

Fermi-Edge Resonance and Tunneling in Nonequilibrium Electron Gas

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Fermi-edge singularity changes in a nonequilibrium system, acquiring features that reflect the structure of energy distribution. In particular, it splits into several components if the energy distribution exhibits multiple steps. While conventional approaches, such as bosonization, fail to describe the nonequilibrium problem, an exact solution for a generic energy distribution can be obtained with the help of the method of functional determinants. In the case of a split Fermi distribution, the “open loop” part of the Greens function possesses power law singularities. At the same time, the resulting tunneling density of states exhibits broadened peaks centered at Fermi sublevels.

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Properties of quantum systems can change drastically when they are driven out of equilibrium. This is especially true for transport in nanodevices [1], such as quantum dots and quantum wires, where energy relaxation takes place outside the device. Transport in interacting systems is often difficult to describe by the methods developed for analyzing equilibrium [2–7], which makes exact solutions outside equilibrium scarce and valuable.

Fermi-edge singularity [8,9] (FES) is a dramatic manifestation of interactions and correlations in electron liquid. It can be observed in a resonant tunneling experiment [10,11] as a power law resonance which peaks at the Fermi level. Being one of the few exactly solvable problems describing transport in strongly interacting systems, FES has been thoroughly explored in a variety of situations, including quantum wires [12–14], quantum Hall edge states [15], and quantum dots [16]. However, apart from recent work by Muzykantskii *et al.* [17] which resolved a long-standing controversy on orthogonality catastrophe in two Fermi seas [18–20], little is known about FES out of equilibrium.

Nonequilibrium electron states with structured energy distribution were demonstrated recently [21] using diffusion-cooled nanoscale wires. In a wire short enough to allow electrons diffuse out without energy relaxation a distribution consisting of two Fermi steps,

$$n(\epsilon) = (1-x)n_F(\epsilon - \mu_1) + xn_F(\epsilon - \mu_2), \quad (1)$$

with $\mu_{1,2}$ potentials in the leads, was created, imaged using tunneling spectroscopy, and employed to study energy relaxation. A similar approach [22] was used to observe splitting of a Kondo resonance in a quantum dot with a mixture of two Fermi steps injected in one of the leads.

Here we study how the FES tunneling density of states is modified by nonequilibrium electron distribution, and find that it can acquire a rich and complex structure. Since FES peaks at the Fermi level, one expects a multiple FES peak profile for a multistep distribution of Refs. [21,22], with each FES peak centered around a corresponding Fermi sublevel. While the standard methods used to describe

FES in equilibrium fail, an exact solution can be obtained with the help of a method proposed below which allows to extend the FES theory to generic nonequilibrium systems.

Although a variety of methods is available to treat the FES problem, applying them outside equilibrium is often problematic. The original approach [9], based on resummation of diagrammatic series, is cumbersome and proves difficult to generalize. Thus alternative techniques, most notably bosonization [23], have been developed. The bosonization approach, however, relies too strongly on the assumption of thermodynamic equilibrium, and thus cannot be used in our problem.

The method used in this article is free of such limitation. The Greens function of a tunneling electron can be represented in terms of an appropriate functional determinant and related quantities which are defined in a *one-particle* Hilbert space. The determinant structure accounts in an exact way for all the effects of Fermi statistics, as well as for the interaction in the final state underpinning the FES phenomenon. Here we employ a generalization of the

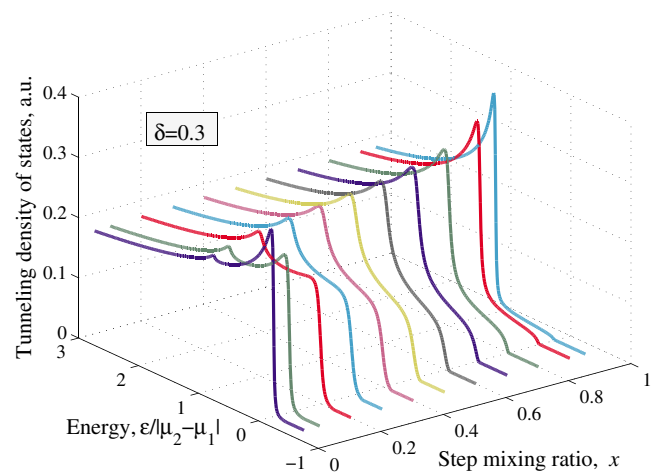


FIG. 1 (color online). Fermi-edge resonance splitting (2) for the two-step Fermi distribution (1), with the scattering phase $\delta = 0.3$.

method of Ref. [17] recently used in nonseparable mesoscopic FES problem [24], allowing one to handle an arbitrary energy distribution. After developing general formalism we focus on the two-step case (1) and obtain a split FES profile $\text{Im}G(\epsilon)$ in terms of the scattering phase shift δ (Fig. 1), where

$$G(\epsilon) \propto \int \frac{1 - n(\epsilon')}{(\epsilon' - \mu_1)^{\alpha_1} (\epsilon' - \mu_2)^{\alpha_2}} \times D(\epsilon - \epsilon') d\epsilon' \quad (2)$$

with complex $\alpha_1 = 2(\delta - \tilde{\delta})/\pi$, $\alpha_2 = 2\tilde{\delta}/\pi$, and

$$\tilde{\delta} = \frac{1}{2i} \ln(1 - x + e^{2i\delta}x). \quad (3)$$

The two factors in Eq. (2) correspond, as we will see, to the well known separation [9] of FES into the ‘‘open line’’ and ‘‘closed loop’’ contributions. The closed loop factor $D(\epsilon)$ equals $e^{(\delta^2/\pi^2 - 1)}$ in equilibrium. We evaluate $D(\epsilon)$ below and find that it describes broadening of nonequilibrium FES, with $\gamma \simeq x(1-x)|\mu_1 - \mu_2|\delta^2/\pi$, which can be attributed to a finite effective temperature $T_* \simeq \int n(1-n) d\epsilon$. The relation $\alpha_1 + \alpha_2 = 2\delta/\pi$ ensures agreement with the equilibrium FES exponent.

Turning to the analysis, the FES Hamiltonian describes band electrons interacting with a localized state:

$$\mathcal{H} = \mathcal{H}_0 \hat{N} + \mathcal{H}_1 (1 - \hat{N}), \quad \mathcal{H}_{0,1} = \sum_{pp'} \hat{h}_{pp'}^{(0,1)} a_p^\dagger a_{p'}, \quad (4)$$

where $\hat{N} = \hat{b}^\dagger \hat{b}$ describes the localized state occupation and $\hat{h}_{pp'}^{(0,1)} = \epsilon_p \delta_{pp'} + V_{p-p'}^{(0,1)}$ are the single-particle operators of band electrons scattering on the charged/uncharged state potential $V^{(0,1)}(r)$. Tunneling from the localized state is described by the Greens function

$$G(\tau) = \text{tr}[\hat{b}^+(0) \hat{\psi}(0) \hat{\psi}^+(-\tau) \hat{b}(-\tau) \hat{\rho}], \quad \tau > 0, \quad (5)$$

where $\hat{\psi}^+(\tau) = \sum_p u_p^* \hat{a}_p^+(\tau)$ creates an electron in the band state $\psi(r) = \sum_p u_p e^{ipr}$. The localized state is filled prior to tunneling, thus the density matrix in Eq. (5) is $\hat{\rho} = \hat{\rho}_e \hat{b}^+ \hat{b}$. Here $\hat{\rho}_e = \prod_p [n_p a_p^\dagger a_p + (1 - n_p) a_p a_p^\dagger]$ describes band electrons with energy distribution $n_p = n(\epsilon_p)$. The latter quantity can also be written as an exponential of a quadratic many-body operator,

$$\hat{\rho}_e = \frac{1}{Z} \exp\left(-\sum_p \lambda_p \hat{a}_p^\dagger \hat{a}_p\right), \quad e^{-\lambda_p} = \frac{n(\epsilon_p)}{1 - n(\epsilon_p)}, \quad (6)$$

with $Z = \prod_p (1 + e^{-\lambda_p})$. One can bring $G(\tau)$ to a standard form which depends only on the band electron variables by summing over the hole states [8,9]. This is achieved by disentangling b and b^+ from Eq. (5), $\hat{\psi}^+(-\tau) \hat{b}(-\tau) = e^{-i\mathcal{H}\tau} \hat{\psi}^+ \hat{b} e^{i\mathcal{H}\tau} = -\hat{b} e^{-i\mathcal{H}_1\tau} \hat{\psi}^+ e^{i\mathcal{H}_0\tau}$, and then using the commutation relations $\hat{a}_p^\dagger \hat{\rho}_e = e^{\lambda_p} \hat{\rho}_e \hat{a}_p^\dagger$, $\hat{a}_p^\dagger e^{i\mathcal{H}_0\tau} = e^{-i\epsilon_p\tau} e^{i\mathcal{H}_0\tau} \hat{a}_p^\dagger$. After summing over b , b^+ we obtain an expression

$$G(\tau) = \sum_{p,p'} u_{p'}^* u_p e^{\lambda_{p'}} e^{-i\epsilon_{p'}\tau} \text{tr}[e^{-i\mathcal{H}_1\tau} e^{i\mathcal{H}_0\tau} \hat{\rho}_e \hat{a}_{p'}^\dagger \hat{a}_p]. \quad (7)$$

The central point of our approach is a relation between the many-body operators in Eq. (7) and appropriate quantities (scattering operators and energy distribution) defined in a single-particle Hilbert space. This relation holds [25] for any electron density matrix of the form of an exponential of a quadratic many-body operator, such as Eq. (6).

The advantage of introducing the single-particle scattering operators in the formalism at an early stage of the calculation is twofold. First, we bypass solution of the single-particle scattering problem which requires resummation of diagrammatic series [9] for band electron in the presence of a time-dependent scattering. Second, we shall be able to construct a nonperturbative solution applicable to an arbitrary energy distribution.

We recall that Ref. [9] treats FES by solving the Dyson integral equation using a decomposition of quantities into analytic and antianalytic functions of complex time variable, made possible by breaking the Hilbert space into the positive and negative frequency components. This approach arises naturally in the equilibrium problem with a pure step $n(\epsilon)$ but fails for a generic distribution. Below we develop a proper replacement of this scheme.

The discussion in the following two paragraphs closely follows that of Ref. [24]. First, we introduce an operator \hat{w} defined in the single-particle Hilbert space of a band electron via the following operator product

$$e^{-i\mathcal{H}_1\tau} e^{i\mathcal{H}_0\tau} \hat{\rho}_e = Z^{-1} \exp\left(\sum_{p,p'} w_{p,p'} \hat{a}_p^\dagger \hat{a}_{p'}\right). \quad (8)$$

The trace in Eq. (7) can be expressed through the operator \hat{w} as follows:

$$\text{tr}(e^{-i\mathcal{H}_1\tau} e^{i\mathcal{H}_0\tau} \hat{\rho}_e \hat{a}_{p'}^\dagger \hat{a}_p) = (\hat{1} + e^{-\hat{w}})_{p,p'}^{-1} \det(\hat{1} + e^{\hat{w}}). \quad (9)$$

Our task is thus reduced to analyzing the quantity $e^{\hat{w}}$ which can be expressed through single-particle operators:

$$e^{\hat{w}} = e^{-i\hat{h}^{(1)}\tau} e^{i\hat{h}^{(0)}\tau} e^{-\hat{\lambda}} \quad (10)$$

with the single-particle Hamiltonian operators $\hat{h}^{(0,1)}$ defined in Eq. (4) and $(e^{-\hat{\lambda}})_{pp'} = e^{-\lambda_p} \delta_{pp'}$. These relations help [25] to bring the determinant $\det(1 + e^{\hat{w}})$ to the form $Z \det[1 - n(\epsilon) + e^{-i\hat{h}^{(1)}\tau} e^{i\hat{h}^{(0)}\tau} n(\epsilon)]$, with the many-body effects fully accounted for by the algebra involved in the determinant construction.

Next, the evolution operator product $e^{-i\hat{h}^{(1)}\tau} e^{i\hat{h}^{(0)}\tau}$ is related to the scattering matrix [24]. For one channel,

$$\hat{S} \equiv e^{-i\hat{h}^{(1)}\tau} e^{i\hat{h}^{(0)}\tau} = \delta_{t,t'} \times \begin{cases} e^{2i\delta} & 0 < t, t' < \tau, \\ 1, & \text{else,} \end{cases} \quad (11)$$

with the phase shift $\delta = \delta_1 - \delta_0$ describing the effect of the resonance level changing occupancy. This gives

$$\det(1 + e^{\hat{w}}) = Z \det[1 + (\hat{S} - 1)\hat{n}]. \quad (12)$$

Similarly, $(1 + e^{-\hat{w}})^{-1} = [n(\epsilon) + (1 - n(\epsilon))\hat{S}^{-1}]^{-1}n(\epsilon)$ where n and S are operators in the Hilbert space of functions of time. The Greens function (7) then becomes

$$G(\tau) = L(\tau)D(\tau), \quad D = \det[1 + (\hat{S} - 1)\hat{n}], \quad (13)$$

$$L = \sum_{\epsilon, \epsilon'} \tilde{u}_{\epsilon'}^* \tilde{u}_{\epsilon} e^{-i\epsilon'\tau} [1 - n(\epsilon)][\hat{n} + \hat{S}^{-1}(1 - \hat{n})]_{\epsilon, \epsilon'}^{-1}, \quad (14)$$

with $\tilde{u}_{\epsilon} = \sum_p u_p \delta(\epsilon - \epsilon_p)$. The factors L and D correspond, in the terminology of Ref. [9], to the open line and closed loop diagram contributions, respectively.

Once the problem is reduced to analyzing certain one-particle operators there are two ways to proceed. Given that \hat{n} is diagonal in the energy domain, while \hat{S} is diagonal in the time domain, one can choose either representation to analyze the quantities in Eq. (13). The former is convenient in equilibrium, since the $T = 0$ Fermi distribution is just a Cauchy kernel [9]. However, since for generic $n(\epsilon)$ the kernel $\hat{n}_{t,t'} = \int n(\epsilon) e^{i\epsilon(t-t')} (d\epsilon/2\pi)$ is fairly complicated, the time representation does not appear to be useful. Here, instead, we employ the energy representation. We note that the operator $(\hat{S} - 1)$ has a double step structure $\theta(t)\theta(\tau - t)$ and argue that the contributions of the two steps can be treated as independent with logarithmic accuracy. For a single step *in the time domain*, the corresponding operator has the form of a Cauchy kernel *in the energy domain*. Such energy-time duality allows to perform calculation in essentially the same way as in the equilibrium problem, with the roles of energy and time interchanged.

Since we are primarily interested in the power law exponent of $G(\tau)$ rather than a prefactor, let us consider replacing the double step $\theta(t)\theta(\tau - t)$ by a sum of almost nonoverlapping contributions $\theta(t)e^{-t/\tau'} + \theta(\tau - t)e^{-(\tau-t)/\tau'}$, $\tau' < \tau$. Such a replacement is reasonable since it preserves the steps at $t = 0, \tau$ and thus affects the corresponding shakeup contributions merely by τ changed to τ' in the cutoff of the logarithms. (In addition, we will have to adjust the extensive part $\ln D_{\text{lin}} \propto \tau$ of the closed loop contribution as described below.) At the same time, since at $\tau' \lesssim \tau$ the two terms do not overlap, the operator quantities in Eq. (13) factor into two independent contributions. Employing this idea, we replace the scattering operator \hat{S} by a product $\hat{T}_1 \hat{T}_2$, where

$$(\hat{T}_1 - 1)_{t,t'} = \delta_{t,t'} \times \theta(t) A e^{-t/\tau'}, \quad (15)$$

$$(\hat{T}_2 - 1)_{t,t'} = \delta_{t,t'} \times \theta(\tau - t) A e^{(\tau-t)/\tau'} \quad (16)$$

($A = e^{2i\delta} - 1$). We note that at $t \approx 0$, where \hat{T}_1 time dependence has a step, the operator \hat{T}_2 is close to unity, while at $t \approx \tau$, where \hat{T}_2 has a step, \hat{T}_1 is close to unity. This transformation allows to treat the contributions of \hat{T}_1, \hat{T}_2 independently, which greatly facilitates analysis.

We first analyze the open line contribution (14). In the $\hat{S} = \hat{T}_1 \hat{T}_2$ approximation, $\tau' \lesssim \tau$, the operator in Eq. (14) is factored into independent contributions as

$$[\hat{n} + \hat{S}^{-1}(\hat{1} - \hat{n})]^{-1} = \prod_{j=1,2} [\hat{1} + \hat{B}_j(\hat{1} - \hat{n})]^{-1}, \quad (17)$$

with $\hat{B}_j = \hat{T}_j^{-1} - \hat{1}$. Let us write \hat{B}_1 in the energy domain:

$$\hat{B}_1 = (e^{-2i\delta} - 1)\hat{\sigma}, \quad \hat{\sigma}_{\epsilon, \epsilon'} = -\frac{i}{2\pi} \frac{1}{\epsilon - \epsilon' - i/\tau'}. \quad (18)$$

Hence $1 + \hat{B}_1(1 - \hat{n}) = 1 - \hat{\sigma} + \hat{\sigma}f(\epsilon)$ with $f(\epsilon) = (e^{-2i\delta} - 1)[1 - n(\epsilon)] + 1$. To invert this operator we use analytic properties of $\hat{\sigma}$. We note that $\hat{\sigma}_{\epsilon, \epsilon'}$ turns into a Cauchy kernel at large τ' . Thus in this limit the operator $\hat{\sigma}$ projects to zero the functions $Y_+(\epsilon)$ analytic in the upper half plane of complex ϵ , $\text{Im}\epsilon > 0$, while $\hat{\sigma}^* = 1 - \hat{\sigma}$ projects to zero the functions $Y_-(\epsilon)$ analytic in the lower half plane, $\text{Im}\epsilon < 0$. Conversely, $\hat{\sigma}^*$ operates as an identity in the subspace of functions $Y_+(\epsilon)$, while $\hat{\sigma}$ is an identity in the subspace of functions $Y_-(\epsilon)$. Hence it is convenient to employ Riemann-Hilbert factorization

$$f(\epsilon) = Y_+(\epsilon)Y_-^{-1}(\epsilon). \quad (19)$$

The factors Y_{\pm} are given in explicit form by

$$\ln Y_{\pm}(\epsilon) = -\frac{1}{2\pi i} \int \frac{\ln f(\epsilon')}{\epsilon - \epsilon' \pm i0} d\epsilon'. \quad (20)$$

Then, taking into account analytic properties of Y_{\pm} ,

$$[1 - \hat{\sigma} + \hat{\sigma}f(\epsilon)]_{\epsilon, \epsilon'}^{-1} = Y_-(\epsilon)[(1 - \hat{\sigma})Y_-^{-1}(\epsilon') + \hat{\sigma}Y_+^{-1}(\epsilon')].$$

Similarly, the inverse $[\hat{1} + \hat{B}_2(\hat{1} - \hat{n})]_{\epsilon, \epsilon'}^{-1}$ is given by

$$e^{-i\epsilon\tau} Y_+^{-1}(\epsilon)[(1 - \hat{\sigma}^*)Y_+(\epsilon') + \hat{\sigma}^*Y_-(\epsilon')] e^{i\epsilon'\tau}, \quad (21)$$

where $\hat{\sigma}_{\epsilon, \epsilon'}^* = (i/2\pi)(\epsilon - \epsilon' + i/\tau')^{-1}$. After summing over ϵ, ϵ' in Eq. (14), we obtain $L(\tau) = \sum_{\epsilon} L(\epsilon) e^{-i\epsilon\tau}$ where

$$L(\epsilon) = |u_{\epsilon}|^2 [1 - n(\epsilon)] Y_+^{-2}(\epsilon). \quad (22)$$

To better understand this general result, let us consider the two-step distribution (1). Using Eq. (20), we obtain

$$\ln Y_+ = \frac{\tilde{\delta}}{\pi} \ln \frac{\tilde{\mu}_2 - \epsilon}{\tilde{\mu}_1 - \epsilon} - \frac{\delta}{\pi} \ln \frac{\xi_0 - i/\tau}{\tilde{\mu}_1 - \epsilon}. \quad (23)$$

Here $\tilde{\mu}_{1,2} = \mu_{1,2} - i/\tau$ and $\tilde{\delta}$ is defined by Eq. (3). Substituting this result into Eq. (22), we obtain a split-peak structure with power law singularities at $\epsilon = \mu_{1,2}$:

$$L(\epsilon) = \frac{|u_{\epsilon}|^2 [1 - n(\epsilon)] (-\xi_0)^{2\delta/\pi}}{(\epsilon - \tilde{\mu}_1)^{2(\delta - \tilde{\delta})/\pi} (\epsilon - \tilde{\mu}_2)^{2\tilde{\delta}/\pi}}. \quad (24)$$

At large $|\epsilon| \gg |\mu_2 - \mu_1|$, the power law form $L \propto \epsilon^{-2\delta/\pi}$ matches the equilibrium result [9].

We now proceed to calculate the closed loop contribution (13). First, consider a quasiclassical result, obtained by treating the time and energy as commuting variables:

$$\text{Indet}(1 - \hat{n} + \hat{S}\hat{n}) = \frac{\tau}{2\pi\hbar} \int \ln[1 + An(\epsilon')]d\epsilon'. \quad (25)$$

Thus we have $\det(1 - \hat{n} + \hat{S}\hat{n}) = e^{-\zeta\tau}$ with complex $\zeta = \gamma + i\epsilon_0$, where the real part γ describes broadening of the FES singularity, while the imaginary part ϵ_0 describes energy offset and can be absorbed in the phase factor $e^{-i\epsilon\tau}$. Evaluating the integral (25) for the two-step energy distribution (1), we obtain

$$-\gamma = \frac{|\mu|}{4\pi\hbar} \ln[1 - 4x(1-x)\sin^2\delta], \quad \mu \equiv \mu_2 - \mu_1. \quad (26)$$

Thus quasiclassical FES energy structure is a broadened step. The power law singularity appears only beyond the quasiclassical approximation. To describe it one has to account for the contributions highly nonlocal in time, corresponding to many low energy particle-hole excitations.

Again using the factorization approximation $S = \hat{T}_1\hat{T}_2$ with soft cutoff $e^{-t/t'}$, we factor the determinant (14) as

$$D = D_1D_2 = \prod_{j=1,2} \det[1 + (\hat{T}_j - 1)\hat{n}] \quad (27)$$

with the two factors accounting for the contributions of abrupt switching at $t = 0$ and $t = \tau$. It is clear that the two determinants $D_{1,2}$ are equal, therefore, it is sufficient to evaluate just one of them. Let us consider

$$D_1 = \det[1 + (\hat{T}_1 - 1)\hat{n}]. \quad (28)$$

The logarithm $\ln D_1$ can be represented as a sum

$$\ln D_1 = \frac{1}{2} C_{\text{lin}} + C_{\text{log}} \quad (29)$$

with $C_{\text{lin}} \propto \tau$ and $C_{\text{log}} \propto \ln\tau$. We have already estimated the former [see Eq. (26)]; to obtain the latter, consider variation $\Delta \ln D_1$ due to a change in the distribution $n(\epsilon)$. Using the formula $\Delta \text{Indet}U = \text{tr}(U^{-1}\Delta U)$, we write

$$\Delta \ln D_1 = A \text{tr}\{[1 - \hat{\sigma}^* + \hat{\sigma}^*(A\hat{n} + 1)]^{-1} \hat{\sigma}^* \Delta \hat{n}\} \quad (30)$$

with variation of n taken with respect to x or any other convenient parameter. To evaluate this expression, one has to invert the operator $1 - \hat{\sigma}^* + \hat{\sigma}^*(A\hat{n} + 1)$. This is accomplished by using Riemann-Hilbert factorization similar to that discussed above (for details, see Ref. [26]), yielding the logarithmic term C_{log} of the form

$$e^{C_{\text{log}}(x,\tau)} = \frac{(1 - i\mu\tau)^{\delta\delta/\pi^2}}{(1 + \mu^2\tau^2)^{\delta^2/2\pi^2}} (-i\tau\xi_0)^{-\delta^2/2\pi^2}. \quad (31)$$

Restoring the exponential from Eqs. (25) and (26), we obtain the closed loop factor $D(\tau) = e^{C_{\text{log}}(x,\tau)} \exp(-\gamma\tau)$.

The function $D(\epsilon) = \int e^{i\epsilon\tau} D(\tau) d\tau$ defines broadening of singularities in the split FES, Eq. (2). We note that the broadening is relatively insignificant at $\delta \ll 1$, since $\alpha_{1,2} \propto \delta$ while both γ and the exponents in (31) are of order δ^2 at small δ . Thus, although FES broadening is

present for a split Fermi step, its magnitude is not large enough to smear the split-peak FES profile.

The FES splitting and broadening have different dependence on the step mixing ratio x (Fig. 1), making it possible to study the complex split FES profile in one device. The many-body broadening can be distinguished in experiment from other FES broadening mechanisms, such as the resonant level width and thermal broadening, which have no dependence on the splitting $\mu_1 - \mu_2$.

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