Fermi edge singularity in a non-equilibrium system

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We report exact 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. We find that the lineshape not only depends on the total scattering phase shift as in the equilibrium case but also on the difference in the phase of the reflection amplitudes on the two sides of the barrier. The out-of-equilibrium spectrum extends below the original threshold as energy can be provided by the power source driving current across the barrier. Our 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 quantum pumps, tunnel junctions and carbon nanotubes. It is often the case that such measurements explore non-equilibrium effects particularly when the potential difference is dropped across a narrow potential barrier or over a short distance inside the metallic region \( \Gamma_r \). While there is often a very good theoretical description of much that has been observed for systems close to equilibrium, the theoretical picture for systems out of equilibrium is less clear with fewer established theoretical results.

A natural point to start, when looking for a description of non-equilibrium effects in many-electron systems is the Fermi Edge Singularity (FES), which is one of the simplest non-trivial many-body effects. The FES is characteristic of the response of a Fermi gas to a rapid switching process. Initially it was associated with the shape of the absorption edge and spectral line found when a core hole is created \( \Gamma_r \). However, it turns out to be a generic feature of a Fermi system’s response to any fast switching process and reflects the large number of low-energy (particle-hole) excitations which exist in Fermi liquids. It has also been shown to be related to Anderson’s orthogonality catastrophe \( \Gamma_r \) 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 \( \Gamma_r \).

We consider a system at zero temperature with two Fermi surfaces separated by a barrier with a potential difference (bias) \( V \) applied across the barrier (see Fig. 1). The barrier contains a defect, which exists in one of two states with energy separation \( E_0 \). Tunneling through the barrier is assumed to be possible only when the defect is 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 \( \xi_0 \) is of order the bandwidth and \( \text{Re}(\Delta(V)) \) is real part of the combined energy shift of the two Fermi seas when the defect is in its excited state. \( \Delta(V) \) is complex for non-zero \( V \) on account of the dissipation in the system.)

Using an approach based on that of Nozières and de Dominicis (ND) \( \Gamma_r \), we solve exactly for the asymptotic behavior of the absorption spectrum in two limiting cases: \( (\omega - \omega_0) \gg V \) and \( (\omega - \omega_0) \ll V \). Our results have a simple interpretation in terms of generalized (complex) phase-shifts at the Fermi energy. Typical lineshapes for the case \( (\omega - \omega_0) \gg V \) illustrating the dependence on the reflection amplitudes and phases are shown in Figure 2.

Our treatment of the problem is based on that of Muzykantskii and Adamov (MA) for the statistics of...
charge transfer in quantum pumps, which uses the relation between the many-particle response to the changing one-body potential and the solution of an associated matrix Riemann-Hilbert (RH) problem \[ \beta \]. This problem was also addressed perturbatively and using the ND approach in \[ \beta \], although the results in \[ \beta \] led the authors to question the validity of the ND approach of \[ \alpha \] (see also \[ \alpha \]). Our solution shows clearly that the ND approach is valid, with the earlier difficulties probably associated with an incomplete analysis of the matrix RH problem associated with their singular integral equation.

We characterize the scattering at the interface between the two subsystems via the unitary \( 2 \times 2 \) matrix, \( S(\epsilon, t) \), connecting scattering states in the two wires for particles with energy \( \epsilon \). This takes one of two values \( S^g \), and \( S^e \) depending on whether the the defect is in its ground (\( g \)) or excited state (\( e \)). In the following, we will take a row/column index equal to one (two) for the left (right) electrode so that the diagonal (off-diagonal) elements correspond to reflection (transmission) amplitudes (see Figure 1). We choose the scattering states to be the eigen states of the system when the defect is in its ground state and the barrier is totally reflecting hence: \( S^g_{ij} = \delta_{ij} \). \( S^e \) is an arbitrary unitary matrix with reflection probability \( R = |S_{11}^e|^2 < 1 \). We will assume that a negative potential \(-V \; (V > 0)\) has been applied to the left electrode with respect to the right electrode.

The spectral function, \( \rho(\omega, V) \), for absorption by the local level is given by \[ \rho \]:

\[
\rho(\omega, V) \sim \text{Re} \int_{-\infty}^{\infty} \chi(t_f, V) e^{i\omega t_f} dt_f
\]

\[
\chi(t_f, V) = \langle 0 | U(t_f, 0) | 0 \rangle.
\]

Here \( |0\rangle \) is the ground state wavefunction 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. \( \chi(t_f, 0) \) is the same as the core hole Green’s function computed in \[ \alpha \] and \[ \beta \].

Before discussing the full non-equilibrium case, we briefly review the known equilibrium results. When \( V = 0 \) the response of the system is that of the core hole problem in a non-separable potential considered in \[ \alpha \] and \[ \beta \]:

\[
\log \chi(t_f, 0) = -i(\mathcal{E}_0 - \Delta(0))t_f - \beta \log t_f \xi_0
\]

where \( \beta = \sum_{j=1,2} \left( \frac{\delta_j}{4} \right)^2 \). Here \( e^{-i\delta_j} \) are the eigen values of \( S^e \). The threshold is shifted from \( \mathcal{E}_0 \), 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 \[ \beta \] 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 \[ \alpha \] from excitations with frequencies between \( t_f^{-1} \) and \( \xi_0 \).

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 is dominated by excitations with frequencies \( \omega \gg V \), involving states which do not sense the potential drop across the barrier. As a result \( \chi(t_f, V) \) is 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

\[
\log \chi(t_f, V) = -i(\mathcal{E}_0 - \Delta(V))t_f - \beta' \log(V t_f) + D \tag{4}
\]

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

\[
\Delta(V) = \int_{-\infty}^{0} \frac{\text{tr} \log (S(E))}{2\pi i} dE + \int_{0}^{V} \frac{\log (S_{11}(E))}{2\pi i} dE \tag{5}
\]

This expression \[ \alpha \] 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 of Fumi’s theorem \[ \alpha \] \[ \alpha \] to the out-of-equilibrium case. The exponent \( \beta' \) in \[ \alpha \] is given by

\[
\beta' = \sum_{j=1,2} \left( -\log(S^e_{jj})/2\pi i \right)^2 \tag{6}
\]

The constant term \( D \) gives the contribution from excitations with frequencies between \( V \) and \( \xi_0 \), which do not sense the potential drop across the barrier. To logarithmic accuracy \[ \alpha \] :

\[
D = \beta \log \xi_0 / V \tag{7}
\]

Writing \( S^e_{jj} = \sqrt{Re^{i\alpha_j}} \) and comparing the forms for \( \beta \) and \( \beta' \) in \[ \alpha \] and \[ \beta \], we see that the quantity

\[-\log(S^e_{jj})/2i = -\alpha_j/2 + i(\log R)/4\pi \]

is acting as a complex phase shift. Its real part, \(-\alpha_j/2\), characterizes the scattering in the \( j \)th electrode and in \[ \alpha \] describes the

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

\[ \text{a} \]

\[ \text{b} \]
effect of particle-hole excitations in the band of width $V$ from the Fermi energy. Its imaginary part $(\log R)/4\pi$ relates to the lifetime of the excitation.

The absorption spectrum is found from the Fourier transform of $\chi(t_f, V)$ in $\mathbf{1}$). Measuring $\omega$ from $\omega_0 = E_0 - \text{Re}(\Delta(V))$, it is given by $\mathbf{17}$:

$$
\rho(\omega) \sim \frac{1}{\Omega^{1-\beta'_1}} e^{-\beta'_2 \phi_{01}} \sin(\beta'_1 \pi - (\beta'_1 - 1) \phi_{01} - \beta'_2 \log \Omega).
$$

(8)

Here we have defined $\Delta = \omega/V - i(\log R)/4\pi$ and written $\beta' = \beta'_1 + i\beta'_2$. The while dependence on $\beta'_1$ reflects the total overall scattering on the two sides of the barrier as in equilibrium, $\beta'_2$ is proportional to the difference in the phases of the two reflection amplitudes $S_{11}$ and $S_{22}$ and its appearance in $\mathbf{3}$ is entirely an out-of-equilibrium effect.

When $R = 1$, the term multiplying $\Omega^{1-\beta'_1}$ in $\mathbf{2}$ is proportional to the theta function $\omega(\omega)$ and describes the usual sharp threshold in $\rho(\omega)$. With $R < 1$ it leads to a smearing of the threshold (see Figure $\mathbf{2}$). As pointed out in $\mathbf{2}$, 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. From an experimental point of view, the below threshold broadening with its functional dependence on the phases of the reflection amplitudes and its overall energy scale fixed by the bias are probably the key signatures of the non-equilibrium effects we are describing. The sensitivity to the difference in scattering phase shifts (this difference is proportional to $\beta'_2$) would show up in changes in the line shape on reversing the bias and should also be observable.

The derivation of the overlap $\chi(t_f)$ follows quite closely that of MA $\mathbf{3}$. We introduce the operators $a_i(\epsilon)$ which annihilate particles on the $i$th side of the barrier with energy $\epsilon$ in eigen states 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 states $a_i^n |\psi\rangle$, where $|\psi\rangle$ is the true vacuum with no particles, is given by

$$
U a_i^n (|\psi\rangle) = \sum_j \int d\epsilon' \sigma_{ij}(\epsilon, \epsilon') a_j^n (|\psi\rangle).
$$

(9)

One can show that for states near the Fermi energy (see $\mathbf{18}$ for example) $\sigma$ is given by:

$$
\sigma_{ij}(\epsilon, \epsilon') = e^{-iE_{0j}t} \frac{1}{2\pi} \int_{-\infty}^{\infty} S_{ij}(t) e^{i(\epsilon-\epsilon')t} dt
$$

(10)

provided that the adiabaticity condition

$$
\hbar \frac{\partial S}{\partial t} \frac{\partial S}{\partial E} \ll 1
$$

(11)

is satisfied. In $\mathbf{19}$, $S(t) = S$ for $t < 0$ and $t > t_f$ and $S(t) = S'$ 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

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

(12)

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 $\mathbf{3}$. With zero chemical potential in the right electrode and treating the (non-equilibrium) Fermi distribution as the diagonal operator $f_{ij}(\epsilon, \epsilon') = \delta_{ij} \delta(\epsilon - \epsilon') \theta(-\epsilon + V(2 - i))$, allows us to write

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

(13)

$$
\log \chi(t_f) = \text{Tr} \log(1 - f + f \sigma) - f \log \sigma + \text{Tr} f \log \sigma
$$

(14)

where the operator determinant is now the full determinant taken over all states and the trace, $\text{Tr}$, is the trace over energy and channels. The last term in the expression $\chi(t_f)$ can be found by explicitly carrying out the integral in $\mathbf{19}$. This gives that $\sigma_{ij}(\epsilon, \epsilon') = \delta_{ij} \delta(\epsilon - \epsilon') - X_{ij}(\epsilon - \epsilon')$. The logarithm can then be expanded as a power series in the matrix $X$ $\mathbf{19}$. After evaluating $X^n$ term by term and then resumming we obtain: $\text{Tr} f \log \sigma = -i (E_0 - \Delta(0)) t_f + (V t_f/2\pi)(\log S)_{11}$. The difference between this and $-i (E_0 - \Delta(V)) t_f$ in $\mathbf{3}$ is contained in the function $C(t_f, V)$.

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

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

(15)

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

$$
a_1(\epsilon) \rightarrow a_1(\epsilon, t) = e^{iL V t} a_1(\epsilon)
$$

(16)

$$
\tilde{S}(t, \lambda) \rightarrow \tilde{S}(t, \lambda) = e^{iL V t} \tilde{S}(t, \lambda) e^{-iL V t}
$$

(17)

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, $\text{Tr}$, becomes a trace over channels and an integral over time) and substituting for $\sigma$ from $\mathbf{19}$, $C(t_f, V)$ can be written

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

(18)

Using a parallel argument to that of $\mathbf{3}$, we find that

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

(19)

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:
\[
Y_- Y_+^{-1} = \tilde{S}(t, \lambda) \quad \text{and} \quad Y(z, \lambda) \rightarrow \text{const for } |z| \rightarrow \infty. \tag{20}
\]
If there is no tunneling between electrodes (\( S' \) diagonal), this matrix RH problem can be shown to be the same as the homogeneous part of that solved in \( \mathbb{E} \). After substituting \( Y \) into \( \mathbb{E} \), using the fact that in the time-representation (after the gauge transformation \( f(t, t') = i(2\pi(t-t'+i0))^{-1} \) and letting \( t' \rightarrow t \) to compute the trace, \( \text{Tr} \), we finally obtain
\[
C(t_f, V) = \frac{i}{2\pi} \int_0^1 d\lambda \int_{t_f}^0 \text{tr} \left\{ \frac{dY}{dt} \tilde{S}^{-1} \frac{dS}{d\lambda} \right\} dt. \tag{21}
\]
Here \( \text{tr} \) 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 \( \mathbb{F} \)) as \( e^{\pm iV \lambda} \). In this case
\[
Y(z, \lambda) = \exp \left[ \frac{1}{2\pi i} \log \left( \frac{z}{z-t_f} \right) \log \tilde{S}(z, \lambda) \right] \tag{22}
\]
solves the RH problem. For \( |z| \rightarrow \infty \), the exponent (and hence \( Y \)) tends to a constant as required. If \( V t_f \ll 1 \) we can insert this result into \( \mathbb{F} \) and compute the integrals over \( t \) and \( \lambda \). This yields the equilibrium result \( \mathbb{H} \). Although there are corrections to the equilibrium \( (V = 0) \) solution for \( Y_+ \), which are linear in \( V t \), these cancel out after taking the trace in \( \mathbb{F} \). Corrections to \( C(t_f, V) \) can therefore only be of order \( (V t_f)^2 \) or higher.

For times \( t_f > V^{-1} \), a general solution to this type of matrix RH problem is not known. The form \( \mathbb{F} \) 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 \( D = \log \left( \frac{\xi_0}{V} \right) \) in \( \mathbb{F} \). However, although the form for \( Y \) in \( \mathbb{F} \) still satisfies the discontinuity condition along the cut, the exponent is unbounded for large \( |z| \) and hence \( \mathbb{F} \) is useless as a starting point for solving for \( Y_+ \) for \( t \gg V^{-1} \). Following the derivation of \( \mathbb{H} \), we find that:
\[
Y_+(t, \lambda) = \left[ \begin{array}{c}
\psi_+(t, \lambda) \quad \text{when} \quad t < 0 \\
0 - \gamma(t, \lambda) \psi_+(t, \lambda) \quad \text{when} \quad 0 < t < t_f \\
\psi_+(t, \lambda) \quad \text{when} \quad t_f < t
\end{array} \right]
\tag{23}
\]
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
\[
\psi(z, \lambda) = \exp \left[ \frac{1}{2\pi i} \int_{t_f}^{0} \log \left( \frac{z}{z-t} \right) \log \tilde{S}(z, \lambda) \right].
\tag{24}
\]

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 \( e^{-V|z-t|} \). (These factors show that we cannot describe the reverse bias case by taking \( V < 0 \) in \( \mathbb{F} \). Instead \( Y_+ \) takes a different form for negative \( V \).) After inserting the solution \( \mathbb{F} \) in \( \mathbb{F} \) and computing the integrals over \( \lambda \) and \( t \), we obtain the first two terms in \( \mathbb{F} \). The term obtained after differentiating \( \gamma \) in \( \mathbb{F} \) and adding to the term from \( \text{Tr} \log \sigma \) in \( \mathbb{F} \), leads after some algebra to the term \( -i(\xi_0 - \Delta(V))t_f \). Differentiating \( \psi_+(t, \lambda) \) in \( \mathbb{F} \) leads to the term proportional to \( \log V t_f \). The constant term is derived using the form \( \mathbb{F} \) for \( Y_+ \) valid for small \( t \) and \( t - t_f \) as discussed above.

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