Fermi-Edge Singularity in the Vicinity of the Resonant Scattering Condition

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Fermi-edge absorption theory predicting the spectrum $A(\omega) \propto \omega^{-2\delta_0/\pi+\delta_0^2/\pi^2}$ relies on the assumption that scattering phase δ_0 is frequency independent. The dependence of δ_0 on ω becomes crucial near the resonant condition, where the phase changes abruptly by π. In this limit, because of the finite time spent by electron on a resonant level, the scattering is dynamic. We incorporate the finite time delay into the theory, solve the Dyson equation with a modified kernel, and find that, near the resonance, $A(\omega)$ behaves as $\omega^{-3/4}|\ln\omega|$. Scattering off the core hole becomes resonant in 1D and 2D in the presence of an empty subband above the Fermi level; then a deep hole splits off a level from the bottom of this subband. Fermi-edge absorption in the regime when resonant level transforms into a Kondo peak is discussed.

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Introduction.—Along with the Kondo effect, the Fermi-edge absorption from the localized level into a continuum is a fundamental many-body effect in the Fermi systems [1]. Its many-body character manifests itself via two mechanisms: scattering of the excited electron from the hole left behind and adjustment of the Fermi sea to the abrupt switch-on of the hole potential. Correspondingly, near the threshold, the spectrum, $A(\omega) = I(\omega)P(\omega)$, is a product [2] of two functions

$$I(\omega) = \left(\frac{D}{\omega}\right)^{2\delta_0/\pi}, \qquad P(\omega) = \left(\frac{D}{\omega}\right)^{-\delta_0^2/\pi^2}, \qquad (1)$$

where D is the bandwidth and δ_0 is the phase shift for s scattering. Phase δ_0 is related to the hole potential strength V as $\tan\delta_0 = \pi\nu_0 V$, where ν_0 is the density of states. The function $I(\omega)$ is the single-electron-line contribution, which describes the first mechanism, while $P(\omega)$ accounts for the shakeup effects.

The essence of the anomalous behavior of $I(\omega)$ can be illustrated using Fig. 1(a). In the first order in scattering by the core-hole potential, the electron is first promoted by a photon from the initial state (i) to the state (ν), and then scattered into the final state (f) by the core-hole potential. Sensitivity to the Fermi edge is due to the fact that the virtual state ν can lie only above the Fermi level. Indeed, in a process when ν is below the Fermi level, the optical transition $i \to \nu$ takes place after the scattering $\nu \to f$. This scattering happens from the occupied core level i and is thus suppressed [3]. Summation over empty virtual states leads to the anomalous contribution $\propto V\ln(\omega/D)$ to $I(\omega)$. Equation (1) emerges upon collecting contributions, $\propto V^n\ln^n(\omega/D)$, in all orders, n.

Derivation of Eq. (1) by Nozieres and De Dominicis (ND) in Ref. [2] strongly relies on the assumption that δ_0 is frequency independent. This assumption implies that the scattering is instantaneous. Below we focus on low-dimensional systems (2D and 1D) and identify a situation when the above assumption is violated. This situation realizes when the Fermi level is close to an empty upper subband, as shown in Fig. 1. In such an arrangement it is important that in 2D and 1D even a deep core hole creates a localized level a distance E_{ex} below the bottom of the upper subband, see Fig. 1. Studies of many-body effects in the arrangement when Fermi level is near the bottom of empty subband have been reported in Refs. [4–10].

Because of hybridization with continuum of lower band, the level E_{ex} acquires a finite width Γ. Then the process underlying the Fermi-edge singularity is not scattering from bare core-hole potential but rather resonant scattering on the quasilocal level. Correspondingly, the scattering phase is given by

$$\delta(\omega) = \arctan\frac{\Gamma}{\omega - \Delta}, \qquad (2)$$

where Δ is the energy distance from localized level to the Fermi level E_F. In the limit $\Delta \to 0$, ω dependence of δ is strong. Indication that in this limit the ND theory is

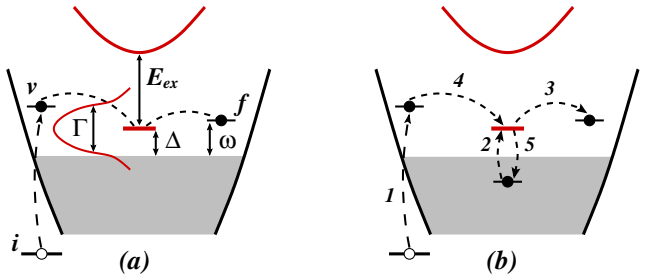

FIG. 1 (color online). (a) In the presence of upper subband, the core-hole potential creates bound state (resonant level) with energy E_{ex} measured from the bottom; its lifetime Γ is due to a coupling to the lower subband. For a photoelectron with energy, $\omega \ll \Gamma$ above the Fermi level, the dynamical character of scattering from resonant level is crucial. (b) In the presence of resonant level, the amplitude of virtual process 2 then 3 is attractive, while the amplitude of virtual process 4 then 5 is repulsive.

inapplicable follows from the fact that at $\omega = \Delta$, the phase jumps by π. Naive assumption that $I(\omega)$ is "local" in frequency leads to a paradoxical conclusion that, as E_F is swept through the bound state, $I(\omega)$ changes abruptly from $I(\omega) \propto 1/\omega$ to $I(\omega) \propto \omega$. By contrast, the shakeup term $P(\omega) \propto \omega^{1/4}$ does not experience a jump.

As a resolution of this paradox, in this Letter we show that abrupt change of $I(\omega)$ does take place in the frequency interval, $\omega \sim |\Delta|$, which gets progressively narrow as Δ goes to 0. We also show that outside this interval, where the ND theory does not apply, a new, dynamical resonant-scattering regime governs the absorption [11]. In this regime, instead of Eq. (1), $I(\omega)$ is given by

$$I(\omega)|_{|\Delta|<\omega<\Gamma} = \frac{\nu_0}{2\pi}\frac{\Gamma}{\omega}\ln\left(\frac{E_{\rm ex}}{\omega}\right), \tag{3}$$

independently of the sign of Δ. Our findings are illustrated in Fig. 2.

Dynamic-scattering regime.—Within the ND theory, the transient Green function $\varphi(\tau, \tau'|t, t')$ satisfies the Dyson equation

$$\varphi(\tau, \tau'|t, t') = G(\tau - \tau') + \int_t^{t'} d\tilde{\tau} K(\tau, \tilde{\tau})\varphi(\tilde{\tau}, \tau'|t, t'), \tag{4}$$

where $G(t) = -\nu_0/t$ is the bare electron Green function, and the kernel is defined as $K(\tau, \tilde{\tau}) = VG(\tau - \tilde{\tau})$. The single-electron-line contribution to $A(\omega)$ is expressed in terms of the transient Green function as

$$I(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\int_{-\infty}^{0} dt e^{-i\omega t}\varphi(0^-, t^+|t, 0). \tag{5}$$

The delicate character of Fermi-edge absorption can be inferred from the structure of nth term,

$$V^n \int_t^0 dt_1 \cdots \int_t^0 dt_n G(-t_1)G(t_1 - t_2)\cdots G(t_n - t), \tag{6}$$

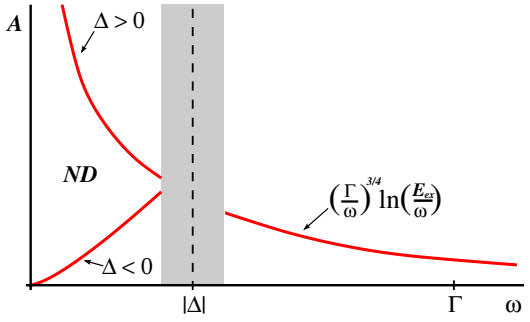

FIG. 2 (color online). Absorption spectrum $A(\omega)$ in the situation when the Fermi level is close to resonant level ($|\Delta| \ll \Gamma$) is shown schematically. For $\omega < |\Delta|$ the ω dependence, Eq. (25), is governed by ND theory. In the "dynamic-scattering" domain $|\Delta| < \omega < \Gamma$ the spectrum is $A(\omega) = (\Gamma/\omega)^{3/4}\ln(E_{\rm ex}/\omega)$ for any sign of Δ. In the domain $\omega \gg \Gamma$, $A(\omega)$ exhibits a jump at $\omega = E_{\rm ex}$, when absorption into the second subband sets in.

of perturbative expansion of $\varphi(0^-, t^+|t, 0)$ in powers of V, which follows from Eq. (4). It appears that contributions of different orderings of times t_i, Fig. 3(a), at which electron is scattered, cancel each other up to $1/n!$.

Frequency dependence of δ, Eq. (2), translates into a time delay τ in the scattering processes, as illustrated in Fig. 3(b). Each delay ranges from $E_{\rm ex}^{-1}$ to $|\Delta|^{-1}$. Then, in the limit $\Delta \to 0$, the above cancellation is completely destroyed. On the quantitative level, the dynamical character of the resonant scattering alters the kernel of Eq. (4).

Resonant-scattering kernel.—In the presence of the empty upper subband, the constant interaction V for electrons of the Fermi sea acquires a frequency dependence,

$$\tilde{V}(\omega) = V_{12}\frac{G_2(\omega)}{1 - V_{22}G_2(\omega)}V_{21}. \tag{7}$$

Here V_{12} and V_{22} are inter- and intrasubband matrix elements of the hole potential, respectively; G_2 is the Green function of the upper subband,

$$G_2(\omega) = \sum_q \frac{1}{\omega - \epsilon_{2q} + i\eta}, \tag{8}$$

and $\epsilon_{2q} = \hbar^2 q^2/2m$ is the spectrum near the bottom. The form Eq. (7) is a result of summation of ladder-type diagrams, see a blowup in Fig. 3. Since $V_{22} < 0$ describes attraction, bound state emerges as a pole in Eq. (7),

$$E_{\rm ex} = \frac{2\pi^2 m}{\hbar^2}|V_{22}|^2 (1\mathrm{D}), \quad E_{\rm ex} = De^{-(2\pi\hbar^2/m|V_{22}|)} (2\mathrm{D}). \tag{9}$$

Expanding near the pole, we simplify $\tilde{V}$ to the form

$$\tilde{V}(\omega) = \left(\frac{\Gamma}{\pi\nu_0}\right)\frac{1}{\omega - \Delta + i\eta}, \tag{10}$$

where the width Γ is given by

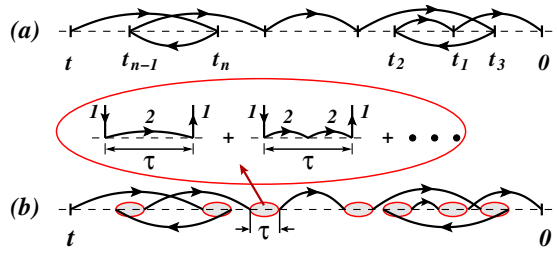

FIG. 3 (color online). (a) Typical contribution, Eq. (6), to the transient Green function in ND theory. Instantaneous scatterings take place at time moments, $t_1, t_2, \ldots, t_n$. (b) In the presence of a resonant level, each scattering act involves a "visit" to the resonant level, and takes a finite time τ. The blowup illustrates a ladder of scatterings off the core hole in the upper subband, 2, which leads to resonant scattering in the lower subband, 1.

$$\Gamma = \frac{2\pi\nu_0 E_{\rm ex}}{|V_{22}|}|V_{12}|^2(1{\rm D}),$$
$$\Gamma = \frac{2\pi^2\hbar^2\nu_0 E_{\rm ex}}{m|V_{22}|^2}|V_{12}|^2(2{\rm D}). \quad (11)$$

Effective interaction Eq. (10) corresponds to repulsion for $\omega > \Delta$ and to attraction for $\omega < \Delta$. In the resonant-scattering regime, the kernel in Eq. (4) instead of the simple product $VG(\tau - \tilde{\tau})$ becomes a convolution

$$K_{\rm res}(\tau, \tau') = \int_t^0 d\tau^* G(\tau - \tau^*) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(\tau^* - \tau')}\tilde{V}(\omega). \quad (12)$$

Integration over ω can be carried out explicitly, yielding

$$K_{\rm res}(\tau, \tau') = i\frac{\Gamma}{\pi}\int_t^0 d\tau^* \frac{\theta(\tau^* - \tau')}{\tau - \tau^*} e^{-i\Delta(\tau^* - \tau')}. \quad (13)$$

For the most interesting case $\Delta = 0$, the expression for the kernel assumes the form

$$K_{\rm res}(\tau, \tau') = -i\frac{\Gamma}{\pi}\ln\left|\frac{\tau}{\tau - \tau'}\right|. \quad (14)$$

We see that $\ln|\tau - \tau'|$ in $K_{\rm res}$ emerges in the place of $1/(\tau - \tau')$ in the ND kernel. This is a consequence of opposite signs of interaction with resonant level for electrons and for holes.

Derivation of Eq. (3).—Substituting Eq. (14) into Eq. (4) and performing the rescaling

$$\varphi(\tau, \tau'|t, 0) = \frac{\nu_0}{t}\phi\left(\frac{\tau}{t}, \frac{\tau'}{t}\right), \quad (15)$$

we arrive to the following dimensionless equation:

$$\phi(x, y) = -\frac{1}{x - y} + i\gamma\int_0^1 dz \ln\left(\frac{x}{|x - z|}\right)\phi(z, y), \quad (16)$$

where $\gamma = \frac{\Gamma}{\pi}t$. Note that the kernel Eq. (16) is much less singular than the ND kernel. As a result, the solution does not contain a ND transient factor, $[(1 - x)y/(1 - y)x]^{\delta/\pi}$, which is singular for $x \to 0$, $y \to 1$. This allows us to search for the solution of Eq. (16) as a linear combination $\phi(x, y) = \sum_m c_m(y, \gamma)u_m(x)$ of the eigenfunctions $u_n(x)$ of the Hermitian integral operator

$$\hat{R}\{u_n(x)\} = \int_0^1 dz \ln|x - z|u_n(z) = \lambda_n u_n(x), \quad (17)$$

where λ_n are the eigenvalues. The kernel in Eq. (17) is symmetric with respect to $x = 1/2$. Correspondingly, $u_n(x)$, $n = 0, 1, 2, \ldots$ are even (for n even) and odd (for n odd) functions of $(x - \frac{1}{2})$. For coefficients $c_m(y, \gamma)$ of the linear expansion Eq. (16) yields $c_m(y, \gamma) = [a_m(y) + b_m d(y, \gamma)]/(1 + i\gamma\lambda_m)$, where

$$a_m(y) = \int_0^1 dz \frac{u_m(z)}{y - z} = \lambda_m u_m'(y), \quad (18)$$

$$b_m = \int_0^1 dz u_m(z)\ln z = \lambda_m u_m(0). \quad (19)$$

In the second identities of (18) and (19) we used Eq. (17).

The kernel, $\ln x - \ln|x - y|$, of Eq. (16), in addition to the difference term, contains a y-independent term. As a result, the coefficient $d(y, \gamma) = i\gamma\int_0^1 dz\phi(z, y)$ is the same for all m. Our key observation is that the relevant values of m are $\gg 1$. For such m, it can be shown that eigenvalues behave as $\lambda_m \approx -1/m$. Concerning the eigenfunctions $u_m(x)$, near the boundaries $x = 0$, 1 they are constants, $u_m(0) = \pm u_m(1)$, while their derivatives diverge logarithmically. Outside of small ($\sim 1/m$) intervals from the boundaries, $u_m(x)$ behave as $\sin(2\pi x/\lambda_m)$ and $\cos(2\pi x/\lambda_m)$. All these large-m properties can be established upon integrating by parts in Eq. (17). Then the result is determined by a narrow domain $|x - z| \sim 1/m$. The same simplification leads to a concise expression for $d(y, \gamma)$, namely, $d(y, \gamma) \simeq -i\gamma\ln(1 - y)$, and subsequently to the solution for $\phi(x, y)$

$$\phi(x, y) \simeq -\ln(1 - y)\sum_n \frac{[u_n(1) + i\gamma\lambda_n u_n(0)]u_n(x)}{1 + i\gamma\lambda_n}. \quad (20)$$

In calculating $I(\omega)$ from Eq. (20) the combination $\sum_n u_n(1)u_n(x)$ appears. This combination is equal to $\delta(1 - x)$ and does not contribute to the absorption. In the ND problem, divergences in the time domain are cut off by iD^{-1}. In our case, the logarithmic divergence in Eq. (20) is terminated at $(1 - y) = i(E_{\rm ex}t)^{-1}$. Correspondingly, the minimal x in Eq. (20) is, in fact, $x_{\rm min} = i(E_{\rm ex}t)^{-1}$. Taking this into account and using Eqs. (5) and (15), we express $I(\omega)$ in the integral form

$$I(\omega) \simeq \frac{2\nu_0\Gamma}{\pi}\,{\rm Im}\int_0^{\infty} dt e^{i\omega t}S(t)\ln(iE_{\rm ex}t), \quad (21)$$

where the sum

$$S(t) = \sum_{\rm odd\ m}\frac{\lambda_m u_m(0)u_m(x_{\rm min})}{\lambda_m\Gamma t + i\pi} \quad (22)$$

is performed over only odd m, for which $u_m(1) = -u_m(0)$. Summation over m requires large-m values of $u_m(0)$. In fact, these values saturate with increasing m. The latter follows from the identity

$$\sum_{\rm odd\ m}\lambda_m u_m(0)u_m(x) = \frac{1}{2}\ln\left(\frac{x}{1 - x}\right), \quad (23)$$

which is a direct consequence of the identity, $\ln x = \sum_m \lambda_m u_m(0)u_m(x)$. The left-hand side behaves as $\ln x$ at $x \to 0$. With $\lambda_m \approx -1/m$, this suggests that $u_m(x) \approx u_m(0) \approx 1$ for $m < x^{-1}$. Comparing Eqs. (22) and (23) we conclude that

$$S(t) \approx \frac{1}{4} + \frac{1}{2\pi i}\ln(i\Gamma t x_{\rm min}) = \frac{1}{4} + \frac{1}{2\pi i}\ln\left(\frac{E_{\rm ex}}{\Gamma}\right). \quad (24)$$

The imaginary part of $S(t)$ is determined by the upper cutoff, while $\mathrm{Re}S(t)$ comes from $m \sim \Gamma t$; relevant values of m are large, as we assumed above. Factor Γt in the argument of the logarithm comes from the terms in sum equation (22) with $m \lesssim \Gamma t$.

With $S(t)$ being time independent for $t \gg \Gamma^{-1}$, integration in Eq. (21) recovers our result Eq. (3). Physical meaning of the enhancement factor Γ/ω in Eq. (3) is the number of virtual visits of the resonant level and returns to the lower subband by electron during the time $1/\omega$. Away from the resonance, V_{12} can be taken into account on a perturbative level, leading to a factor $[1 + \Gamma/\omega \ln(D/\omega)]$, in $I(\omega)$. Nontriviality of Eq. (3) is that this factor is essentially unchanged near the resonance, when the number of visits to resonant level is large, $\Gamma/\omega \gg 1$.

Concluding remarks.—(i) Our main result, Eq. (3), was obtained by setting $\Delta = 0$ in the kernel equation (13). Finite-Δ correction to $A(\omega)$ is small as $(\Delta/\omega)^2$. Let us briefly discuss the opposite limit, $\omega \ll |\Delta| \ll \Gamma$. In this limit, the characteristic time t in Fig. 3 is $\gg |\Delta|^{-1}$. Then, our above consideration for $\Delta = 0$ applies only in the time domain $(-|\Delta|^{-1}, 0)$. In the remaining domain $(t, -|\Delta|^{-1})$ time intervals $t_i - t_{i+1}$ in Fig. 3 are much bigger than $|\Delta|^{-1}$. This makes scattering "instantaneous," and ND theory applicable in the domain $(t, -|\Delta|^{-1})$; corresponding time-independent scattering amplitude and effective bandwidth are $\Gamma/(\pi\nu_0\Delta)$ and Δ, respectively. Separation of time scales leads to the absorption coefficient in the form of a product of $(\omega/|\Delta|)^{-2\arctan(\Gamma/\Delta)/\pi} \approx (\omega/|\Delta|)^{-\mathrm{sgn}\Delta}$ (from long times), and $\Gamma/|\Delta|$ (from short times, $|t_i| < |\Delta|^{-1}$). With shakeup included, the overall result for absorption coefficient,

$$A(\omega)|_{\Delta>0} \propto \frac{\Gamma}{\omega}\left(\frac{\omega}{\Gamma}\right)^{1/4}, \qquad A(\omega)|_{\Delta<0} \propto \frac{\omega\Gamma}{\Delta^2}\left(\frac{\omega}{\Gamma}\right)^{1/4}, \tag{25}$$

is illustrated in Fig. 2. At $\omega \sim \Delta$, Eq. (25) matches Eq. (3) with logarithmic accuracy.

(ii) Ovals in Fig. 3 can overlap; this corresponds to double occupancy of the resonant level, which our theory does not prohibit. This implies that the Hubbard repulsion U is smaller than Γ. Since U is inversely proportional to the radius of the level wave function, this condition can be met for a shallow level.

Even more interesting is the situation when resonant level, which is split off the upper band by the core hole, is well below the Fermi level ($|\Delta| \gg \Gamma$), and U is not small. Then the level gets occupied, and after time $\sim T_K^{-1} \sim \exp[\pi\Delta/2\Gamma]$ a Kondo peak of width $\sim T_K$ is formed at the Fermi level [13]. The photoexcited electron will experience dynamical resonant scattering from this peak. One can argue that our result for dynamical resonant-scattering regime will apply in this situation, with replacement $(\Gamma/\omega) \to (T_K/\omega)$. However, we cannot make this analogy rigorous because the Kondo scattering of the state ω leads to finite lifetime $\sim T_K/\omega^2$.

Another interesting possibility is when the core hole possesses spin [14]. Then a Kondo peak at the Fermi level will form even without the upper subband, so that the scattering off the core hole will become a Kondo scattering with ω-dependent scattering phase.

(iii) Fermi-edge physics manifests itself also in resonant-tunneling via an impurity [3,15]. However, the regime $\Delta \ll \Gamma$, considered here, cannot be realized in this setting since at long times impurity gets reoccupied.

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