

Fermi-Edge Singularity in a Nonequilibrium System

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We report exact nonperturbative results for the Fermi-edge singularity in the absorption spectrum of an out-of-equilibrium tunnel junction. We consider two metals with chemical potential difference V separated by a tunneling barrier containing a defect, which exists in one of two states. When it is in its excited state, tunneling through the otherwise impermeable barrier is possible. Our nonperturbative solution of this nonequilibrium many-body problem shows that, as well as extending below the equilibrium threshold, the line shape depends on the difference in the phase of the reflection amplitudes on the two sides of the barrier. These results have a surprisingly simple interpretation in terms of known results for the equilibrium case but with (in general complex-valued) combinations of elements of the scattering matrix replacing the equilibrium phase shifts.

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Developments in the fabrication and manipulation of mesoscopic systems have allowed detailed and well-characterized transport measurements for a large range of devices including photon detectors, quantum pumps, tunnel junctions, and carbon nanotubes. It is often the case that such measurements explore nonequilibrium effects particularly when the potential difference is dropped across a narrow potential barrier or over a short distance inside the metallic region [1–4]. While there is often a very good theoretical description of much that has been observed for systems close to equilibrium, there are few exact nonperturbative theoretical results for systems out of equilibrium.

A natural point to start, when studying nonequilibrium effects in many-electron systems, is the Fermi-edge singularity (FES). It is probably the simplest nontrivial many-body effect and is a generic feature of a Fermi system's response to any fast switching process as seen, for example, in a photon-absorption experiment [5] and a resonant tunneling device [6]. It is related to the orthogonality catastrophe [7] and can be used to reformulate the Kondo problem in terms of a succession of spin flips which are treated as the switching of a one-body potential between two different values [8].

Here we present exact nonperturbative results for the FES in a nonequilibrium system. We obtain the asymptotic behavior of the absorption spectrum of a tunneling device as a function of the applied bias V (see Fig. 1). In this device, light is assumed to couple to a defect within the barrier. The defect exists in one of two states with energy separation E_0 . Tunneling is possible only with the defect in its excited state. We compute the absorption spectrum close to the threshold at $\omega_0 = E_0 - \text{Re}(\Delta(V))$, for frequencies $(\omega - \omega_0) \ll \xi_0$, where ξ_0 is of order the bandwidth and $\text{Re}(\Delta(V))$ is the combined energy shift of the two Fermi seas when the defect is in its excited state [9].

Typical line shapes for the case $(\omega - \omega_0) \ll V$ illustrating the dependence on the reflection amplitudes and phases are shown in Fig. 2. We find that the FES is smoothed out on a frequency scale given by $V \log R$ where R is the reflection probability of the barrier in its excited state. This is in line with expectations from perturbative treatments of other nonequilibrium tunneling problems (these suggest that $V \log R$ plays the role of an effective decoherence rate [10]). However, we also find that the spectrum is sensitive to the difference in phases of the matrix elements S_{11}^e and S_{22}^e . This gives rise to a dependence on the sign of the voltage V and is entirely an

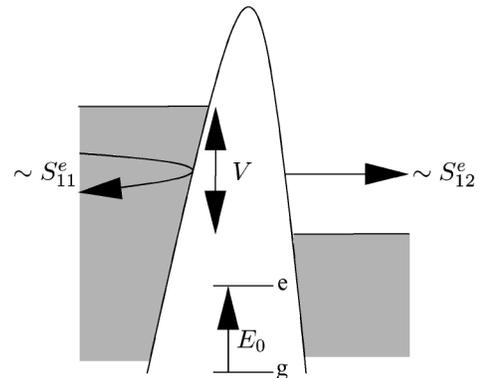


FIG. 1. Energy levels in an idealized device to demonstrate the out-of-equilibrium FES. The scattering potential for electrons is characterized via the 2×2 matrix, $S(\epsilon)$, connecting scattering states in the two wires for particles with energy ϵ . $S = S^g$ or S^e depending on whether the defect is in its ground (g) or excited (e) state (with excitation energy E_0). S^g is the identity matrix and S^e is an arbitrary unitary matrix. S_{11}^e and S_{12}^e correspond to the reflection and transmission amplitudes, respectively. We will refer to the device operating as illustrated here, with a negative potential $-V$ ($V > 0$) applied to the left electrode, as the forward-biased case.

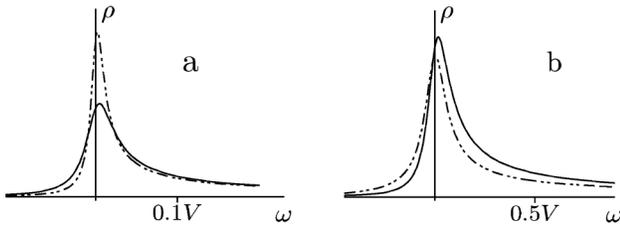


FIG. 2. Typical absorption spectra, $\rho(\omega)$, in arbitrary units for the out-of-equilibrium device sketched in Fig. 1. The spectra depend on $S_{11}^e = \sqrt{R}e^{i\alpha_1}$ and $S_{22}^e = \sqrt{R}e^{i\alpha_2}$ [see (8) and (6)], where R is the reflection probability. (a) $(\alpha_1, \alpha_2) = (0, 1.5)$ with $R = 0.9$ (broken line) and $R = 0.8$ (solid line). As the reflection probability decreases, the spectrum broadens but retains its asymmetric shape. (b) $R = 0.5$ with $(\alpha_1, \alpha_2) = (0, 1.5)$ (solid curve) and $(\alpha_1, \alpha_2) = (1.5, 0)$ (broken curve). The spectrum is sensitive to the difference in α_1 and α_2 . The difference between the two curves would show up as differences in the spectra on reversing the bias.

out-of-equilibrium effect, which we explain in terms of generalized (complex) phase shifts at the Fermi energy.

The spectral function, $\rho(\omega, V)$, for absorption by the local defect in the barrier is given by [7]

$$\rho(\omega, V) \sim \text{Re} \int_0^\infty \chi(t_f, V) e^{i\omega t_f} dt_f, \quad (1)$$

$$\chi(t_f, V) = \langle 0 | U(t_f, 0) | 0 \rangle. \quad (2)$$

Here $|0\rangle$ is the ground state wave function of the complete system (the filled Fermi seas in the two electrodes and the defect in its ground state), while $U(t_f, 0)$ is the time-evolution operator for the system between $t = 0$ and $t = t_f$ with the defect in its excited state.

When $V = 0$ the response of the system is that of the core hole problem considered in [5,7,11,12]

$$\log \chi(t_f, 0) = -i[E_0 - \Delta(0)]t_f - \beta \log i t_f \xi_0, \quad (3)$$

where $\beta = \sum_{j=1,2} (\delta_j / \pi)^2$. Here $e^{-i2\delta_j}$ are the eigenvalues of the scattering matrix S^e (see Fig. 1). The threshold is shifted from E_0 , the energy separation in the two-level system, by $\Delta(0)$, which is the shift of the ground state energy of the two Fermi seas when the scattering defect is in its excited state. This standard equilibrium result (3) is well understood in terms of the low-lying particle-hole excitations created by the rapid switching of the potential, with the principal contributions to the logarithm in (3) from excitations with frequencies between t_f^{-1} and ξ_0 .

When a voltage is applied across the barrier with the defect in its excited state and $R \neq 1$, a current will flow and the system will become dissipative. For $t_f \ll V^{-1}$, the spectral response will be dominated by excitations with frequencies $\omega \gg V$, involving states which do not sense the potential drop across the barrier. As a result, $\chi(t_f, V)$ will be unchanged from its value in equilibrium.

When $t_f \gg V^{-1}$, the response is controlled by electrons within the band of width V about the mean Fermi energy. We find that

$$\log \chi(t_f, V) = -i[E_0 - \Delta(V)]t_f - \beta' \log(Vt_f) + D. \quad (4)$$

Here the function $\Delta(V)$ is given by

$$\Delta(V) = \int_{-\infty}^0 \frac{\text{tr} \log(S(E))}{2\pi i} dE + \int_0^V \frac{\log(S_{11}(E))}{2\pi i} dE. \quad (5)$$

This expression (5) for the (in general complex) energy shift of the two Fermi seas, when the defect is in its excited state, can be thought of as the generalization to the out-of-equilibrium case of Fumi's theorem [13]. The first term (which is real) and the real part of the second term describe the energy shift of the occupied states of the two electrodes. The imaginary part of the second term describes the finite lifetime of occupied states in the left electrode, with energies between 0 and V , which can decay by tunneling through the barrier.

The exponent β' in (4) is given by

$$\beta' = \left(\frac{-\log(S_{11}^e)}{2\pi i} \right)^2 + \left(\frac{-\log(S_{22}^{e*})}{2\pi i} \right)^2. \quad (6)$$

The constant term D gives the contribution from excitations with frequencies between V and ξ_0 , which do not sense the potential drop across the barrier. To logarithmic accuracy [15],

$$D = \beta \log \xi_0 / V. \quad (7)$$

Writing $S_{11}^e = \sqrt{R}e^{i\alpha_1}$ and comparing the forms for β and β' in (3) and (6), we see that the quantity $-\log(S_{11}^e)/2i = -\alpha_1/2 + i(\log R)/4\pi$ is acting as a complex phase shift in the left electrode. Its real part, $-\alpha_1/2$, characterizes the scattering in the electrode and in (4) describes the effect of particle-hole excitations in the band of width V from the Fermi energy. Its imaginary part $(\log R)/4\pi$ characterizes the lifetime of the excitation.

The absorption spectrum is found from the Fourier transform of $\chi(t_f, V)$ in (1). Measuring ω from $\omega_0 = E_0 - \text{Re}(\Delta(V))$, it is given by [16]

$$\rho(\omega) \sim \frac{1}{\Omega^{1-\beta'_1}} e^{-\beta'_2 \phi_\Omega} \sin[\beta'_1 \pi - (\beta'_1 - 1)\phi_\Omega - \beta'_2 \log \Omega]. \quad (8)$$

Here we have defined $\Omega \exp i\phi_\Omega \equiv \omega/V - i(\log R)/4\pi$ and written $\beta' = \beta'_1 + i\beta'_2$. While the dependence on β'_1 reflects the strength of the overall scattering on the two sides of the barrier as in equilibrium, β'_2 is proportional to $\log R$ and to the difference in the phases of the two reflection amplitudes S_{11}^e and S_{22}^e . The sensitivity to the sign of the phase shift difference, while unexpected, is quite easy to understand. The exponent β' in (6) is related via Friedel's sum rule to the charge, which the system pulls in or ejects from the two electrodes in order

to screen the potential characterized by S^e [7,14]. In the case of Fig. 2(b) with $\alpha_2 = 0$ and $\alpha_1 > 0$, the corresponding potential in the left electrode is repulsive and will expel charge $\sim \alpha_1/\pi$. In the forward-biased case (Fig. 1) this charge moves away in both electrodes. However, when the device is reverse biased, the states in the right electrode are occupied and block the expulsion of charge in this channel. As a result, the line shape [the solid line in Fig. 2(b)] is sharper than in the forward-biased case (dash-dotted line).

When $R = 1$, the term multiplying $\Omega^{1-\beta_i}$ in (8) is proportional to the theta function $\theta(\omega)$ and describes the usual sharp threshold in $\rho(\omega)$. With $R < 1$ it leads to a smearing of the threshold (see Fig. 2). As pointed out in [17], where a similar model was treated perturbatively (see also [18,19]), this broadening of the threshold reflects the existence of “negative energy excitations” in the system involving a hole in the left electrode and a particle in the right electrode.

The effects we are describing should be visible in the voltage dependence of the absorption line shape of devices like the single-photon detector of [4], which consists of a quantum dot in the quantum Hall regime coupled via tunneling barriers to two electrodes on either side of the dot. For magnetic fields in the range 3.4–4.2 T, the conductance through the dot can change from zero to around $0.3e^2/h$ when a photon is absorbed via cyclotron resonance in the dot. From the perspective of the two electrodes, the dot behaves as a tunneling barrier which allows tunneling only in its excited state. Our approach would actually need further development to account for the momentum dependence of the scattering states (these are the edge states in the quantum Hall liquids of the source and drain) in this particular device, although the qualitative arguments will still apply.

The derivation of the overlap $\chi(t_f)$ follows quite closely that of Muzykantskii and Adamov [20]. We introduce the operators $a_i(\epsilon)$ which annihilate particles on the i th side of the barrier with energy ϵ in eigenstates of the system with the defect in its ground state ($S = 1$). The effect of the time-evolution operator U acting between $t = 0$ and t_f on single-particle states $a_i^\dagger|\rangle$, where $|\rangle$ is the true vacuum with no particles, is given by

$$U a_i^\dagger(\epsilon)|\rangle = \sum_i \int d\epsilon' \sigma_{ij}(\epsilon, \epsilon') a_j^\dagger(\epsilon')|\rangle. \quad (9)$$

One can show that, for states near the Fermi energy (see [21], for example), σ is given by

$$\sigma_{ij}(\epsilon, \epsilon') = e^{-iE_0 t_f} \frac{1}{2\pi} \int_{-\infty}^{\infty} S_{ij}(t) e^{i(\epsilon - \epsilon')t} dt \quad (10)$$

provided that the adiabaticity condition $\hbar \frac{\partial S}{\partial t} \frac{\partial S}{\partial E} \ll 1$ is satisfied. In (9) $S(t) = S^g$ for $t < 0$ and $t > t_f$, $S(t) = S^e$ for $0 < t < t_f$, and we have suppressed the explicit dependence of S on energy. When computing the low frequency

asymptotics, this becomes a slow dependence on $(\epsilon + \epsilon')/2$, and can be neglected.

The overlap $\chi(t_f)$ can be written

$$\chi(t_f) = \langle 0|U|0\rangle = \det' \sigma, \quad (11)$$

where the prime indicates that the operator determinant is to be taken only over the occupied states in the two filled Fermi seas. This reduces in the equilibrium case to the determinant in [11]. With zero chemical potential in the right electrode and treating the (nonequilibrium) Fermi distribution as the diagonal operator $f_{ij}(\epsilon, \epsilon') = \delta_{ij} \delta(\epsilon - \epsilon') \theta\{\epsilon - [\epsilon + V(2 - i)]\}$ allows us to write

$$\chi(t_f) = \det(1 - f + f\sigma), \quad (12)$$

$$\begin{aligned} \log \chi(t_f) &= \text{Tr}[\log(1 - f + f\sigma) - f \log \sigma] + \text{Tr} f \log \sigma \\ &\equiv C(t_f, V) + \text{Tr} f \log \sigma, \end{aligned} \quad (13)$$

where the operator determinant is now the full determinant taken over all states and the trace, Tr , is the trace over energy and channels. The last term in the expression (13) can be found by explicitly carrying out the integral in (10). This gives $\sigma_{ij}(\epsilon, \epsilon') = \delta_{ij} \delta(\epsilon - \epsilon') - X_{ij}(\epsilon - \epsilon')$. The logarithm can then be expanded as a power series in the matrix X [22]. After evaluating X^n term by term and then resumming we obtain $\text{Tr} f \log \sigma = -i[E_0 - \Delta(0)]t_f + (Vt_f/2\pi i)(\log S)_{11}$. The difference between this and $-i[E_0 - \Delta(V)]t_f$ in (5) is contained in the function $C(t_f, V)$.

To evaluate $C(V, t_f)$ we introduce $\tilde{S}(t, \lambda)$ where

$$\tilde{S}(t, \lambda) = \exp(\lambda \log S(t)), \quad (14)$$

so that $\tilde{S}(t, 1) = S(t)$. We now apply the following gauge transformation:

$$\mathbf{a}(\epsilon) \rightarrow \mathbf{a}(\epsilon, t) = e^{iLVt} \mathbf{a}(\epsilon), \quad (15)$$

$$\tilde{S}(t, \lambda) \rightarrow \tilde{S}(t, \lambda) = e^{iLVt} \tilde{S}(t, \lambda) e^{-iLVt}. \quad (16)$$

Here L is the diagonal matrix with $L_{11} = 1$ and $L_{22} = 0$. This has the advantage of eliminating the chemical potential difference between the two electrodes at the expense of an added time dependence for \tilde{S} when $t \in [0, t_f]$. After switching to the time representation (in which the trace, Tr , becomes a trace over channels and an integral over time) and substituting for σ from (10), $C(t_f, V)$ can be written as

$$C(t_f, V) = \text{Tr} \int_0^1 d\lambda \left[(1 - f + f\tilde{S})^{-1} f - f\tilde{S}^{-1} \right] \frac{d\tilde{S}}{d\lambda}. \quad (17)$$

Using a parallel argument to that of [20], we find that

$$(1 - f + f\tilde{S})^{-1} = Y_+ ((1 - f)Y_+^{-1} + fY_-^{-1}). \quad (18)$$

where $Y_\pm = Y(t \pm i0, \lambda)$. Here $Y(z, \lambda)$ is an analytic (matrix) function of complex z in the complement of the cut

along the real axis between $z = 0$ and $z = t_f$, and satisfies

$$Y_- Y_+^{-1} = \tilde{S}(t, \lambda) \quad \text{and} \quad Y(z, \lambda) \rightarrow \text{const} \quad \text{for} \quad |z| \rightarrow \infty. \quad (19)$$

If there is no tunneling between electrodes (S^e diagonal), this matrix Riemann-Hilbert (RH) problem can be shown to be the same as the homogeneous part of that solved in [7]. After substituting (18) into (17), using the fact that in the time representation [after the gauge transformation (15)] $f(t, t') = i[2\pi(t - t' + i0)]^{-1}$ and letting $t' \rightarrow t$ to compute the trace, Tr , we finally obtain

$$C(t_f, V) = \frac{i}{2\pi} \int_0^1 d\lambda \int_0^{t_f} \text{tr} \left\{ \frac{dY_+}{dt} Y_+^{-1} S^{-1} \frac{dS}{d\lambda} \right\} dt. \quad (20)$$

Here tr denotes a trace over channel indices.

Solving for $\chi(t_f, V)$ is equivalent to solving for the quantity $Y(z, \lambda)$. For small V , we can expand the exponential factors in $\tilde{S}(z, \lambda)$ (see [14]) as $e^{\pm iVz} = 1 \pm iVz$. In this case

$$Y(z, \lambda) = \exp \left[\frac{1}{2\pi i} \log \left(\frac{z}{z - t_f} \right) \log \tilde{S}(z, \lambda) \right] \quad (21)$$

solves the RH problem. For $|z| \rightarrow \infty$, the exponent (and hence Y) tends to a constant as required. If $Vt_f \ll 1$ we can insert this result into (20) and compute the integrals over t and λ . This yields the equilibrium result (3). Although there are corrections to the equilibrium ($V = 0$) solution for Y_+ which are linear in Vt , these cancel out after taking the trace in (20). Corrections to $C(t_f, V)$ can therefore be only of order $(Vt_f)^2$ or higher.

For times $t_f > V^{-1}$, a general solution to this type of matrix RH problem is not known. The form (21) for Y_+ is still valid for $0 < t < V^{-1}$ and $t_f > t > t_f - V^{-1}$. The integral over times close to the branch points of Y then gives the contribution varying as $D = \log(\xi_0/V)$ in (7). However, although the form for Y in (21) still satisfies the discontinuity condition along the cut, the exponent is unbounded for large $|z|$ and hence (21) is useless as a starting point for solving for Y_+ for $t \gg V^{-1}$. Following the derivation of [20], we find that

$$Y_+(t, \lambda) = \begin{cases} \psi_+(t, \lambda) & \text{when } t < 0 \\ \begin{pmatrix} 1 & -\gamma(t, \lambda) \\ 0 & 1 \end{pmatrix} \psi_+(t, \lambda) & \text{when } 0 < t < t_f \\ \psi_+(t, \lambda) & \text{when } t_f < t \end{cases} \quad (22)$$

is asymptotically correct for $t \gg V^{-1}$. Here $\gamma(t, \lambda) = \tilde{S}_{12}(t, \lambda)/\tilde{S}_{11}(t, \lambda)$ and $\psi_+(t, \lambda) = \psi(t + i0, \lambda)$ where

$$\psi(z, \lambda) = \exp \left(\left[\frac{\log \tilde{s}_{11}/\tilde{s}_{22}^*}{4\pi i} \tau_0 + \frac{\log(\tilde{s}_{11}\tilde{s}_{22}^*)}{4\pi i} \tau_3 \right] \log \frac{z}{z - t_f} \right). \quad (23)$$

The corresponding function $Y(z, \lambda)$ is not analytic across

vertical cuts in the complex z plane through the points $z = 0$ and $z = t_f$, with discontinuities which decay as $e^{-V|z|}$ or $e^{-V|z-t_f|}$. (These factors show that we cannot describe the reverse bias case by taking $V < 0$ in (22). Instead, Y_+ takes a different form for negative V .) After inserting the solution (22) in (20) and computing the integrals over λ and t , we obtain the first two terms in (4). The term obtained after differentiating γ in (22) and adding to the term from $\text{Tr} f \log \sigma$ in (13) leads after some algebra to the term $-i[E_0 - \Delta(V)]t_f$. Differentiating $\psi_+(t_f, \lambda)$ in (22) leads to the term proportional to $\log V t_f$. The constant term is derived using the form (21) for Y_+ valid for small t and $t - t_f$ as discussed above.

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