

Fermi-edge singularities in x-ray spectra of strongly correlated fermions

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We discuss the problem of x-ray absorption in a D -dimensional system of interacting fermions and, in particular, those features in the x-ray spectra that can be used to discriminate between conventional Fermi liquids and “strange metals.” We find that the x-ray Fermi edge singularities can still be present, although modified, even if the density of states vanishes at the Fermi energy, and that, in general, the relationship between the two appears to be quite subtle.

Since its foundation in the late 1950s, the theory of Fermi liquids has come a long way exploring the limits of its own applicability. However, the quest for possible departures from conventional Fermi-liquid behavior still remains one of the mainstays of modern condensed-matter theory.

It is well known that Fermi liquids can be more easily destroyed in low dimensions. As a common example, in one spatial dimension (1D) the Fermi-liquid theory utterly fails even for a seemingly innocuous arbitrary weak short-range repulsion. The corresponding non-Fermi-liquid (NFL) metallic state is characterized by power-law decaying correlation functions and is referred to as the Luttinger liquid (LL) which can be thought of as a marginal deformation of the Fermi liquid.

It is generally believed that in higher ($D > 1$) spatial dimensions a NFL behavior can stem from sufficiently long-ranged and/or retarded (“singular”) interactions. However, the necessary criteria remain unknown, which leaves room for a NFL regime to occur even as a result of nonsingular (e.g., screened) repulsive interactions.

In theory, a NFL behavior is commonly expected to manifest itself in single electron spectroscopy and, in particular, in angular resolved photoemission at low energies of incident photons. However, even for such a widely recognized candidate for a “strange metal” as the normal state of the high T_c cuprates, direct deduction of any ultimate evidence of the NFL behavior (e.g., electron self-energy) from the photoemission data has proven to be a tedious task.¹

In the present paper, we discuss a different kind of feature that has already been extensively studied in a variety of conventional metals: the Fermi-edge singularities (FES) in high-energy x-ray absorption. First predicted theoretically for weakly interacting (Fermi-liquid-like) metals back in 1967,^{2,3} the FES became one of the hallmarks of many-body Fermi systems. However, the effect of interactions in the conduction band on the FES has not drawn much attention, except for the case of the 1D LL’s studied by a number of authors.^{4,5}

In retrospect, the FES provided the first example of a much more generic phenomenon of the “orthogonality catastrophe” (OC). The latter implies that in the presence of a

sudden perturbation the ground states of an infinite Fermi system before and after the perturbation was switched on appear to be strictly orthogonal to each other.

In the problem of the x-ray-induced photoemission such a steplike time-dependent perturbation $V(t) = V\Theta(t)$ corresponds to the attractive potential of a deep core level stripped off its electron by an incident x-ray photon. Following the instantaneous shakeup, the initial ground state $|0\rangle$ of the Fermi system tends to readjust and evolves into the final one $|V\rangle$ by virtue of creating coherent multiple particle-hole pairs. These bosonic excitations dominate in the action $S_{oc}(t)$ describing the process of relaxation of the initial ground state and lead to the suppression of the time-dependent overlap between the two ground states: $\langle 0|V\rangle \sim \exp[-S_{oc}(t)]$ at times $t \rightarrow \infty$.

Being closely related to the Green function of a localized core hole described by the operator $d(t)$,³ the overlap factor controls the shape of the photoemission peak corresponding to the absorption of hard x-ray photons that knock core electrons out of the system

$$P(\omega) \propto \text{Im} \int_0^\infty dt e^{i\omega t} \langle T d(t) d^\dagger(0) \rangle. \quad (1)$$

Here ω is the photon energy measured from the threshold equal to the sum of the binding energy of the core level and the exit work function for the runaway electron.

In the standard Fermi-liquid case the action $S_{oc}(t)$ diverges logarithmically, which gives rise to the asymmetrical power-law singularity of the absorption peak^{2,3}

$$P(\omega) \propto \Theta(\omega) |\omega|^{-1+2 \sum_l \delta_l^2 / \pi^2} \quad (2)$$

that would have been absent in an insulating state where at zero temperature the peak remains sharp: $P(\omega) \propto \delta(\omega)$.

The partial phase shift δ_l in Eq. (2) is equal to the product of one of the angular momentum harmonics of the Fourier transformed core hole potential: $\int d\mathbf{r} V(\mathbf{r}) e^{i\mathbf{r}(\mathbf{k}-\mathbf{k}')} = \sum_l Y_l(\hat{\Omega} - \hat{\Omega}') V_l(k_F)$ (throughout this paper we include all the angular momentum quantum numbers into the definition of “ l ”) and the density of states (DOS) in the conduction band $\nu(\omega) = 1/\pi \int d\mathbf{k} \text{Im} G(\mathbf{k}, \omega)$ taken at the Fermi energy $\nu_F = \nu(\omega=0)$:

$$\tan \delta_l = -V_l \nu_F. \quad (3)$$

At first sight, Eq. (3) seems to imply that DOS must remain finite for the divergence (2) to occur. In order to find a possible caveat in this seemingly unavoidable conclusion, we consider the simplest, short-range isotropic, core-hole potential $V(\mathbf{r}) = V\delta(\mathbf{r})$ and, following the original work by Noziers and De Dominicis,⁶ introduce a transient Green function $\mathcal{G}(t, t'|V)$ which allows the OC action to be cast in the form $S_{oc}(t) = \int_0^V dV' \int_0^t dt' \mathcal{G}(t, t'|V')$.

For free fermions this Green function obeys the equation

$$\mathcal{G}(t, t'|V) = G(\mathbf{0}, t - t') + V \int_0^t dt'' \mathcal{G}(t, t''|V) G(\mathbf{0}, t'' - t'), \quad (4)$$

which relates it to the time dependence of the propagator $G(\mathbf{r}, t)$ of the conduction-band fermions in the absence of the core hole potential.

The above, naive, conclusion would then imply that even with the interaction effects taken into account, the local value of the propagator $G(\mathbf{0}, t)$ would have to retain its Fermi-liquid-like $\propto 1/t$ behavior, the exponent in the power-law divergence (2) being determined by the corresponding prefactor.

However, this condition would be much too stringent, because Eq. (4) appears to be missing important vertex corrections that describe the effect of the electron interactions on the coupling to the core hole potential $V(\mathbf{r})$.

In the extensively studied case of the 1D LL, for example, crucial relevance of the vertex corrections can be seen from the fact that although the faster-than- $1/t$ decay of the fermion propagator $G(0, t) \propto t^{-(2+g+g^{-1})/4}$, where g is the Luttinger parameter ($0 < g < 1$ for short-range repulsive interactions), does imply a vanishing DOS, the FES retain their algebraic behavior with the g -dependent exponents.⁴

In the 1D case of purely forward scattering off the core-hole potential, one can relate the robustness of the FES to the fact that the density of particle-hole pairs with small momenta given by the integral of the density correlation function $\chi(\omega, q)$ maintains its noninteracting functional form: $\int_0^{Q \ll k_F} \text{Im} \chi(\omega, q) dq \propto \omega$.⁴

This property is due to the known asymptotically exact cancellation between the self-energy and vertex interaction corrections to the density correlation function at small momenta. In order to account for both types of corrections the previous studies⁴ resorted to the standard method of 1D bosonization.

Inspired by the success of 1D bosonization, there has been a strong recent effort toward extending this method to higher dimensions.^{7,8} In what follows we employ the ‘‘tomographic’’ version of this technique (see Ref. 7), which is capable of yielding asymptotically exact results provided that fermions undergo predominantly forward scattering due to the interactions in the conduction band and the core-hole potential.

Under these conditions the Lagrangian of the problem can be expressed solely in terms of the bosonic partial densities $\rho_{\hat{\Omega}}^{\sigma}(\mathbf{r}, t)$ associated with different points on the Fermi surface parametrized by the unit vector $\hat{\Omega}$. These degrees of freedom obey the infinite algebra

$$[\rho_{\hat{\Omega}}^{\sigma}(\mathbf{r}, t), \rho_{\hat{\Omega}'}^{\sigma'}(\mathbf{r}', t)] = K_{\sigma\sigma'} \delta(\hat{\Omega} - \hat{\Omega}') (\nabla \hat{\Omega}) \delta(\mathbf{r} - \mathbf{r}'). \quad (5)$$

Noncommutativity of the density operators at the same point of the Fermi surface can be interpreted as the ‘‘chiral anomaly’’ which reflects, in compliance with the Luttinger theorem, conservation of the total number of states enclosed by the nominal Fermi surface in the presence of interactions between fermions.

In the case of sufficiently weak spin-independent interactions the K matrix reduces to the unit $K_{\sigma\sigma'} = \delta_{\sigma\sigma'}$. By introducing the K matrix into the theory one can incorporate strong correlations between fermions of opposite spins which modify the very kinematics of the system and cannot be treated as regular quadratic Landau-type terms in the effective Lagrangian.

Although the conduction-band fermions $\psi_{\sigma}(\mathbf{r}, t)$ couple to the forward-scattering core hole potential only via the charge density operator $\int d\mathbf{r} \sum_{\sigma} \psi_{\sigma}^{\dagger}(\mathbf{r}) V(\mathbf{r}) \psi_{\sigma}(\mathbf{r}) \approx V \sum_{\hat{\Omega}} \sum_{\sigma} \rho_{\hat{\Omega}}^{\sigma}$, we keep the spin degrees of freedom as well, thereby leaving open the possibility of incorporating the above-mentioned exclusion principle-type spin-dependent correlations in the conduction band. Then the relevant part of the Lagrangian reads as

$$\begin{aligned} L = & \sum_{\hat{\Omega}} \int d\mathbf{q} \rho_{\hat{\Omega}}^{\sigma}(\mathbf{q}) K_{\sigma\sigma'}^{-1}(\mathbf{q}) \frac{i\partial_t - v_F \hat{\Omega} \cdot \mathbf{q}}{\hat{\Omega} \cdot \mathbf{q}} \rho_{\hat{\Omega}}^{\sigma'}(-\mathbf{q}) \\ & - \frac{1}{2} \sum_{\hat{\Omega}, \hat{\Omega}'} \int d\mathbf{q} \rho_{\hat{\Omega}}^{\sigma}(\mathbf{q}) F_{\hat{\Omega}, \hat{\Omega}'}(\mathbf{q}) \rho_{\hat{\Omega}'}^{\sigma}(-\mathbf{q}) \\ & + d^{\dagger} (i\partial_t - E_d) d - (V d^{\dagger} d - E_F) \sum_{\hat{\Omega}} \int d\mathbf{q} \rho_{\hat{\Omega}}^{\sigma}(\mathbf{q}), \quad (6) \end{aligned}$$

where we introduced a generalized (momentum and/or frequency-dependent) Landau function $F_{\hat{\Omega}, \hat{\Omega}'}(\mathbf{q})$ to describe the spin-independent (‘‘residual’’) part of the forward scattering between the conduction-band fermions.

The quantity of primary physical interest is the x-ray absorption/emission intensity in the processes of electron transfer from the core level to the conduction band and vice versa

$$I(\omega) \propto \text{Im} \int_0^{\infty} dt e^{i(\omega + E_F - E_d)t} D(t),$$

$$D(t - t') = \langle T d(t) \psi_{\sigma}(\mathbf{0}, t) \psi_{\sigma'}^{\dagger}(\mathbf{0}, t') d^{\dagger}(t') \rangle. \quad (7)$$

The amplitude (7) can be conveniently expressed as a Gaussian average that has to be taken with respect to the Lagrangian (6)

$$\begin{aligned} D(t) \propto & \left\langle \exp \left[i \sum_{\hat{\Omega}} \int d\mathbf{q} \int d\omega (J_{\hat{\Omega}}(t, \omega, \mathbf{q}) \phi_{\hat{\Omega}}^{\sigma}(-\mathbf{q}) \right. \right. \\ & \left. \left. + V j(t, \omega) \rho_{\hat{\Omega}}^{\sigma}(-\mathbf{q}) \right) \right] \right\rangle, \quad (8) \end{aligned}$$

where the source densities

$$J_{\hat{\Omega}}(t, \omega, \mathbf{q}) = \frac{1 - e^{i\omega t}}{\omega - v_F \hat{\Omega} \cdot \mathbf{q}}, \quad j(t, \omega) = \frac{1 - e^{i\omega t}}{\omega} \quad (9)$$

represent a conduction-band fermion and an immobile core hole, respectively, while $\phi_{\hat{\Omega}}^{\sigma}(\mathbf{q})$ is an auxiliary Hubbard-Stratonovich variable conjugate to $\rho_{\hat{\Omega}}^{\sigma}(\mathbf{q})$.

In order to perform the averaging explicitly one first has to compute the kernel of the angular decomposition for the density correlator $\chi(\omega, \mathbf{q}) = \sum_{\hat{\Omega}, \hat{\Omega}'} \sum_{\sigma, \sigma'} \chi_{\hat{\Omega}, \hat{\Omega}'}^{\sigma, \sigma'}(\omega, \mathbf{q})$. In practice, this amounts to inverting the operator

$$\chi_{\hat{\Omega}, \hat{\Omega}'}^{-1}(\omega, \mathbf{q}) = \delta(\hat{\Omega} - \hat{\Omega}') \mathbf{K} \frac{\omega - v_F(\hat{\Omega} \mathbf{q})}{(\hat{\Omega} \mathbf{q})} - \mathbf{1} F_{\hat{\Omega}, \hat{\Omega}'}(\mathbf{q}). \quad (10)$$

Having carried out the Gaussian functional averaging one arrives at the result $D(t) \propto \exp[-S(t)]$ where the total bosonic action $S(t)$ consists of the three different contributions that can be identified with, respectively, the time dependence of the local conduction-band propagator $G(\mathbf{0}, t)$ which is directly related to DOS:

$$S_{dos}(t) = \int d\omega (1 - \cos \omega t) \text{Im} \int d\mathbf{q} \frac{\chi_{\hat{\Omega}, \hat{\Omega}'}(\omega, \mathbf{q})}{v_F^2(\mathbf{q} \hat{\Omega})^2}, \quad (11)$$

the ‘‘excitonic’’ term due to the interaction between the conduction band and the core hole in the final state:

$$S_{ex}(t) = V \int d\omega \frac{1 - \cos \omega t}{\omega} \text{Im} \sum_{\hat{\Omega}'} \int d\mathbf{q} \frac{\chi_{\hat{\Omega}, \hat{\Omega}'}(\omega, \mathbf{q})}{v_F(\mathbf{q} \hat{\Omega})} \quad (12)$$

and the OC term *per se*:

$$S_{oc}(t) = V^2 \int d\omega \frac{1 - \cos \omega t}{\omega^2} \text{Im} \sum_{\hat{\Omega}, \hat{\Omega}'} \int d\mathbf{q} \chi_{\hat{\Omega}, \hat{\Omega}'}(\omega, \mathbf{q}). \quad (13)$$

We first comment on the use of Eqs. (11)–(13) in the free limit where one is supposed to recover the known results of Refs. 2 and 3 by simply putting the Landau function equal to zero.

Although for a sufficiently weak attractive core hole potential ($0 < \delta_l \ll 1$) we do reproduce the expected results for $S_{dos} = \log t$ and $S_{ex} = (2V\nu_F/\pi) \log t$, the expression for S_{oc} turns out to be formally divergent. This nonphysical divergence is solely due to our assumption of a strictly forward scattering off the core-hole, for in this extreme limit all the angular harmonics of the core-hole potential become equal: $V_l = V$, and therefore the sum

$$\sum_{\hat{\Omega}} V^2 = \sum_l V_l^2 \quad (14)$$

diverges. As a result, the vanishing OC factor $\exp(-S_{oc})$ in $I(\omega)$ outpowers any divergence that may result from the excitonic DOS enhancement at the location of the core hole, and, as a result, all the FES are gone.

However, for any realistic core-hole potential $V(\mathbf{r})$ the sum (14) is finite, and the overall energy dependence of the x-ray absorption near the threshold assumes its classical form: $I(\omega) \propto \Theta(\omega) |\omega|^{-2\delta_0/\pi + 2\sum_l \delta_l^2/\pi^2}$.^{2,3}

It is worthwhile mentioning that the opposite case of an isotropic core hole potential ($\delta_l = 0$ for all $l \neq 0$) allows one

to construct an alternate bosonization scheme, thanks to the effectively 1D character of the radial motion of noninteracting fermions in the s -wave orbital channel.⁹

Turning now to the applications of the above formalism, we first consider the limit of an exclusively ‘‘intratomograph’’ spin-independent interaction that can only couple fermions with the same direction of the momenta: $\mathbf{K} = \mathbf{1}$ and $F_{\hat{\Omega}, \hat{\Omega}'}(\mathbf{q}) \propto \delta(\hat{\Omega} - \hat{\Omega}')$. A straightforward analysis shows that, similarly to the chiral 1D case, the only effect of such an interaction is a multiplicative renormalization of the Fermi velocity v_F and, accordingly, the phase shifts: δ_l that determine the, otherwise unaltered, FES exponents.

Therefore, in order for a quasi-1D LL-like behavior to occur in $D > 1$ -dimensions, the spin-independent fermion interaction must couple each tomograph $\hat{\Omega}$ to its antipodal one at $-\hat{\Omega}$: $F_{\hat{\Omega}, \hat{\Omega}'}(\mathbf{q}) \propto \delta(\hat{\Omega} - \hat{\Omega}') + \delta(\hat{\Omega} + \hat{\Omega}')$.

In this situation the effective Luttinger parameter appears to be given by the ratio $g = v_F/c$ between the Fermi velocity and the speed of zero sound that can be read off from the low- q limit of the density correlator: $\chi(\omega, \mathbf{q}) = \sum_{\hat{\Omega}} (\hat{\Omega} \mathbf{q})^2 / [\omega^2 - c^2(\hat{\Omega} \mathbf{q})^2]$.

Then, in a close analogy with the situation in the 1D LL, coupling between the opposite points on the Fermi surface gives rise to, both, vanishing DOS [$\nu(\omega) \sim |\omega|^{(g+1/g-2)/4}$] and modified, yet nonzero, FES exponents

$$P(\omega) \propto |\omega|^{-1 + 2g^3 \sum_l \delta_l^2 / \pi^2},$$

$$I(\omega) \propto \nu(\omega) |\omega|^{-2g\delta_0/\pi + 2g^3 \sum_l \delta_l^2 / \pi^2}, \quad (15)$$

where the phase shifts δ_l are given by Eq. (3) with a finite ν_F corresponding to the noninteracting case $g = 1$.

As follows from Eqs. (15), repulsive interactions weaken the OC exponent via the reduced compressibility, thereby enhancing the overlap $\langle 0|V \rangle$ between the initial and the final ground states.

An effective 1D LL-like behavior was conjectured in the very beginning of the high T_c saga on the basis of such suggestive experimental findings about the normal state of the high T_c cuprates as the anomalous power-law decay of the optical conductivity $\sigma(\omega) \propto \omega^{-1+2\alpha}$ with $\alpha = 0.15 \pm 0.05$, the $\propto 1/T^2$ temperature dependence of the low-frequency limit of the magnetic susceptibility at momentum $\mathbf{q} = (\pi, \pi)$, the $\propto \omega^{-1/2}$ tail of the electron spectral function $\text{Im} G(\mathbf{k}, \omega)$, the linear c -axis tunneling density of states $dI/dV \sim V$, and others.¹⁰

Thus far, traditional perturbative analyses did not provide supporting evidence that the above quasi-1D regime may indeed occur in a low-density weakly interacting system of fermions with a spherical Fermi surface. Nonetheless, one can expect the situation to be different in paramagnetic lattice systems close to half filling where the Hubbard-like no-double-occupancy constraint gives rise to the off-diagonal matrix elements $K_{\sigma, -\sigma} = \phi/\pi$ in Eq. (5) which are proportional to the on-shell phase shift $-\pi/2 \leq \phi \leq 0$ for a pair of fermions with opposite spins.⁷

Indeed, even in the absence of any coupling between different tomographs the modified commutation relations (5) alone give rise to the anticipated spin-charge separation and

change the OC exponent that enters both $P(\omega)$ and $I(\omega)$ from $2\sum_l \delta_l^2/\pi^2$ to $[1 + 2\phi/\pi + \sqrt{1 + (2\phi/\pi)^2}]\sum_l \delta_l^2/\pi^2$ while leaving DOS unaltered.

In principle, the asymmetrical profile of the photoemission peak $P(\omega)$ can be measured in absorption of hard x rays that knock core electrons out of the system, whereas measuring $I(\omega)$ requires soft x rays that can only promote core electrons up to the conduction band. In practice, however, for the exponents in question to be reliably deduced from a real x-ray spectrum, all the absorption lines and thresholds must be sufficiently sharp and well separated from one another.

Furthermore, if the core-hole potential can be approximated by the first two orbital harmonics, $V(\hat{\Omega} - \hat{\Omega}') \approx V_0 + V_1 Y_1(\hat{\Omega} - \hat{\Omega}')$, then by measuring the two exponents in Eqs. (15) and invoking the Friedel sum rule ($2\sum_l \delta_l = \pi$) one might be able to extract the numerical values of both the relevant phase shifts $\delta_{0,1}$ and the Luttinger parameter g that serves as a measure of the strength of the LL-like correlations in the conduction band.

Yet another evidence in favor of the above quasi-1D behavior would be the presence of the FES in the x-ray spectra even if the core hole has a finite, as opposed to infinite, mass. Such an observation would be in a marked contrast with the situation in the $D > 1$ Fermi liquids, where the hole recoil is known to reduce the number of density excitations, thereby smearing the FES out.¹¹

Therefore, one indirect manifestation of the ‘‘tomographic’’ picture of fermion scattering would be an observation of the FES in valence-band photoemission which creates a mobile hole in the valence band.¹²

The above results are valid as long as the core-hole potential can be considered as a predominantly forward scatterer, and the bosonized theory (6) remains Gaussian. For a

realistic core-hole potential, however, the non-forward-scattering contribution is likely to become increasingly more and more important at $\omega \rightarrow 0$.

Indeed, in the framework of the conventional cluster expansion that does not rely on any bosonic representation, Eq. (13) appears to be merely the first significant ($k=2$) term in the infinite series $S_{oc} = \sum_k S_{oc}^{(k)}$, where $S_{oc}^{(k)} \propto V^k$ is given by a convolution of the $k-1$ functions $\chi(\omega, \mathbf{q})$.

In analogy with the 1D backscattering problem where Eq. (13) yields $S_{oc}^{(k)} \propto t^{2(1-g)(k-1)}$,⁵ it is conceivable that the re-summation of the formally divergent series may result in $S_{oc} \propto \log t$, and therefore at the lowest energies a universal algebraic behavior would set in, which then would be controlled by a universal (independent of the strength of a generic non-forward-scattering core-hole potential) exponent.

However, regardless of whether or not this regime could be washed out by the photoemission line broadening, the universal exponents themselves cannot provide much insight into the nature of electron correlations in the conduction band.

To summarize, in this paper we considered the problem of x-ray absorption in the presence of interactions in the conduction band. By restricting our attention to the case of the forward-scattering core-hole potential we were able to incorporate the fermion interactions in the framework of the tomographic bosonization approach. We found that a vanishing single-particle DOS does not necessarily preclude the existence of the FES in the x-ray spectra, which then offer an independent way of probing the many-body correlations in strongly interacting Fermi systems.

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