

$$p_\mu(j) \to 1 \tag{21}$$

while the probabilities with lower and higher indices vanish:

$$\begin{aligned} p_\mu(j-r) &\to \frac{1}{\xi_{j-1}\xi_{j-2}\ldots\xi_{j-r}} \sim 0 \\ p_\mu(j+r) &\to \xi_j \ldots \xi_{j+r-1} \sim 0. \end{aligned} \tag{22}$$

Therefore at $T = 0$ it follows that the system has j, and no more than j particles, i.e.

$$\lim_{T=0} p_\mu(j) = \Theta(\mu - \mu(j-1)) - \Theta(\mu - \mu(j)). \tag{23}$$

The number of particles can be found using Eq. (23) and $\bar{N}(\mu) = \sum_{m=1}^{N_s} m\, p_\mu(m)$. Shifting the sum in one of the terms and simplifying, we deduce the $T = 0$ thermodynamic number sumrule Eq. (2).

Note the crucial role played by concavity of the free energy, it implies a $1 \leftrightarrow 1$ relationship between m and $\mu(m)$. This rules out double bends  , i.e a non monotonic relation which prevents inversion. The assumed monotonicity allows the relationship to be inverted, yielding m from $\mu(m)$ uniquely and hence giving the sum-rule. In order to deal with degeneracies of $\mu(m)$, usually arising from discrete symmetries (spin, parity, rotation, ...), we relax the strictly increasing condition Eq. (13) to the weaker

$$\mu(m) \geq \mu(m-1), \tag{24}$$

we obtain a second form of the sumrule:

$$\bar{N}(\mu) = \sum_{m}{}' g_m \Theta(\mu - \mu(m)), \tag{25}$$

where g_m is the degeneracy of the particular $\mu(m)$, and the primed sum is over unequal $\mu(m)$'s.

3. Log-derivative of the Greens function

The log-derivative in Eq. (3) can be written as a ratio

$$\gamma_{\vec{k}\sigma} = \beta_{\vec{k}\sigma}/\alpha_{\vec{k}\sigma}, \tag{26}$$

where

$$\alpha_{\vec{k}\sigma}(\mu, T) = -G_\sigma(\vec{k}, \frac{\beta}{2}|\mu) \tag{27}$$

$$\beta_{\vec{k}\sigma}(\mu, T) = -\lim_{\tau \to \frac{1}{2}\beta} \partial_\tau G_\sigma(\vec{k}, \tau|\mu). \tag{28}$$

In terms of the convenient variable

$$\mathbf{f}(m, a, b) \equiv e^{\beta\left(\mu(m+\frac{1}{2}) - \frac{1}{2}(E_a(m)+E_b(m+1))\right)}/Z(\mu),$$

we find

$$\alpha_{\vec{k}\sigma}(\mu, T) = \sum_{m,a,b} \mathbf{f}(m, a, b)|\langle m, a|C_{\vec{k}\sigma}|m+1, b\rangle|^2, \tag{29}$$

and

$$\beta_{\vec{k}\sigma}(\mu, T) = \sum_{m,a,b} \mathbf{f}(m, a, b)\,(\mu + E_a(m) - E_b(m+1)) \\ |\langle m, a|C_{\vec{k}\sigma}|m+1, b\rangle|^2 \tag{30}$$

These spectral representations imply that at low T *both initial and final states* are limited to their ground states in their respective number sectors.

We take the low temperature limit and the thermodynamic limit in two distinct ways, by comparing k_BT with an energy scale Δ_E representing the excited state energy level separation in gapless systems:

$$\Delta_E \sim \frac{2\pi\hbar v}{L}, \tag{31}$$

where $v \sim v_F$ the band velocity. We distinguish between two ways of taking the limit

- **Limit (I) :** $\Delta_E > k_BT \gtrsim 0$, or equivalently $\{\frac{1}{L} \to 0, T \to 0\}$
- **Limit (II):** $k_BT > \Delta_E \gtrsim 0$, or equivalently $\{T \to 0, \frac{1}{L} \to 0\}$.

The two limits can be taken with different sets of tools, **Limit**(**I**) leads to Eq. (4), and can be taken employing ideas and tools relevant to finite size systems, while **Limit**(**II**) leading to Eq. (5) allows the use of electronic spectral functions that are continuous functions of ω. The results of [29,30] imply Eq. (6), i.e. that the two limits coincide asymptotically.

4. Zero temperature Limit (I), i.e. $\{\frac{1}{L} \to 0, T \to 0\}$

In this section we consider Fermi liquids of TLM systems and take the $T = 0$ limit in Eqs. (26), (29), (30). Upon taking the stated limit, we project the sum over the intermediate states a, b to the ground state, and write $e^{\beta(\mu m - E_0(m))} \to p_\mu(m) \times Z(\mu)$, whereby

$$\begin{aligned}
\alpha_{\vec{k}\sigma}(\mu, 0) &= \sum_m \Phi_m(\vec{k}\sigma), \\
\beta_{\vec{k}\sigma}(\mu, 0) &= \sum_m \Phi_m(\vec{k}\sigma) \times \{\mu - \mu(m)\}, \\
\gamma_{\vec{k}\sigma}(\mu, 0) &= \mu - \sum_m \widetilde{\Phi}_m(\vec{k}\sigma)\mu(m),
\end{aligned} \tag{32}$$

the normalized weight function $\widetilde{\Phi}_m = \Phi_m / \sum_r \Phi_r$ is normalized to unity $\sum_m \widetilde{\Phi}_m = 1$) and its un-normalized counterpart

$$\Phi_m(\vec{k}\sigma) = p_\mu(m) e^{\frac{1}{2}(\beta - \mu(m))} \; Z_{\sigma N_s}(\vec{k}, m), \tag{33}$$

$$Z_{\sigma N_s}(\vec{k}, m) = |\langle m, 0 | C^\dagger_{\vec{k}\sigma} | m + 1, 0\rangle|^2. \tag{34}$$

$Z_{\sigma N_s}$ is the ground state CE quasiparticle weight of a state with m particles in N_s. In Eq. (32) by writing $\mu(m)\langle m, 0|C^\dagger_{\vec{k}\sigma}|m+1, 0\rangle = \langle m, 0|[C^\dagger_{\vec{k}\sigma}, H]|m+1, 0\rangle$ and evaluating the kinetic piece explicitly, we obtain

$$\gamma_{\vec{k}\sigma}(\mu, 0) = \mu - \varepsilon(\vec{k}) - \mathcal{M}(\vec{k}\sigma, \mu), \tag{35}$$

$$\mathcal{M}(\vec{k}\sigma, \mu) = \sum_m \frac{\widetilde{\Phi}_m(\vec{k}\sigma)}{Z^{\frac{1}{2}}(\vec{k}, m)} \langle m, 0|[C^\dagger_{\vec{k}\sigma}, V]|m + 1, 0\rangle. \tag{36}$$

We require Z in Eq. (34) to be non-zero at *finite* N_s, although it could vanish as $N_s \to \infty$, in such a way that the normalized $\widetilde{\Phi}$ and $\mathcal{M}$ involving the ratios of Z-like objects remain non-zero. Let us also observe that $\mathcal{M}$ vanishes on turning off interactions. We comment on its relation to the conventional Dyson selfenergy below after Eq. (45).

We next argue that Eq. (32) implies Eq. (4) provided the interacting system is continuously connected to the gas limit. For the strictly monotonic case $\mu(m) < \mu(m + 1)$, there is a $1 \leftrightarrow 1$ map between the $\vec{k}\sigma$ and the $\mu(m)$, extending the obvious map in the gas. Hence $\widetilde{\Phi}_m = \delta_{m,m_0}$ for some m_0, whereby $\gamma_{\vec{k}\sigma} = \mu - \mu(m_0)$. Summing over all $\vec{k}\sigma$ leads to Eq. (4). This property of a sum over all $\vec{k}\sigma$ recovering the sum over all $\mu(m)$ follows from the completeness of Fermi operators with the $\vec{k}\sigma$ labels, i.e. there is no state in the Hilbert space that is inaccessible by a combination of these operators.

We might relax strict monotonicity of $\mu(m)$ and allow for the merging of a set of $\mu(m)$ at different m with say $\mu(m_0)$. In this case $\widetilde{\Phi}(m)$ are non-zero for the set of m with non vanishing matrix elements in $Z_{\sigma N_s}(\vec{k}, m)$. Summing over these m's we again get $\gamma_{\vec{k}\sigma} = \mu - \mu(m_0)$. Further summing over all $\vec{k}\sigma$ gives us back Eq. (4), with a suitable degeneracy factor, provided we use completeness of the sum. We verify completeness in the noninteracting case (including shell type degeneracies) by using the representation Eq. (35), with $\mathcal{M} = 0$. In an interacting theory this completeness requires invoking isothermal continuity.

5. Zero temperature Limit (II), i.e. $\{T \to 0, \frac{1}{L} \to 0\}$

We now consider the log-derivative $\gamma_{\vec{k}}(\mu, T)$ for Fermi liquids as well as 1-d TLM. We are interested in calculating the $T \to 0^+$ limit of $\gamma_{\vec{k}}(\mu, T)$ near its root.

In order to calculate α (Eq. (27)) and β (Eq. (28)) (dropping the explicit spin label below) we use the spectral function representations for the time dependent G detailed in Appendix A. We start

with Eq. (A.4) where we put $\tau = \frac{1}{2}\beta$ so that

$$\alpha_{\vec{k}}(\mu, T) = \int_{-\infty}^{\infty} \frac{d\omega}{2\cosh(\beta\omega/2)}\, \rho_G(\vec{k}, \omega), \tag{37}$$

$$\beta_{\vec{k}}(\mu, T) = -\int_{-\infty}^{\infty} \frac{\omega\, d\omega}{2\cosh(\beta\omega/2)}\, \rho_G(\vec{k}, \omega), \tag{38}$$

$$\gamma_{\vec{k}}(\mu, T) = \beta_{\vec{k}}/\alpha_{\vec{k}}. \tag{39}$$

5.1. Fermi liquids

The spectral function in a Fermi liquid can be expressed for low T, $|\omega| \ll T_F$ as a Lorentzian [4]

$$\rho_G(\vec{k}, \omega) \sim \frac{Z(\vec{k})}{\pi} \frac{\Gamma_k}{\Gamma_k^2 + (\omega - E(\vec{k}, T))^2}, \tag{40}$$

where the quasiparticle weight

$$Z^{-1}(\vec{k}) = 1 - \partial_\omega \Sigma(\vec{k}, \omega)\big|_{\omega\to 0}, \tag{41}$$

and the width of the peak $\Gamma_k = -Z(\vec{k})\Sigma''(\vec{k}, 0, T)$, these are implicitly functions of k, T, μ etc. Note that $\Gamma_k \sim T^2$ is the standard Fermi liquid result for this object. The quasiparticle energy is defined as usual from the root of the nonlinear equation

$$E(\vec{k}, T) = \varepsilon(\vec{k}) + \Sigma'(\vec{k}, E, T) - \mu(T), \tag{42}$$

and Σ' (Σ'') denotes the real (imaginary) part of Σ. From Eq. (B.7) and Eq. (B.5) and using the convenient symbol

$$W(\vec{k}, T) = \frac{1}{2} + \frac{\Gamma_k + iE(\vec{k}, T)}{2\pi T} \tag{43}$$

we deduce that

$$\begin{aligned}
\alpha_{\vec{k}}(\mu, T) &= \frac{Z(\vec{k})}{\pi} \Re e\, \xi(W) \\
\beta_{\vec{k}}(\mu, T) &= -E(\vec{k}, T)\alpha_{\vec{k}}(\mu, T) - \frac{Z(\vec{k})\Gamma_k}{\pi} \Im m\, \xi(W) \\
\gamma_{\vec{k}}(\mu, T) &= -E(\vec{k}, T) - \Gamma_k \frac{\Im m \xi(W)}{\Re e \xi(W)}.
\end{aligned} \tag{44}$$

In the limit $T \to 0^+$ the width Γ_k vanishes and we obtain

$$\gamma_{\vec{k}}(\mu, 0^+) = -E(\vec{k}, 0). \tag{45}$$

Comparing the relations Eqs. (42), (45) with Eqs. (35), (36), we observe that the variable $\mathcal{M}$ is essentially the selfenergy Σ' from the perspective of **Limit-I**. A change in the sign of $\gamma_{\vec{k}}$ therefore occurs at the zero of $E(\vec{k}, 0)$. Close to this root, i.e. with small E Eq. (42) and the Dyson expression for the Greens function give us

$$\Theta(\gamma_{\vec{k}}(\mu, 0^+)) = \Theta(G^{-1}(\vec{k}, \omega = 0|\mu)), \tag{46}$$

and by replacing the static Greens function $G^{-1} \to G$ we obtain the sumrule Eq. (5). We return to these expressions later in Section 7, where we carry out a detailed analysis of the volume of the Fermi surface in connection with ARPES experiments.

5.2. Non-Fermi liquids in 1-d

In this section we apply our method to the case of Tomonaga–Luttinger systems. This is an extensively studied area where many methods for exact solution are available [37–39]. In these

systems the quasiparticle weight Z vanishes, in parallel to the discussion for **Limit (I)** after Eq. (36). We show below that as $T \to 0$ in **Limit(II)**, $\alpha_{\vec{k}}$ vanishes as well, and so does $\beta_{\vec{k}}$ in such a way that $\gamma_{\vec{k}}$ remains finite and switches sign at the true Fermi wave-vector.

For the canonical example of a spinless model, the spectral function is severely constrained by the Lorentz invariance of the theory and conformal invariance of the effective 2-d classical theory at finite T [37,38,40]. It can be expressed as a scaling function valid at low T, ω and $\hat{k}$ defined as $\hat{k} = k - \zeta k_*$ near the left ($\zeta = -1$) and right ($\zeta = 1$) Fermi points $\mp k_*$ [37,39,40]

$$\rho_G(k,\omega) = \frac{1}{T^{\alpha_0}} \sum_{\zeta=\pm 1} \mathcal{F}(\frac{\omega - \zeta V\hat{k}}{T}), \tag{47}$$

where V the renormalized Fermion velocity is related to the bare Fermi velocity V_F by a non singular scaling factor, and we set $k_B = 1$ in this section. Here and in the following we should retain only one of the two terms of the ζ sum, where $\hat{k}$ is small. Although we did not specify the value of k_* yet, it will turn out that $k_* = k_F$ below, thanks to the sumrule. The exponent $\alpha_0 < 1$, both α, V depend on the interaction strength, and the positive definite scaling function is peaked at the origin. It satisfies $\mathcal{F}(0) = 1$ and $\mathcal{F}(\xi) \to 1/|\xi|^{\alpha_0}$ for $|\xi| \gg 1$. As $T \to 0^+$ we obtain

$$\rho_G(k,\omega) \sim \sum_{\zeta=\pm 1} \frac{\mathcal{A}}{|\omega - \zeta V\hat{k}|^{\alpha_0}}, \tag{48}$$

with $\mathcal{A} > 0$. From the above spectral function and Eq. (A.5) we can calculate the Greens function near zero frequency close to the Fermi points with $T \to 0^+$ as

$$G(k,0|\mu) = -\mathcal{B}\frac{\zeta V\hat{k}}{|V\hat{k}|^{\alpha_0+1}}, \tag{49}$$

where $\mathcal{B} > 0$, and $\zeta = \pm 1$ for the right and left Fermi points.

We next calculate Eqs. (37) and (38) using Eq. (47). The $\cosh(\frac{1}{2}\beta\omega)$ factor in Eq. (37) cuts off frequencies with $|\omega| > T$, and if we restrict $|V\hat{k}| \lesssim T$ as well, then the dimensionless argument of the scaling function $\mathcal{F}$ in Eq. (47) is at most of $\mathcal{O}(1)$, and we get no contribution to the integrals from a regime where $\mathcal{F}(\xi) \to 1/|\xi|^{\alpha_0}$. We can therefore reasonably replace $\mathcal{F}$ by a Lorentzian

$$\mathcal{F} \sim \frac{\mathcal{C}T}{\pi} \frac{\mathcal{C}T}{(\mathcal{C}T)^2 + (\omega - \zeta V\hat{k})^2}, \tag{50}$$

where $\mathcal{C}$ is a positive constant. This enables the convenience of an explicit evaluation of the integrals. If needed it can be supplanted by a more lengthy and tedious argument that avoids this replacement, giving the same answer.

We therefore use the results Eq. (B.7) and Eqs. (B.8), (B.9) to explicitly perform the integrals and write down at low T the results when $V\hat{k}$ is small;

$$\alpha_{\vec{k}}(\mu,T) = \frac{\mathcal{C}}{\pi} T^{1-\alpha_0}\, \Re e\, \xi\left(\frac{1}{2} + \frac{\mathcal{C}T + iV\hat{k}}{2\pi T}\right) \tag{51}$$

$$\gamma_{\vec{k}}(\mu,T) = -\zeta V\hat{k} - \mathcal{C}T \frac{\Im m\, \xi\left(\frac{1}{2} + \frac{\mathcal{C}T + i\zeta V\hat{k}}{2\pi T}\right)}{\Re e\, \xi\left(\frac{1}{2} + \frac{\mathcal{C}T + iV\hat{k}}{2\pi T}\right)} \tag{52}$$

and $\beta_{\vec{k}}(\mu,T) = \gamma_{\vec{k}}(\mu,T)\alpha_{\vec{k}}(\mu,T)$. Here $\zeta = \pm 1$ for the right and left Fermi points. Note that these equations closely resemble Eq. (44). At finite T both terms in Eq. (52) vanish when $V\hat{k}$ vanishes. As $T \to 0^+$ the second term in Eq. (52) drops out identically, and we get

$$\gamma_k(\mu,0^+) = -\zeta V\hat{k}. \tag{53}$$

Comparing with the static Greens function Eq. (49) we obtain

$$\lim_{T\to 0^+} \Theta(\gamma_{\vec{k}}(\mu,T)) = \Theta\left(G(k,0|\mu)\right) \tag{54}$$

we get the sumrule Eq. (5).

We note that the vanishing of the quasiparticle weight Z in this model is reflected in the vanishing of $\alpha_{\vec{k}}$ in Eq. (51) at $T \to 0$. Away from the Fermi points $\beta_{\vec{k}}$ also vanishes but their ratio $\gamma_{\vec{k}}$ in Eq. (52) is finite. It follows that

$$2\sum_k \Theta\left(G(k,0|\mu)\right) = 2\sum_k \Theta\left(G_0(k,0|\mu)\right) \tag{55}$$

since each side equals the number of particles and therefore equates the Fermi diameter of the interacting and non interacting theories. Therefore the unspecified k_* can now be identified with the bare Fermi momentum k_F.

6. Sumrules in the singlet superconducting state

The volume theorem can be generalized to singlet superconductors. Our work is inspired by an observation regarding Gor'kov's (diagonal) Greens function describing the superconducting state [32] (see Eq. (14))

$$G(\vec{k},\omega) = \frac{1}{2}\frac{u^2(\vec{k})}{\omega - E(\vec{k}) + i0^+} + \frac{1}{2}\frac{v^2(\vec{k})}{\omega + E(\vec{k}) + i0^+}, \tag{56}$$

$$u^2(\vec{k}) = \frac{1}{2}\left(1 + \frac{\varepsilon(\vec{k})-\mu}{E(\vec{k})}\right) \text{ and } v^2(\vec{k}) = \frac{1}{2}\left(1 - \frac{\varepsilon(\vec{k})-\mu}{E(\vec{k})}\right). \tag{57}$$

Here $\varepsilon(\vec{k})$ is the band energy, $E(\vec{k}) = \sqrt{\varepsilon^2(\vec{k}) + \Delta^2(\vec{k})}$ the (positive) quasiparticle energy and $\Delta(\vec{k})$ the gap function. It is remarkable to note that this expression contains in its innards, a precise encoding of the (submerged) normal state Fermi surface. Setting $\omega = 0$ we find

$$G(\vec{k},0) = \frac{\mu - \varepsilon(\vec{k})}{E^2(\vec{k})}. \tag{58}$$

Therefore in system exhibiting superconductivity, the submerged normal state Fermi surface is revealed by a change in sign of $G(\vec{k},0)$ occurring at

$$\varepsilon(\vec{k}) = \mu, \tag{59}$$

and at the root,

$$u(\vec{k}_F) = v(\vec{k}_F). \tag{60}$$

The latter condition expresses an emergent particle–hole symmetry on the Fermi surface of the weak coupling BCS solution. While the above relations are true at the mean-field (BCS) level of description, it is not clear if this encoding survives the effects of strong interactions, and further refinements of the theory. It is also not entirely clear as to how one might probe this encoding, since there is no known method for probing the static G directly. The first question is treated here with an affirmative answer for a fully gapless superconductor. For a partially or fully gapped case, it is subject to the survival of the particle–hole symmetry as at least an approximate symmetry for arbitrary coupling. The second is answered in Section 7, where we relate an observable first moment of frequency with a suitable weight function to this observation, thereby suggesting a potentially useful photoemission experiment.

The strategy used for the normal state is extended to the superconductors as follows. We first establish the thermodynamic sumrule Eq. (7), under the assumption that (Cooper) pairs of electrons exhibit mutual repulsion, when viewed as composite particles. We then take the $T = 0$ limit to

obtain the sumrule Eq. (8). The main assumption here, used without a direct proof, is that of nearly particle–hole symmetric matrix elements for the interacting system, analogous to Eq. (60) for the free case. Finally we take the $L \to \infty$ limit and using results from the Nambu–Gorkov formalism, obtain Eq. (75) and hence the sumrule Eq. (5). This completes the set of sumrules needed to establish Eq. (1) for the superconducting state as well.

6.1. Superconducting phase: Thermodynamic sumrule

We next study the thermodynamic sumrule for a superconducting state, using the canonical ensemble. This approach is familiar from the nuclear physics context [41,42] and has been recently applied in the context of mesoscopic superconductivity [43]. Our treatment initially assumes a finite gap such as s-wave BCS superconductors, and later generalized to include d-wave case relevant for cuprate superconductors. We define the CE chemical potentials remaining within the *even-canonical* ensemble [41,43]:

$$\mu_e(2m) \equiv \frac{1}{2}(F_{2m+2} - F_{2m}), \tag{61}$$

and require the monotonic property $\mu_e(2m+2) > \mu_e(2m)$ leading to an ordering

$$\mu_e(0) < \mu_e(2) < \cdots \mu_e(2j) \cdots < \mu_e(N_{max}). \tag{62}$$

This clearly implies a concavity condition on the free energies $2F_{2n} < F_{2n-2} + F_{2n+2}$, arising from represents repulsion between pairs, so that further clusters of electrons are forbidden, i.e. *the pairing stops with pairs*. This results in a homogeneous many-body eigenstate of pairs, qualitatively similar and continuously connected to a gas of (repulsive) Bosons as envisaged in Ref. [44,45]. Assuming the ordering Eq. (62) we may repeat the discussion leading to Eq. (2), yielding Eq. (7), the number sum-rule for paired superconductors at $T = 0$, with the extra factor of 2 from skipping odd fillings.

6.2. Superconducting phase: $T = 0$ sumrule

We now consider the low T log-derivative Greens function as in Eq. (3) with $F_m \sim E_0(m)$. For this we also need the odd sector energies F_{2n+1}, these are expressed in terms of the even energies and a gap function Δ[41–43,46–54]:

$$E_0(2n+1) = \frac{1}{2}(E_0(2n) + E_0(2n+2)) + \Delta(2n+1). \tag{63}$$

Here Δ playing the role of the BCS gap is assumed non-zero initially. It is interpretable as the energy of an unpaired electron in an otherwise paired state. It is essentially the lowest energy Bogoliubov–Valatin [55] quasiparticle in the CE.

We consider the **Limit(I)** of α, β of Eqs. (11), (12), (13), (14) of the main paper. We proceed to calculate Eqs. (13), (14) by grouping pairs of terms $\{2m, 2m+1\}$, rewriting p_μ's using Eqs. (27) and (29) as $p_\mu(2m) = e^{\beta(2m\mu - F_{2m})}/Z(\mu)$ and $p_\mu(2m+1) = e^{-\beta\Delta(2m+1)} p_\mu^{\frac{1}{2}}(2m) p_\mu^{\frac{1}{2}}(2m+2)$. We further define the matrix elements:

$$\begin{aligned} V^{ab}_{\vec{k}\sigma}(2m+1) &= \langle 2m+1, a | C_{\vec{k}\sigma} | 2m+2, b \rangle, \\ U^{ab}_{\vec{k}\sigma}(2m+1) &= \langle 2m, a | C_{\vec{k}\sigma} | 2m+1, b \rangle. \end{aligned} \tag{64}$$

The ground state $|2m+1, 0\rangle$ has one unpaired quasiparticle (with 2-fold degeneracy), while $|2m, 0\rangle$ and $|2m+2, 0\rangle$ are the fully paired non-degenerate ground states. These matrix elements are therefore analogs of the familiar GCE coefficients $(u_k, v_k) = \sqrt{\frac{1}{2}(1 \pm \frac{\xi_k}{E_k})}$ of the BCS–Gor'kov theory [32,55,56] noted in Eq. (57), with $\xi = \varepsilon - \mu$. Recall that $\xi_k = 0$ at the Fermi momentum, therefore the relation $u_{k_F} = v_{k_F}$ noted in Eq. (60) holds good in weak coupling [32,55,56]. This relation also underlies the Majorana zero modes discussed in [57], and is often viewed as expressing an emergent particle–hole symmetry. Following this we assume the more general ground states

matrix elements satisfy $|U^{00}_{\vec{k}\sigma}| \sim |V^{00}_{\vec{k}\sigma}|$, for the correct bridging momentum. For finite systems we require it to hold within a tolerance that is discussed below.

We closely follow the procedure in the Fermi liquid case, and express α, β in terms of the matrix elements U, V.

$$\beta_{\vec{k}}(\mu, T) = \sum_m e^{\frac{1}{2}\beta(\mu-\mu_e(2m)-\Delta)} p_\mu^{\frac{1}{2}}(2m) p_\mu^{\frac{1}{2}}(2m+2)\ \mathcal{B}(m),$$

and

$$\alpha_{\vec{k}}(\mu, T) = \sum_m e^{\frac{1}{2}\beta(\mu-\mu_e(2m)-\Delta)} p_\mu^{\frac{1}{2}}(2m) p_\mu^{\frac{1}{2}}(2m+2)\ \mathcal{A}(m), \tag{65}$$

where

$$\mathcal{A}(m) = \left\{(U^{00}_{k\sigma}(2m+1))^2 + e^{-\beta(\mu-\mu_e(2m))}(V^{00}_{k\sigma}(2m+1))^2\right\}, \tag{66}$$

$$\mathcal{B}(m) = (\mu - \mu_e(2m))\mathcal{A}(m) + \Delta(2m+1)\left\{(U^{00}_{k\sigma}(2m+1))^2 - e^{-\beta(\mu-\mu_e(2m))}(V^{00}_{k\sigma}(2m+1))^2\right\}. \tag{67}$$

In computing $\gamma_{\vec{k}}(\mu, T)$ as $T \to 0$, our calculation proceeds similar to the non-superconducting case but with the role of $Z(\vec{k}, m)$ now played by the matrix elements U, V. Assuming continuity from the Fermi gas via the weak coupling BCS–Gor'kov theory, the given wave vector $\vec{k}$ picks out a single particle number m contributing to both α, β. In the gapless case for the given $\vec{k}$, Δ vanishes as an inverse power of L. Thus $\mathcal{B}/\mathcal{A} = \mu - \mu_e(2m)$ with negligible corrections. If the gap is non-zero the ratio $\mathcal{B}/\mathcal{A} = \mu - \mu_e(2m) + \Delta\,\mathcal{C}$ where on dropping indices:

$$\mathcal{C} = \frac{e^{\beta(\mu-\mu_e(2m))}U^2 - V^2}{e^{\beta(\mu-\mu_e(2m))}U^2 + V^2}.$$

We require the correction $\Delta\,\mathcal{C}$ to be small relative to the separation between $\mu_e(2m)$ and $\mu_e(2m+2)$. If particle–hole symmetry were exactly true then $U = V$, $\Delta\,\mathcal{C} = 0$ and the node in γ is situated exactly at $\mu = \mu_e(2m)$ even if $\Delta \neq 0$. In practice an approximate equality between U and V suffices for this condition with a specified tolerance. If we require that

$$\frac{|U^2 - V^2|}{U^2 + V^2} < \frac{|\mu_e(2m \pm 2) - \mu_e(2m)|}{\Delta(2m+1)}, \tag{68}$$

the node in γ at $\mu \sim \mu_e(2m)$ is essentially unshifted. Assuming this relation and summing over $\vec{k}$, it follows that

$$\sum_{\vec{k}\sigma} \Theta(\gamma_{\vec{k}\sigma}(\mu, 0)) = 2 \sum_m \Theta(\mu - \mu_e(2m)) = \bar{N}(\mu),$$

as noted in Eq. (8), where the factor of 2 comes from the equal contribution from $\vec{k}\sigma$ and its time reversed partner $-\vec{k}\bar{\sigma}$.

6.3. Superconducting phase: $T \to 0^+$ sumrule using Nambu–Gor'kov formalism

We next take the limit $\{T \to 0, \frac{1}{L} \to 0\}$ in the superconducting state. In order to go beyond the mean-field treatment in the Gor'kov's paper [32], we use the formally exact Nambu formalism [31]. It contains all possible many body effects, including those neglected in mean field theory. We start with the Nambu–Gor'kov [31–33] four component theory where the selfenergy in the superconducting state is expanded as

$$\Sigma(\vec{k}, z) = (1 - Z_{\vec{k}}(z))z\ \mathbb{1} + \phi(\vec{k}, z)\ \tau_1 + \chi(\vec{k}, z)\ \tau_3, \tag{69}$$

with $z = i\omega_n$ where the Nambu selfenergies Z, χ, ϕ are even functions of z. In this notation for superconductors $Z \sim 1-\partial_\omega \Sigma$, i.e the inverse of the normal state convention where $Z \sim (1-\partial_\omega \Sigma)^{-1}$. From this the matrix Greens function $\mathbf{G}$ is written as

$$\mathbf{G}(\vec{k}, z|\mu) = \frac{zZ_{\vec{k}}(z)\mathbb{1} + \tau_3(\varepsilon(\vec{k}) - \mu + \chi_{\vec{k}}(z)) + \tau_1\phi_{\vec{k}}(z)}{z^2Z^2_{\vec{k}}(z) - E^2_{\vec{k}}(z)}. \tag{70}$$

We are only interested in the diagonal Greens function G_{11}, which we shall denote by G below. This is the component of the Greens function relevant to the volume theorem and also to photoemission studies. It can be found within the quasiparticle approximation by expanding Eq. (70) near the poles of the Greens function [31,33–35]. The poles of $G(\vec{k}, \omega)$ are located at the Bogoliubov–Valatin (B–V) [55] quasiparticle energies $\omega = \pm E_{r\vec{k}}$ where

$$E_{r\vec{k}} = \Re e(E_{\vec{k}}(\eta_{\vec{k}})/Z_{\vec{k}}(\eta_{\vec{k}})), \quad \text{with} \quad \eta_{\vec{k}} = E_{r\vec{k}} + i0^+, \tag{71}$$

and have a width

$$\Gamma_{\vec{k}} = Z^{-1}_{\vec{k}}\Im m\{\eta_{\vec{k}}Z_{\vec{k}}(\eta_{\vec{k}}) - \frac{1}{E_{\vec{k}}}(\tilde{\varepsilon}_{\vec{k}}\chi_{\vec{k}}(\eta_{\vec{k}}) + \phi_{\vec{k}}\phi_{\vec{k}}(\eta_{\vec{k}}))\},$$

expressed in terms of the following set of real constants (Eq. (2.25,2.26,2.27) of [34]).

$$\begin{aligned}
&\tilde{\varepsilon}_{\vec{k}} = \varepsilon(\vec{k}) - \mu + \Re e\, \chi_{\vec{k}}(\eta_{\vec{k}}),\ \phi_{\vec{k}} = \Re e\, \phi_{\vec{k}}(\eta_{\vec{k}}) \\
&E_{\vec{k}} = (\tilde{\varepsilon}^2_{\vec{k}} + \phi^2_{\vec{k}})^{\frac{1}{2}},\ Z_{\vec{k}} = \Re e Z_{\vec{k}}(\eta_{\vec{k}}).
\end{aligned} \tag{72}$$

In the above expression $\phi_{\vec{k}}$ plays the role of a gap function, $\tilde{\varepsilon}_{\vec{k}}$ the dispersion of a gapless underlying Fermi liquid renormalized with selfenergy $\chi_{\vec{k}}$, and $E_{\vec{k}}$ is proportional to the quasiparticle energy $E_{r\vec{k}}$.

For energies close to the BV quasiparticle energies, the quasiparticle Greens function is given by the asymptotic expressions

$$G(\vec{k}, i\omega_n|\mu) \sim \sum_{\alpha=\pm1}\left\{\frac{1}{2} + \alpha\frac{\tilde{\varepsilon}_{\vec{k}}}{2E_{\vec{k}}}\right\}\frac{Z^{-1}_{\vec{k}}}{i\omega_n - \alpha E_{r\vec{k}} + i\Gamma_{\vec{k}}}, \tag{73}$$

$$\rho_G(\vec{k}, \omega) \sim \frac{1}{\pi}\sum_{\alpha=\pm1}\left\{\frac{1}{2} + \alpha\frac{\tilde{\varepsilon}_{\vec{k}}}{2E_{\vec{k}}}\right\}\frac{Z^{-1}_{\vec{k}}\Gamma_{\vec{k}}}{(\omega - \alpha E_{r\vec{k}})^2 + \Gamma^2_{\vec{k}}} \tag{74}$$

The spectral function has a similar status for superconducting systems as Eq. (40) for Fermi liquids; both expressions capture the various many-body renormalizations in terms of a few parameters.

We calculate $\alpha_{\vec{k}}, \beta_k$ from Eqs. (37), (38) using the spectral function Eq. (74) in greater detail below in Eq. (92) in Section 7.2. However as $T \to 0^+$ it is known [34] that $\Gamma_{\vec{k}} \to 0$, i.e. one has sharp poles, and ρ_G is a sum over two delta functions. In this case we easily calculate

$$\alpha_{\vec{k}} \sim \frac{1}{Z_k\cosh(\frac{1}{2}\beta E_{r\vec{k}})},\ \beta_{\vec{k}} \sim \frac{-\tilde{\varepsilon}_{\vec{k}}}{Z^2_{\vec{k}}\cosh(\frac{1}{2}\beta E_{r\vec{k}})}$$

therefore $\gamma_{\vec{k}}(\mu, T) \to -\frac{\tilde{\varepsilon}_{\vec{k}}}{Z_{\vec{k}}}$. Now $G(\vec{k}, 0|\mu) = -\frac{\tilde{\varepsilon}_{\vec{k}}}{E^2_{\vec{k}}}$ from Eq. (73), and therefore

$$\Theta\left(\gamma_{\vec{k}}(\mu, 0^+)\right) = \Theta\left(G(\vec{k}, 0|\mu)\right), \tag{75}$$

and therefore by summing over $\vec{k}$ we obtain the sumrule Eq. (5). This result is argued to be valid for all flavors of singlet pairing, including the gapless d-wave case. We combine Eq. (75) or Eq. (5) with Eq. (8) and infer the sumrule Eq. (1) in the superconductor.

7. The pseudo Fermi surface at finite T

Extending the ground state sum-rule to finite T, we define a "pseudo-Fermi surface" and an effective density $n_{eff}(T)$ from the changes in sign with $\vec{k}$ of $\gamma_{\vec{k}\sigma}(\mu, T)$. These tend to the true Fermi surface and particle density when $T \to 0$, and can be extracted from experimental photoemission data as follows. In terms of a dipole matrix-element M and the Fermi function $f(\omega) = (\exp \beta\omega + 1)^{-1}$, the photoelectron intensity is given by $\mathcal{I}(\vec{k}, \omega) = M(\vec{k})\rho_G(\vec{k}, \omega)f(\omega)$. From Eqs. (3), (37), (38) it follows that γ is a suitably weighted *first moment of frequency*:

$$\gamma_{\vec{k}\sigma}(\mu, T) = -\langle\omega\rangle_{\vec{k}}, \tag{76}$$

where

$$\langle\omega\rangle_{\vec{k}} = \int d\omega\, \mathcal{I}(\vec{k}, \omega)e^{\frac{1}{2}\beta\omega}\omega \Big/ \int d\omega\, \mathcal{I}(\vec{k}, \omega)e^{\frac{1}{2}\beta\omega}, \tag{77}$$

$$= \int \rho_G(\vec{k}, \omega)\frac{\omega\, d\omega}{\cosh(\frac{1}{2}\beta\omega)} \Big/ \int \rho_G(\vec{k}, \omega)\frac{d\omega}{\cosh(\frac{1}{2}\beta\omega)}, \tag{78}$$

the two expressions Eqs. (77), (78) are equivalent since the $\vec{k}$ dependent matrix element and other factors cancel out. This weight function was already mentioned in Eq. (9) in Section 1. In averaging over ω, the weight factors provide exponential cutoffs for high $|\omega|$. By replacing ω by ω^m in Eq. (76), one can generates the mth moment $\langle\omega^m\rangle_{\vec{k}}$. This novel set of moments characterize the low energy excitations of the spectral function, unlike the moments without the T dependent weight functions, and seem promising for further study.

From γ we define the effective density

$$n_{eff}(T) = 1/N_s \sum_{\vec{k}\sigma} \Theta\left(\gamma_{\vec{k}\sigma}(\mu, T)\right). \tag{79}$$

We can now define the pseudo-Fermi surface at any T; it is defined as the set of Fermi points $\vec{k}$ satisfying

$$\langle\omega\rangle_{\vec{k}} = 0. \tag{80}$$

The sign changes of γ with $\vec{k}$ occur on this surface, and $n_{eff}(T)$ counts the number of particles within this surface from Eq. (79). It reduces to the true Fermi-surface at $T = 0$. We next discuss the content of this sum-rule at finite T for two important cases.

7.1. Finite T volume sumrule: Fermi liquids

We note that Eqs. (76), (77) are identical to Eq. (39) in Section 6.3. Therefore for Fermi liquids at finite (but low) T, we can use the quasiparticle approximation for the spectral function Eq. (40), so that

$$\langle\omega\rangle_{\vec{k}} = E(\vec{k}, T) + \Gamma_k \frac{\Im m\xi(\frac{1}{2} + \frac{\Gamma_k + iE(\vec{k},T)}{2\pi T})}{\Re e\xi(\frac{1}{2} + \frac{\Gamma_k + iE(\vec{k},T)}{2\pi T})}, \tag{81}$$

following Eq. (44). In order to deduce the pseudo Fermi points, we observe that when $E(\vec{k}, T)$ vanishes in Eq. (39), the imaginary part of ξ vanishes as well. Thus at any T the pseudo Fermi point is located by

$$E(\vec{k}, T) = 0, \tag{82}$$

where $E(\vec{k}, T)$ is defined in Eq. (42). At $T = 0$ it reduces to

$$E(\vec{k}_F, 0) = \varepsilon(\vec{k}_F) + \Sigma'(\vec{k}_F, 0, 0) - \mu(0) = 0, \tag{83}$$

where we set $\vec{k} = \vec{k}_F$, the corresponding $T = 0$ Fermi momentum upon using the volume theorem. In Eq. (42) we expand the selfenergy at low ω and write E as

$$Z^{-1}(\vec{k}, T)E(\vec{k}, T) = \varepsilon(\vec{k}) + \Sigma'(\vec{k}, 0, T) - \mu(T) \tag{84}$$

$$= \varepsilon(\vec{k}) + (\Sigma'(\vec{k}, 0, T) - \Sigma'(\vec{k}, 0, 0)) + \Sigma'(\vec{k}, 0, 0) + (\mu(0) - \mu(T)) - \mu(0) \tag{85}$$

The vanishing of the right hand side locates the pseudo FS. Using Eq. (83) we obtain

$$(\mu(T) - \mu(0)) = (\varepsilon(\vec{k}) - \varepsilon(\vec{k}_F)) + (\Sigma'(\vec{k}, 0, T) - \Sigma'(\vec{k}, 0, 0)) + (\Sigma'(\vec{k}, 0, 0) - \Sigma'(\vec{k}_F, 0, 0)). \tag{86}$$

As expected this equation is satisfied identically by setting $\vec{k} = \vec{k}_F$ at $T = 0$. At low T we perturb by expanding $\vec{k}$ about $\vec{k}_F$,

$$\vec{k} = \vec{k}_F + \delta\vec{k}, \tag{87}$$

and linearize in $\delta\vec{k}$ to find

$$\delta\vec{k}.\vec{V}_{\vec{k}_F} = (\mu(T) - \mu(0)) - (\Sigma'(\vec{k}_F, 0, T) - \Sigma'(\vec{k}_F, 0, 0)), \tag{88}$$

where $\vec{V}_{\vec{k}} = \vec{\nabla}_{\vec{k}}[\varepsilon(\vec{k}) + \Sigma'(\vec{k}, 0, 0)]$ is related to the Fermi velocity. The variation $\delta\vec{k}$ is normal to the true (i.e. T = 0) FS, and can be determined from this relation. Proceeding further we may write the change in FS area with T as a line integral over the true FS in 2-d

$$\delta A(T) = \oint_{FS} dk_\perp \frac{(\mu(T) - \mu(0)) - (\Sigma'(\vec{k}_F, 0, T) - \Sigma'(\vec{k}_F, 0, 0))}{|\vec{V}_k|}, \tag{89}$$

where $dk_\perp$ is the wave-vector element tangential to the FS.

The effective density at T differs from the true particle density by the usual counting rules leading to

$$n_{eff}(T) - n = 2 \times \delta A(T)/(2\pi)^2. \tag{90}$$

The variation Eq. (89) is driven by the T dependent shifts of $\mu(T)$ and of the real part of the selfenergy $\Sigma'(k_F, 0, T)$. The shift of μ with T is the smaller of the two, and can in principle be estimated experimentally. For example in ARPES the apparent change of excitation energy with T of some fixed (T independent) feature, such as a band edge can be used for this purpose. The variation $\delta A(T)$ is amplified when the quasiparticle Fermi velocity is reduced from the bare one, as it often happens in strongly correlated matter. An example of the T dependence of n_{eff} in the t-J model is shown in Ref. [58], where the variation with T is quite significant due to strong correlations. revealing emergent low-energy scales in the problem.

The expression Eq. (89) allows us to explore the T dependent shift of the real part of Σ. This object is of great interest in strongly correlated materials. In the strange metal regime of the d = ∞ Hubbard model, it has been reported in Ref. [59] (Fig (12.c)) to have a strong T dependence, which in turn leads to a linear T resistivity

7.2. Finite T volume sumrule: Superconductors

In parallel to the treatment of the normal case above, we calculate the first moment Eq. (78) in the superconducting phase, using the quasiparticle spectral function in Eq. (74), and the useful integrals noted in Eq. (B.7). Canceling common factors we write

$$\langle\omega\rangle_{\vec{k}} = \mathcal{N}/\mathcal{D},$$

$$\mathcal{N} = \sum_{\alpha=\pm1} \left\{\frac{1}{2} + \alpha\frac{\tilde{\varepsilon}_{\vec{k}}}{2E_{\vec{k}}}\right\} \left[\alpha E_{r\vec{k}}\, \Re e\, \xi\left(\frac{1}{2} + \frac{\Gamma_{\vec{k}} + i\alpha E_{r\vec{k}}}{2\pi T}\right) + \Gamma_{\vec{k}}\, \Im m\, \xi\left(\frac{1}{2} + \frac{\Gamma_{\vec{k}} + i\alpha E_{r\vec{k}}}{2\pi T}\right)\right]$$

$$\mathcal{D} = \sum_{\alpha=\pm1} \left\{\frac{1}{2} + \alpha\frac{\tilde{\varepsilon}_{\vec{k}}}{2E_{\vec{k}}}\right\} \Re e\, \xi\left(\frac{1}{2} + \frac{\Gamma_{\vec{k}} + i\alpha E_{r\vec{k}}}{2\pi T}\right) \tag{91}$$

We now use the properties of the ξ function Eqs. (B.8) and (B.9) to simplify Eq. (91). This gives the final formula for the first moment:

$$\langle\omega\rangle_{\vec{k}} = \frac{\tilde{\varepsilon}_{\vec{k}}}{E_{\vec{k}}}\left(E_{r\vec{k}} + \Gamma_{\vec{k}}\frac{\Im m\,\xi\left(\frac{1}{2}+\frac{\Gamma_{\vec{k}}+iE_{r\vec{k}}}{2\pi T}\right)}{\Re e\,\xi\left(\frac{1}{2}+\frac{\Gamma_{\vec{k}}+iE_{r\vec{k}}}{2\pi T}\right)}\right). \tag{92}$$

The $\Gamma_{\vec{k}}$ term in the above expression is expected to be exponentially small for the gapped states and a power law for gapless singlet paired states. This expression resembles Eq. (81) for the Fermi liquid state with the energy dispersion $\tilde{\varepsilon}_{\vec{k}}$ replacing the quasiparticle energy $E(\vec{k}, T)$. The vanishing of the first moment locates the pseudo-FS for the superconductor through the condition

$$\tilde{\varepsilon}_{\vec{k}} = \varepsilon(\vec{k}) - \mu + \Re e\,\chi_{\vec{k}}(E_{r\vec{k}}) \to 0, \tag{93}$$

which replaces the simple relation of Gor'kov's theory Eq. (59). This implies that the shift in the chemical potential from the noninteracting value due to pairing effects is exactly canceled by the selfenergy term $\Re e\,\chi_{\vec{k}}(E_{r\vec{k}})$. This cancellation is analogous to exact cancellation in the normal state.

Our treatment of the pseudo FS of the superconducting state has a few precedents. The closely related papers [60,61] discuss the surface formed by $\vec{k}$ with $G(\vec{k}, 0) = 0$, using a phenomenological model of G for superconductors in strongly correlated cuprate materials. The model uses a "renormalized" mean field theory [62] for this calculation. This method incorporates effects of strong correlations through a rescaled version of the BCS effective Hamiltonian with density dependent scale factors. The area of the above surface in these works is found to be only approximately the number density, even at T = 0. Their results are in contrast to the findings of the present work, where the pseudo FS area must match the particle density exactly at T = 0. The discrepancy could be due to missing a cancellation between the shifts of the selfenergy and the chemical potential, or due to a lack of the (unproven) particle–hole symmetry at strong coupling. Experimental checks of the particle–hole symmetry, as suggested in this work would be of considerable interest.

In the present work we propose a new suggestion for probing the pseudo-Fermi surface for superconductors. It differs from the signatures proposed earlier [60,61], advocating either locating the maxima of the spectral weight, or the maxima of the gradient of the momentum distribution function $|\nabla_k n_k|$. Our proposal involves studying the first moment of the frequency $\langle\omega\rangle_{\vec{k}}$, defined in Eq. (78). Its vanishing as in Eq. (80) defines the pseudo FS. As explained above this moment can be constructed from the dynamical information in ARPES. For singlet superconductors such as the cuprates, the pseudo-Fermi surface is definable on both sides of the superconducting transition using the moment in both phases Eqs. (81), (92). Apart from (usually small) T dependent corrections, its area is the same in both phases, being related to the number of particles.

8. Discussion

Given the importance of the Fermi volume theorem, and the attendant complexities of deriving it, a fresh approach seems relevant. This work presents a non-perturbative derivation of the volume sum-rule Eq. (1) in a broad setting. We avoid using the traditional number sum-rule

$$\bar{N}(\mu) = \sum_{k\sigma} G_\sigma(\vec{k}, \tau = 0^-|\mu); \tag{94}$$

instead we use different ways to compute the zero T limit of the log-derivative $\gamma_{\vec{k}}$. This is a major departure from the L–W route, where the introduction of the Luttinger–Ward functional is an essential second step. This functional can only be defined in perturbation theory, and leads to difficulties for strong coupling problems, as explicitly demonstrated in recent work [63].

In 1-d Ref. [17] uses adiabatic evolution of the system with a magnetic flux parameter, to give a non-perturbative argument for the invariance of Fermi diameter. Ref. [16] extends this to arbitrary dimensions d > 1 assuming that the system is a Fermi liquid. In contrast to the 1-d result, Ref. [16] also requires adiabatic evolution through a large number $\mathcal{O}(L^{d-1})$ of level crossings, arising from a large accumulation of phase with increasing flux.

More generally the use of adiabatic theorem in gapless situations, particularly for d $>$ 1 is risky, and often requires extra symmetry for justification. A well known example is provided by a gapless metal for d $>$ 1, with a varying interaction strength. When the symmetry is less than circular (or spherical), k-space redistribution always occurs upon varying the interaction constant. This results in a change of shape of the Fermi surface [7,64,65], implying that adiabaticity is violated.

We note a few points regarding perturbative arguments. The $T = 0$ Brueckner–Gammel–Goldstone formalism [66] is based on the adiabatic theorem and uses the non-interacting Greens function G_0 as the foundation for the perturbation expansion. Therefore the invariance of the Fermi volume, as well as its shape, are automatic byproducts, we get back what we initially put in. A critique of this method by Kohn and Luttinger [67] led to the L–W work. They used finite T perturbation theory instead, allowing for a k-space redistribution of occupied states [7,64,65]. However the problem of strong coupling remains. It is hard to see how the L–W method can be justified in strong coupling, recalling that it is predicated on the existence of the Luttinger–Ward functional, defined term by term in powers of the coupling. Recent work explicitly displays pathologies of the L–W functional in Hubbard type models at strong coupling [63].

The present work utilizes continuity, instead of perturbation, to bypass the strong coupling problem. Isothermal continuity breaks down at level crossing transitions with tuning, and is signaled by a jump in expectation values. Therefore the guarantor of isothermal continuity is the absence of jump discontinuities in expectation values. In summary we may assume isothermal continuity within a continuously connected phase of matter, thus requiring the absence of first order quantum transitions. As our example of the superconductor shows, the isothermal argument works through the normal to superconducting transition, where the dependence on coupling is non-analytic (but continuous). Here the adiabatic methods seem to fail.

We use continuity in a parameter for linking the interacting system with the Fermi gas. The parameter used is most often, but not necessarily, the coupling constant in the Hamiltonian. In the case of the t-J model with extreme coupling $U = \infty$, a more general interaction type parameter $\lambda \in [0, 1]$ is invoked [25]. Continuous evolution with λ ensures the volume theorem for the t-J model [25].

Our extension of the volume theorem to singlet superconductor is based on two assumptions. Firstly we assume that pairs of electrons act repulsively with respect to other pairs, thereby giving a monotonically increasing chemical potential $\mu_e(m)$ in Eq. (62). This is certainly true in the BCS theory and in exactly solvable models [46,48] for superconductivity in finite size systems. It would break down if an as yet undiscovered glue were to result in say Cooper-quartets, instead of Cooper-pairs. The other main assumption is that of an approximately valid particle–hole symmetry Eq. (68) for the case of fully or partially gapped superconductors. This leads to U$\sim$V in the correlated superconductors, extending the known result Eq. (60) in the weak coupling BCS–Gor'kov case. This symmetry has been assumed to be true in other contexts, e.g. for the recently discussed Majorana Fermions [57]. For strongly coupled systems, this symmetry is hard to establish analytically. However numerical tests of the condition Eq. (68) involving ground-state to ground state matrix elements of the Fermi operators may be feasible for small systems using exact diagonalization, and are planned for future work. Finally since we establish a direct connection with observable variables, one could test the resulting sumrule experimentally in a variety of superconducting materials. The results would indicate if this symmetry holds good, and how widely, if so.

The present work leads to the notion of a pseudo-Fermi surface defined finite T. This surface is shown here to be accessible to ARPES studies from moments of the observed intensities. It seems well worth exploring this object and its T dependence experimentally to throw light on interesting issues in strongly correlated matter. For superconductors such measurements could complement information from the high magnetic field setups used to study the same submerged normal state Fermi surface by destroying the superconducting order using strong magnetic fields [68].

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Appendix A. Spectral function and its relation to the Greens function

With $-\beta < \tau \leq \beta$, we recall the (Matsubara) imaginary time Greens function [2–4]

$$G_\sigma(k,\tau) = -\frac{1}{Z(\mu)} \mathrm{Tr}\, e^{-\beta\mathcal{H}} \left(T_\tau C_{k\sigma}(\tau) C^\dagger_{k\sigma} \right), \tag{A.1}$$

where the time dependence is $Q(\tau) = e^{\tau\mathcal{H}} Q e^{-\tau\mathcal{H}}$. Using the usual antiperiodicity $G(\tau) = -G(\tau+\beta)$ we define the Fourier version as usual $G(i\omega_n) = \frac{1}{2}\int_{-\beta}^{\beta} G(\tau) e^{i\omega_n\tau} d\tau$. We may express G as

$$G(\vec{k}, i\omega_n) = \int d\omega \, \frac{\rho_G(\vec{k},\omega)}{i\omega_n - \omega}, \tag{A.2}$$

where the spectral function $\rho_G(\vec{k},\omega)$ can be conveniently found from the analytic continuations $i\omega_n \to z$ followed by $z \to \omega + i0^+$ as $\rho_G(\vec{k},\omega) = -\frac{1}{\pi}\Im m G(\vec{k}, \omega + i0^+)$.

The spectral function has a further representation [4]

$$\begin{aligned}\rho_G(k,\omega) = (1+e^{-\beta\omega}) \sum_{n,m,a,b} & p_\mu(n) |\langle n,a|C^\dagger_{\vec{k}}|m,b\rangle|^2 \\ & \times \delta(\omega + E_a(n) - E_b(m) + \mu) e^{-\beta E_a(n) + \beta F_n},\end{aligned} \tag{A.3}$$

where F_n is the n-particle free energy.

In terms of $\Delta_E \sim |E_a(n) - E_{a'}(n)|$, i.e. a typical excitation energy at a fixed number for a finite system, we may distinguish between two regimes. At zero T, or more generally for $\Delta_E/k_B \gtrsim T$, the spectral function is a sum over separated delta functions and hence is very grainy. On the other hand provided $(T,\omega) \gtrsim \Delta_E/k_B$, the sum over the delta functions is taken over several states and hence the resulting spectral functions are smooth functions of ω. This is therefore a complementary regime to the earlier one.

In terms of the spectral functions we may write the time dependent functions as

$$G(\vec{k},\tau) = \int_{-\infty}^{\infty} d\omega \, \rho_G(\vec{k},\omega) e^{-\tau\omega} \left(f(\omega)\theta(-\tau) - \bar{f}(\omega)\theta(\tau) \right) \tag{A.4}$$

with the Fermi functions $f(\omega) = \frac{1}{e^{\beta\omega}+1}$ and $\bar{f} = 1 - f$. We will need the following relation for the real part of the Greens function

$$G(k,0) = -\mathcal{P}\int \frac{d\omega}{\omega} \rho_G(k,\omega), \tag{A.5}$$

where $\mathcal{P}$ denotes the principal value.

Appendix B. Some useful integrals arising in the sum-rule Eq. (78)

We outline the calculation of integrals that arise in Eq. (78):

$$\mathcal{J}_m = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega \, \frac{(-\omega)^m}{\cosh(\frac{1}{2}\beta\omega)} \frac{\Gamma}{\Gamma^2 + (\omega - E)^2}, \tag{B.1}$$

for real parameters Γ, E with $m = 0, 1$. A simple way to do these integrals is to use the Mittag-Leffler expansion

$$\frac{1}{\cosh(\pi z)} = \frac{2}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^n (n+\frac{1}{2})}{z^2 + (n+\frac{1}{2})^2}, \tag{B.2}$$

so that we can integrate term by term using the simple result for convolution of two Lorentzians. This yields

$$\mathcal{J}_0 = \frac{1}{\pi}\sum_{n=0}^{\infty}(-1)^n \frac{\Gamma/(2\pi T)+n+\frac{1}{2}}{E^2/(2\pi T)^2+(\Gamma/(2\pi T)+n+\frac{1}{2})^2}$$
$$\mathcal{J}_1 = -\frac{1}{\pi}\sum_{n=0}^{\infty}(-1)^n \frac{(n+\frac{1}{2})E}{E^2/(2\pi T)^2+(\Gamma/(2\pi T)+n+\frac{1}{2})^2}. \tag{B.3}$$

These sums can be performed using the digamma function

$$\Psi(z) = \frac{d}{dz}\log\Gamma(z) = \lim_{M\to\infty}\left(\log M - \sum_{n=0}^{M}\frac{1}{z+n}\right). \tag{B.4}$$

We define a meromorphic function $\xi(z)$ via the alternating infinite sum

$$\xi(z) = \sum_{n=0}^{\infty}\frac{(-1)^n}{z+n} = \frac{1}{2}\left(\Psi(\frac{1}{2}+\frac{z}{2}) - \Psi(\frac{z}{2}).\right), \tag{B.5}$$

In the complex z plane $\xi(z)$ has a pole at the origin and at every negative integers, and is analytic everywhere else. Writing $z = x+iy$ we record the useful corollaries

$$\Re e\,\xi(x+iy) = \sum_{n=0}^{\infty}(-1)^n\frac{x+n}{(x+n)^2+y^2}$$
$$\Im m\,\xi(x+iy) = -\sum_{n=0}^{\infty}(-1)^n\frac{y}{(x+n)^2+y^2}. \tag{B.6}$$

Using these we can perform the required summations in Eq. (B.3) analytically as

$$\mathcal{J}_0 = \frac{1}{\pi}\Re e\,\xi\left(\frac{1}{2}+\frac{\Gamma+iE}{2\pi T}\right)$$
$$\mathcal{J}_1 = -\frac{E}{\pi}\Re e\,\xi\left(\frac{1}{2}+\frac{\Gamma+iE}{2\pi T}\right) - \frac{\Gamma}{\pi}\Im m\,\xi\left(\frac{1}{2}+\frac{\Gamma+iE}{2\pi T}\right). \tag{B.7}$$

From the series defining $\xi(z)$ in Eq. (B.5), it is real for real z. Using the Schwarz reflection principle we deduce relations needed in the text; for $\alpha = \pm 1$

$$\Re e\,\xi\left(\frac{1}{2}+\frac{\Gamma+i\alpha E}{2\pi T}\right) = \Re e\,\xi\left(\frac{1}{2}+\frac{\Gamma+iE}{2\pi T}\right) \tag{B.8}$$
$$\Im m\,\xi\left(\frac{1}{2}+\frac{\Gamma+i\alpha E}{2\pi T}\right) = \alpha\,\Im m\,\xi\left(\frac{1}{2}+\frac{\Gamma+iE}{2\pi T}\right). \tag{B.9}$$

References

[1] J.M. Luttinger, J.C. Ward, Phys. Rev. 118 (1960) 1417.
[2] T. Matsubara, Progr. Theoret. Phys. 14 (1955) 351.
[3] A. Abrikosov, L. Gor'kov, I.E. Dzyaloshinski, Sov. Phys. J.E.T.P. 36 (1959) 900.
[4] A. Abrikosov, L. Gor'kov, I.E. Dzyaloshinski, Methods of Quantum Field Theory in Statistical Physics, Prentice-Hal, Englewood-Cliffs, NJ, 1963.
[5] J.M. Luttinger, Phys. Rev. 119 (1960) 1153, (esp. Eqs. (31, 32, 35)).
[6] L.D. Landau, Sov. Phys. J.E.T.P. 30 (1956) 1058, Sov. Phys. J.E.T.P. 32, 59.
[7] P. Nozières, Theory of Interacting Fermi Systems, W. A. Benjamin, New York, 1964.
[8] C. De Dominicis, J. Math. Phys. 3 (1964) 983;
C. De Dominic, P.C. Martin, J. Math. Phys. 5 (14) (1964) 31.
[9] M. Dahmen, G. Jona-Lasinio, Il Nuovo Cimento LII A (1967) 807.
[10] J.S. Langer, V. Ambegaokar, Phys. Rev. 121 (1961) 1090.
[11] D.C. Langreth, Phys. Rev. 150 (1966) 516.

[12] B.L. Altshuler, A.V. Chubukov, A. Dashevskii, A.M. Finkel'stein, D.K. Morr, E.P.L. 41 (1998) 401.
[13] I. Dzyaloshinskii, Phys. Rev. B 68 (2013) 085113.
[14] K.B. Blagoev, K.S. Bedell, Phys. Rev. Lett. 79 (1997) 1106.
[15] K.B. Dave, P.W. Phillips, C.L. Kane, Phys. Rev. Lett. 110 (2013) 090403.
[16] M. Oshikawa, Phys. Rev. Lett. 84 (2000) 3370.
[17] M. Yamanaka, M. Oshikawa, I. Affleck, Phys. Rev. Lett. 79 (1997) 1110.
[18] T. Senthil, S. Sachdev, M. Vojta, Phys. Rev. Lett. 90 (2003) 216403;
T. Senthil, S. Sachdev, M. Vojta, Physica B 359 (2005) 9;
T. Senthil, M. Vojta, S. Sachdev, Phys. Rev. B 69 (2004) 035111.
[19] J. Kokalj, P. Prelovsek, Eur. Phys. J. B 63 (2008) 431; Phys. Rev. B 78 (2008) 153103.
[20] B. Farid, A.M. Tsvelik, arXiv:0909.2886 (2009).
[21] O.J. Curtin, Y. Nishikawa, A.C. Hewson, J. Phys. Commun. 2 (2018) 031001.
[22] Y. Nishikawa, O.J. Curtin, A.C. Hewson, D.J.G. Crow, Phys. Rev. B 98 (2018) 104419.
[23] E. Quinn, Phys. Rev. B 97 (2018) 115134.
[24] K. Seki, S. Yunoki, Phys. Rev. B 96 (2017) 085124.
[25] B.S. Shastry, Phys. Rev. Lett. 107 (2011) 056403, http://physics.ucsc.edu/~sriram/papers/ECFL-Reprint-Collection.pdf.
[26] B.S. Shastry, Phys. Rev. B 81 (2010) 045121.
[27] W.V. Liu, F. Wilczek, Phys. Rev. Lett. 90 (2003) 047002; Phys. Rev. Lett. 94 (2005) 017001.
[28] N. Trivedi, M. Randeria, Phys. Rev. Lett. 75 (1995) 312;
M. Randeria, N. Trivedi, A. Moreo, R.T. Scalettar, Phys. Rev. Lett. 69 (1992) 2001;
N. Trivedi, R.T. Scalettar, M. Randeria, Phys. Rev. B 54 (1996) R3756.
[29] L. van Hove, Physica 16 (1950) 137;
C.N. Yang, T.D. Lee, Phys. Rev. 87 (1952) 404;
M.E. Fisher, Physics 3 (1967) 255;
Joel L. Lebowitz, International Symposium on Mathematical Problems in Theoretical Physics, Kyoto, Japan, 1975.
[30] J.L. Lebowitz, E.H. Lieb, Phys. Rev. Lett. 22 (1969) 13;
E.H. Lieb, J.L. Lebowitz, Adv. Maths. 9 (1972) 316;
E.H. Lieb, R. Seiringer, The Stability of Matter in Quantum Mechanics, Cambridge University Press, 2010.
[31] Y. Nambu, Phys. Rev. 117 (1960) 648.
[32] L.P. Gor'kov, Sov. Phys.—JETP 7 (1958) 505.
[33] J.R. Schrieffer, Theory of Superconductivity, Benjamin, New York, 1964.
[34] L. Tewordt, Phys. Rev. 128 (1962) 12.
[35] D.J. Scalapino, J.R. Schrieffer, J.W. Wilkins, Phys. Rev. 148 (1966) 263.
[36] S. Kivelson, S. Chakravarty, Europhys. Lett. 16 (1991) 751;
S.R. White, S. Chakravarty, M.P. Gelfand, S.A. Kivelson, Phys. Rev. B 45 (1992) 5062.
[37] A.O. Gogolin, A.A. Nersesyan, A.M. Tsvelik, Bosonization and Strongly Correlated Systems, Cambridge University Press, Cambridge, 1998.
[38] F.H.L. Essler, H. Frahm, F. Göhmann, A. Klümper, V.E. Korepin, The One-Dimensional Hubbard Model, Cambridge University Press, Cambridge, 2005.
[39] T. Giamarchi, Quantum Physics in One Dimension, Clarendon Press, Oxford, 2004.
[40] S. Eggert, A. Mattsson, J. Kinaret, cond-mat/9705157 (vide Eq. (15)).
[41] A.B. Migdal, Nuclear Phys. 13 (1959) 655.
[42] A. Bohr, B.R. Mottleson, D. Pines, Phys. Rev. 110 (1958) 936.
[43] B. Janko, A. Smith, V. Ambegaokar, Phys. Rev. B 50 (1994) 1152;
R.A. Smith, V. Ambegaokar, Phys. Rev. Lett. 77 (1996) 4962.
[44] A.J. Leggett, J. Phys. (Paris) 41 (1980) C7–19.
[45] P. Nozières, S. Schmitt-Rink, J. Low. Temp. Phys. 59 (1985) 195.
[46] R.W. Richardson, J. Math. Phys. 18 (1977) 1802;
R.W. Richardson, N. Sherman, Nucl. Phys. 52 (1964) 221; Nucl. Phys. 52 (1964) 253.
[47] M.T. Tuominen, J.M. Hergenrother, T.S. Tighe, M. Tinkham, Phys. Rev. Lett. B 9 (1992) 1997;
D.C. Ralph, C.T. Black, M. Tinkham, Phys. Rev. Lett. 74 (1995) 3241;
C.T. Black, D.C. Ralph, M. Tinkham, Phys. Rev. Lett. 76 (1996) 688.
[48] M. Gaudin, La Fonction dònde de Bethe, Masson, Paris, 1983;
M.C. Cambiaggio, A.M.F. Rivas, M. Saraceno, Nucl. Phys. A 424 (1997) 157.
[49] J. von Delft, A.D. Zaikin, D.S. Golubev, W. Tichy, Phys. Rev. Lett. 77 (1996) 3189.
[50] K.A. Matveev, A.I. Larkin, Phys. Rev. Lett. 78 (1997) 3749.
[51] L. Amico, A. Osterloh, Phys. Rev. Lett. 88 (2002) 127003.
[52] L. Amico, A. Di Lorenzoa, A. Mastellonea, A. Osterloh, R. Raimondi, Ann. Phys. 299 (2002) 228.
[53] A. Faribault, P. Calabrese, J-S. Caux, Phys. Rev. B 77 (2008) 064503.
[54] E.A. Yuzbashyan, A.A. Baytin, B.L. Altshuler, Phys. Rev. B 71 (2005) 094505; Phys. Rev. B 26 (2003) 214509.
[55] N. Bogoliubov, Sov. Phys.—JETP 34 (1958) 73;
J.G. Valatin, Il Nuovo Cimento 7 (1958) 883.
[56] J. Bardeen, L.N. Cooper, J.R. Schriefer, Phys. Rev. 108 (1957) 1175.
[57] S.R. Elliott, M. Franz, Rev. Modern Phys. 87 (2015) 137.
[58] P. Mai, B.S. Shastry, arXiv:1808.09788, Phys. Rev. B, 98, 2018, 205106. See especially Figures 9-12.
[59] B.S. Shastry, E. Perepelitsky, arXiv:1605.08213, Phys. Rev. B, 94, 2016, 045138.

[60] C. Gros, B. Edegger, V.N. Muthukumar, P.W. Anderson, P.N.A.S. 103 (2006) 14298.
[61] R. Sensarma, M. Randeria, N. Trivedi, Phys. Rev. Lett. 98 (2007) 027004.
[62] F.C. Zhang, C. Gros, T.M. Rice, H. Shiba, Superconductivity Sci. Tech. Vol. 1, 1988.
[63] E. Kozik, M. Ferrero, A. Georges, Phys. Rev. Lett. 114 (2015) 156402.
[64] I.J. and Pomeranchuk, Sov. Phys.—JETP 8 (1958) 361.
[65] W. Metzner, D. Roher, S. Andergassen, Phys. Rev. Lett. 91 (2003) 066402.
[66] K.A. Brueckner, J.L. Gammel, Phys. Rev. 109 (1958) 1023;
J. Goldstone, Proc. Roy. Soc. (London) A 293 (1957) 267;
M. Gell-Mann, F. Low, Phys. Rev. 84 (1951) 350.
[67] W. Kohn, J.M. Luttinger, Phys. Rev. 118 (1960) 41.
[68] G.S. Boebinger, Phys. Today 49 (1996) 36.