Fermi gas response to time-dependent perturbations

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We describe the Riemann-Hilbert (RH) approach to computing the long-time response of a Fermi gas to a time-dependent perturbation. The approach maps the problem onto a noncommuting RH problem. The method is nonperturbative, quite general, and can be used to compute the Fermi gas response in driven (out of equilibrium) as well as equilibrium systems. It has the appealing feature of working directly with scattering amplitudes defined at the Fermi surface rather than with the bare Hamiltonian. We illustrate the power of the method by rederiving standard results for the core-hole and open-line Green's functions for the equilibrium Fermi edge singularity (FES) problem. We then show that the case of the nonseparable potential can be solved nonperturbatively with no more effort than for the separable case. We compute the corresponding results for a biased (nonequilibrium) model tunneling device, similar to those used in single-photon detectors, in which a photon absorption process can significantly change the conductance of the barrier. For times much larger than the inverse bias across the device, the response of the Fermi gases in the two electrodes shows that the equilibrium Fermi edge singularity is smoothed, shifted in frequency, and becomes polarity dependent. These results have a 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. We also consider the shot noise spectrum of a tunnel junction subject to a time-dependent bias and demonstrate that the calculation is essentially the same as that for the FES problem. For the case of a periodically driven device we show that the noise spectrum for coherent states of alternating current can be easily obtained using this approach.

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I. INTRODUCTION

An approach to the study of the quantum statistics of an *arbitrary* single-particle observable in a Fermi gas has been recently described in Ref. 1. We refer to it as the RH approach, as it reduces the calculation of a determinant describing the quantum statistics of an observable to the solution of an (in general) non-Abelian Riemann-Hilbert (RH) problem. The relation between such determinants and RH problems has been known for a long time, and has been used extensively in studies of quantum inverse scattering problems.² As a result, a lot is known about the non-Abelian RH problem,³ and much of this can be taken over directly to the study of the quantum statistics of Fermi gases.

The RH approach gives an expression for the distribution function of an observable in a Fermi gas perturbed by a time-dependent potential. To illustrate the method, one of us used it to prove a long-standing conjecture, first stated in Ref. 4, that the two sources of shot noise in a biased point contact, namely fluctuations in the number of attempts to tunnel through the barrier and fluctuations in the number of reflections, are statistically independent.¹ We have also used the method to study how nonequilibrium effects alter the fermi edge singularity in a tunnel junction.⁵

The response of a Fermi gas to a time-dependent perturbing potential is a central problem in condensed matter physics. It has been tackled in many different contexts often with different approaches. For systems out of equilibrium, such as quantum pumps, perturbative approaches, based on the Keldysh formalism, have been used, while for systems in equilibrium it has been possible to find exact solutions in some limiting cases by solving the equations of motion directly.^{6–9} One of the advantages of the RH method is that it applies equally to all such problems and therefore offers the prospect of a unified approach to computing the time-dependent response of all observables in Fermi gases.

Setting up the description of a problem in the RH framework is quite straightforward. Given the solution of the single-particle scattering problem, the response of the Fermi gas reduces to the computation of a determinant of an operator taken over single-particle states occupied in the initial configuration. (The generalization of the method to the more general case in which the initial state is given in terms of a density matrix rather than a single quantum state should be possible but has not yet been formulated.) The evaluation of this determinant then reduces to the solution of a Riemann-Hilbert problem. The solution is in general a matrix-valued function analytic everywhere except across a cut, along which the function is discontinuous. The discontinuity is fixed by the driving force or perturbation acting upon the system.¹ From the point of view of the Keldysh formalism the method performs a nontrivial resummation of all relevant diagrams with the help of the solution of the corresponding RH problem. In the Abelian case, when the discontinuity function commutes with itself at all points along the cut, the solution is given in terms of an integral. The classic solution of the FES problem^{7,8} is the simplest example of this solution. In the non-Abelian case, the solution to the RH problem is not known in general, although asymptotic solutions exist. These are valid for response frequencies small compared to those present in the discontinuity function.

Here we explain the RH approach in some detail. To illustrate the power of the method we start by showing how the solution of the equilibrium FES problem^{7,8,10} is derived. We then show the generalization of this problem to include the case where the "impurity" potential mixes scattering states of the unperturbed problem-the case of a nonseparable potential-and deal explicitly with the case when the impurity potential gives rise to a bound state. This problem was treated initially in Refs. 9 and 11, in a calculation that solved directly the Dyson-like equation for the appropriate Green's functions. In the RH formulation of this problem the discontinuity function, although matrix-valued, is constant and commutes with itself. As a consequence, the solution to the RH problem is trivial to derive and yields the standard results of Refs. 9 and 11 with no more work than for the case separable potential case. We show how these results are changed in a nonequilibrium situation. In both the equilibrium and nonequilibrium cases, we compute both the corehole Green's function reported in Ref. 5 and the open line contribution. Finally we show how the states that minimize the shot noise in a periodically driven quantum pump-the so-called coherent states of alternating current¹² (CSAC's) can be described using the RH method.

II. PERTURBING THE FERMI GAS

We consider a system in which particles impinge upon a localized potential. The potential takes the same timeindependent form at times t with t < 0 and $t > t_f$. For $0 < t < t_f$ the potential varies as a function of time. We take our basis to be the eigenstates of the system when t < 0. The states are labeled by their single-particle energy ϵ (\hbar =1) and a channel index i=1, ..., N. We will consider the corresponding annihilation operator, $a_{i\epsilon}$, as the *i*th component of the vector $\hat{\mathbf{a}}_{\epsilon}$. The Hamiltonian of the system is then

$$\hat{H}(t) = \hat{H}_0 + \sum_{\boldsymbol{\epsilon}, \boldsymbol{\epsilon}'} \hat{\mathbf{a}}_{\boldsymbol{\epsilon}}^{\dagger} M(t, \boldsymbol{\epsilon}, \boldsymbol{\epsilon}') \hat{\mathbf{a}}_{\boldsymbol{\epsilon}'},$$
$$\hat{H}_0 = \sum_{\boldsymbol{\epsilon}} \boldsymbol{\epsilon} \hat{\mathbf{a}}_{\boldsymbol{\epsilon}}^{\dagger} \hat{\mathbf{a}}_{\boldsymbol{\epsilon}}.$$
(1)

Here $M(t, \epsilon, \epsilon')$ is an $N \times N$ matrix with M=0 for t<0 and $t>t_f$. (In the following, for any operator \hat{O} , we will denote by O the matrix of \hat{O} taken between the single-particle basis states.)

We will be interested in the total effect of the perturbation, i.e., what is the final state of the system for $t > t_f$ given the initial state at t=0. This requires a knowledge of the effect on the initial many-body state of the time-evolution operator $\hat{U}(t_f)$, where

$$i\frac{d\hat{U}}{dt} = \hat{H}(t)\hat{U}(t), \quad \hat{U}(0) = 1.$$
 (2)

Because the Hamiltonian $\hat{H}(t)$ in (1) is quadratic, the effect of $\hat{U}(t_f)$ is fully characterized by its effect on the set of *single-particle* scattering states, $a_{ie'}^{\dagger}|\rangle$:

$$\hat{U}(t_f)\hat{\mathbf{a}}_{\epsilon'}^{\dagger}|\rangle = \sum_{\epsilon} e^{-i\epsilon t_f} \sigma(\epsilon, \epsilon') \hat{\mathbf{a}}_{\epsilon}^{\dagger}|\rangle, \qquad (3)$$

where $\sigma(\epsilon, \epsilon')$ is some unitary $N \times N$ matrix and $|\rangle$ is the true vacuum with no particles in the system.¹³

When computing the response of the Fermi gas to the time-dependent potential, we will need to compute expectation values of the type

$$\chi_R = \langle 0 | \hat{R} | 0 \rangle. \tag{4}$$

Here $|0\rangle$ is the state of the Fermi gas before the perturbation is applied and \hat{R} is an operator (or operator product) related to an obvervable of interest. In general, the \hat{R} in Eq. (4) will involve the time-evolution operator $\hat{U}(t_f)$. For example, in the case of the shot noise spectrum of a tunneling barrier,¹ the interest is in the statistics of the charged transferred from one electrode to the other. If \hat{Q}_1 is the charge in the first Ŕ electrode, then the expectation value of $=\hat{U}^{\dagger}(t_{f})e^{-i\lambda Q_{1}}\hat{U}(t_{f})e^{i\lambda Q_{1}}$ yields the generating function for moments of the distribution of charge transferred out of channel 1 (into channel 2) during the period between t=0and $t=t_f$. In the case of the FES problem,⁵ the core-hole Green's function (see below) is related to the overlap $\langle 0 | \hat{U}_0^{\dagger}(t_f) \hat{U}(t_f) | 0 \rangle$, where $\hat{U}_0(t_f)$ is the time-evolution operator for \hat{H}_0 in Eq. (1). This overlap is an expectation value of the type (4) with $\hat{R} = \hat{U}_0^{\dagger}(t_f)\hat{U}(t_f)$.

The effect of $\hat{U}(t_f)$ acting on the single-particle states of the basis is given by the unitary matrix $\sigma(\epsilon, \epsilon')$ defined in Eq. (3). The matrix $\sigma(\epsilon, \epsilon')$ can be related to the scattering matrix, S(t, E), for a particle with energy E evaluated on the *instantaneous* value of the potential M(t) in Eq. (1). This reflects the fact that S(t, E) encodes all the information in the potential variations M(t). This relation will be complicated in general. However, if

and

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

 $(\boldsymbol{\epsilon} - \boldsymbol{\epsilon}') \frac{\partial S}{\partial E} \ll 1$

the relation between σ and S becomes simple:

a

$$S_{l\epsilon l'\epsilon'} = S_{l\epsilon l'\epsilon'}$$

$$S_{l\epsilon l'\epsilon'} = \frac{1}{2\pi\sqrt{\nu_l\nu_{l'}}} \int dt S_{ll'}(t,E) e^{i(\epsilon-\epsilon')t},$$
(6)

(5)

where $E = (\epsilon + \epsilon')/2$ and ν_i is the density of states in channel *i*. The result (6) shows that the total scattering amplitude from state ϵ in channel *l* to ϵ' in channel *l'* is just the Fourier transform of the scattering matrix S(t) evaluated on the instantaneous value of the potential. This result was used implicitly to solve the FES problem in the presence of a separable potential.¹⁰

A brief derivation of the condition (5) is given in Ref. 1. The condition can be understood heuristically as follows (see also Ref. 12). We consider the incoming wave packet to be a sum over partial waves in channel l' of the basis, in which S is diagonal before the perturbation is switched on. After impinging on the potential, the partial waves scattered from channel l' into channel l will take a time of the order of the corresponding Wigner delay time to pass out of the region where the potential acts. The condition (5) is equivalent to the requirement that the scattering matrix does not change significantly during this delay time. If this condition is satisfied, relation (6) also has a simple interpretation: the effect of the slowly varying scattering potential on an incident partial wave is just multiplication by the scattering matrix computed on the instantaneous value of the potential M(t). This can be seen by considering a wave packet, with average energy ϵ' and corresponding wave number k' in channel l', incident at time t on the potential (which is assumed to be localized around the origin). This will have amplitude at the origin proportional to $e^{-i\epsilon' t}$. Scattered wave packets will emanate from the source at the origin with amplitudes $S_{ll'}(t)e^{-i\epsilon' t}$ in channels labeled by l. If dispersion effects are small, this will lead to wave forms a distance x from the origin of the form $S_{ll'}(t-(x/v_l))e^{-ik'v_l[t-(x/v_l)]}$, where $v_l = \partial \epsilon / \partial k$ is the velocity of states in channel *l*. Decomposing this into waves of the form $e^{ik(x-v_lt)}$ as $t \to t_{\infty}$ gives the result (6). The normalization factor $1/\sqrt{\nu_l \nu_l'}$ is included so that in the case where the incoming flux $(\sim v |\psi_n|^2)$ is totally scattered into channel n' the scattering amplitude is 1.

A. Fermi sea at T=0

The calculation of the response of the Fermi gas to the time-dependent perturbation reduces to the computation of the expectation value $\chi_R = \langle 0 | \hat{R} | 0 \rangle$ in Eq. (4). In the following we will assume that $| 0 \rangle$ is a single Slater determinant. In this case the computation of χ_R requires the evaluation of a single determinant:

$$\langle 0|\hat{R}|0\rangle = \det'|R|, \qquad (7)$$

where the elements of R are given by

$$R_{ii'}(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}') = \langle |\hat{a}_{i\boldsymbol{\epsilon}} R \hat{a}_{i'\boldsymbol{\epsilon}'}^{\dagger} | \rangle.$$
(8)

and where the prime on det indicates that the determinant is taken only over states occupied in $|0\rangle$.

When the initial Slater determinant $|0\rangle$ corresponds to a filled Fermi sea, it is useful to introduce the Fermi distribution as an operator with elements:

$$f_{\epsilon l,\epsilon' l'} = \frac{\delta(\epsilon - \epsilon')}{\sqrt{\nu_l \nu'_l}} \delta_{ii'} \theta(-(\epsilon - \mu)).$$
(9)

Here μ is the chemical potential, which we take to be zero. For the nonequilibrium problems discussed later the chemical potential can vary according to the channel index [see the discussion around Eq. (57)]. In a block notation that separates the states with positive and negative energies f and Rbecome

$$f = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad R = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix}$$
(10)

and

$$1 - f + fR = \begin{pmatrix} R_{11} & R_{12} \\ 0 & 1 \end{pmatrix}.$$
 (11)

It then follows that

$$\chi_R = \det' |R_{11}| = \det|1 - f + fR|, \qquad (12)$$

where det is now a determinant taken over all states in the basis.

Expressing χ_R as the determinant of 1-f+fR taken over all states in the basis, allows us to write

$$\ln \chi_R = \operatorname{Tr}(f \ln R) + \operatorname{Tr}[\ln(1 - f + fR) - f \ln R]. \quad (13)$$

In Eq. (13), we have added and subtracted the term $\ln \chi_R^{(1)} \equiv \text{Tr}(f \ln R)$. This term consists of the diagonal elements of $\ln R$ summed over all occupied states in $|0\rangle$ and gives the contributions linear in t_f . It often has a simple physical interpretation. In the FES problem it yields the threshold shift (or change in the ground state energy of the Fermi gas after the core hole is created), while in the shot noise spectrum of the tunneling barrier it can be shown to be related to the average transfer of charge across the barrier (the Brouwer formula^{1,14}).

The second term in Eq. (13),

$$\ln \chi_R^{(2)} \equiv \text{Tr}[\ln(1 - f + fR) - f \ln R], \quad (14)$$

accounts for all the nontrivial effects associated with excitations close to the Fermi surface induced by the perturbation. (States far from the Fermi energy, when f=1 or f=0, make no contribution to this term. As a result there are no problems associated with effects of the band edge or short time cutoff when computing this term.) In the case of the FES problem it describes the line shape, while in the shot noise spectrum it gives all the higher moments of the charge transfer distribution. When computing this term, we will later switch to the time representation in which

$$R_{l\epsilon l'\epsilon'} = \frac{1}{2\pi\sqrt{\nu_l\nu_{l'}}} \int dt R_{ll'}(t,E) e^{i(\epsilon-\epsilon')t}, \qquad (15)$$

with [as in Eqs. (6)] $E = (\epsilon + \epsilon')/2$. *R* will normally involve σ or some simple combination of σ with itself and its inverse. Provided the condition (5) is satisfied, we will be able to evaluate σ by ignoring the dependence of S(t, E) on *E*. (This *E* dependence is not important as states far from the Fermi energy do not contribute to $\ln \chi_R^{(2)}$). As a result the term $\ln \chi_R^{(2)}$ will depend only on the time dependence of the scattering matrix evaluated at the Fermi energy, which we will denote by S(t).

The Riemann-Hilbert problem

Computing the second term in Eq. (13), $\ln \chi_R^{(2)}$, is the central task in the evaluation of the response of the Fermi gas. The nontrivial part of this is finding the inverse of (1

-f+fR), which can then be used in an integral representation for its logarithm. This inverse can be written in terms of the solution of an $N \times N$ matrix Riemann-Hilbert problem, where N is the length of the vector $\hat{\mathbf{a}}_{\epsilon}$, i.e., the number of channels in the problem [see Eq. (1)].

A standard procedure for representing the logarithm of an infinite matrix, such as the one on the right hand side of Eq. (14), introduces a λ dependence for *R* via¹⁵

$$R(\lambda) = \exp(\lambda \ln R) \tag{16}$$

and then uses an integral over λ to represent the logarithm:

$$\ln \chi_R^{(2)} = \int_0^1 d\lambda \, \mathrm{Tr} \left[\left[(1 - f + fR)^{-1} f - fR^{-1} \right] \frac{dR}{d\lambda} \right]. \quad (17)$$

[The λ dependence of *R* introduced in Eq. (16) is assumed in Eq. (17) although not written explicitly.]

To compute the trace in Eq. (17), we switch to a time representation in which a quantity A becomes

$$A_{ll'}(t,t') = \frac{1}{2\pi\sqrt{\nu_l\nu_{l'}}} \int_{-\infty}^{\infty} \nu_l d\epsilon \int_{-\infty}^{\infty} \nu_{l'} d\epsilon' A_{ll'}(\epsilon,\epsilon') e^{i\epsilon't'-i\epsilon t}.$$
(18)

Now, the Fermi distribution Eq. (9) is no longer diagonal:

$$f_{ll'}(t,t') = \frac{i}{2\pi} \frac{\delta_{ll'}}{t-t'+i0}.$$
 (19)

However, as we can neglect the *E* dependence of $R(\lambda, t, E)$ and S(t, E) [see discussion after Eq. (15)], *R* and *S* are now diagonal in *t* and equal to $R(\lambda, t, 0)\delta(t-t')$ and $S(t, 0)\delta(t-t')$ respectively. In the time representation, the product of two quantities requires matrix multiplication in the space of scattering channels together with an integral over the intermediate time coordinate. Where one of the quantities in the product is diagonal in *t* (for example *S*), the integral over the intermediate time coordinate is of course trivial and the product reduces to the simple matrix multiplication in the channel space. Tr now becomes a trace over the scattering channels, which we denote by tr, and an integral over the time coordinate, so that

$$\ln \chi_{R}^{(2)} = \int_{0}^{1} d\lambda \int dt \, \text{tr} \bigg[[(1 - f + fR)^{-1}f - fR^{-1}] \frac{dR}{d\lambda} \bigg].$$
(20)

Here, when computing the diagonal (equal time) elements of O, one should take $\lim_{t\to t'} O(t, t')$. If A and B are diagonal in the time representation, it follows that

$$\int dt \operatorname{tr}[A, f]B = \int dt \lim_{t' \to t} \operatorname{tr} \frac{i}{2\pi} \left[\frac{A(t) - A(t')}{t - t' + i0} \right] B(t')$$
$$= \frac{i}{2\pi} \int dt \operatorname{tr} \frac{dA(t)}{dt} B(t), \qquad (21)$$

which is a result we use later.

The quantity $(1-f+fR)^{-1}$ can be written in terms of the function Y(z), which is a matrix in the channel space and

which solves an auxiliary Riemann-Hilbert problem. Y(z) should be analytic everywhere in the complex z plane except on the interval $[0, t_f]$ on the real axis along which it satisfies

$$Y_{-}(t)Y_{+}^{-1}(t) = R(t)$$
 where $Y_{\pm} = Y(t \pm i0)$. (22)

In addition Y should satisfy

$$Y \to 1$$
 when $|z| \to \infty$. (23)

These analytic properties together with Eq. (19) yield the useful identities

$$fY_{-}f = fY_{-},$$

 $fY_{+}f = Y_{+}f.$ (24)

Using these relations (and assuming that Y^{-1} is also analytic everywhere except along the cut), it is then easy to verify that

$$(1 - f + fR)^{-1} = Y_{+}[(1 - f)Y_{+}^{-1} + fY_{-}^{-1}].$$
 (25)

As an aside, we note that $(1-f+fR)^{-1}$ is the solution to a singular integral equation, with *f* playing the role of the singular kernel of the Cauchy type. It is well known that such integral equations can be solved using Carleman's method, which writes the solution in terms of an analytic function satisfying a Riemann-Hilbert problem.¹⁶ In the one-channel case the corresponding singular integral equation for the case when R(t) is constant between t=0 and $t=t_f$ is the problem solved in Refs. 7 and 8 when describing the equilibrium FES.

Inserting Eq. (25) into Eq. (20) and using Eq. (21) we obtain

$$\ln\chi_R^{(2)} = \frac{i}{2\pi} \int_0^1 d\lambda \int dt \, \mathrm{tr} \left\{ \frac{dY_+}{dt} Y_+^{-1} R^{-1} \frac{dR}{d\lambda} \right\}.$$
 (26)

The integral over t is over all times. However, as $dR/d\lambda$ normally vanishes for $t > t_f$ and t < 0, one often only needs to integrate from 0 to t_f .

Equations (26) and (13) map the characterization of the response χ_R in Eq. (4) onto an integral involving the solution, Y(t), of a RH problem [Eqs. (22) and (23)]. An appealing feature of this formulation is that these formulas apply for any choice of variable χ_R provided that the Fermi gas (or gases) is initially in its ground state and apply for many nonequilibrium cases as well. If R(t) commutes with itself at different values of t, the solution of the RH problem can be written in closed form. Although there is no solution for the general case, a lot is known about such noncommuting problems including some asymptotic solutions valid when t_f^{-1} is much smaller than any characteristic frequency in $R(t)^3$.

III. FERMI EDGE SINGULARITY

In this section we show how all the known results for the equilibrium FES follow directly from the formula (26). Within our formalism the case of nonseparable channels considered in Ref. 9 and again in Ref. 11 is no more complicated

than the separable case. We will then discuss how these results are changed in the nonequilibrium case.

A. Equilibrium

The FES problem was first considered in the context of the x-ray absorption spectrum of a metal.⁶ When a photon creates a core hole in a metal, the Fermi gas is affected by the potential of the core hole, leading to the excitation of particle-hole pairs. The absorption line expected in the absence of the Fermi gas becomes a threshold with a singularity in the absorption spectrum as a function of $\omega - \omega_0 > 0$:

$$I(\omega) \sim |\omega - \omega_0|^{-\alpha}, \tag{27}$$

where ω_0 is the threshold frequency for absorption. It turns out that similar singularities are seen in the distribution of energy absorbed by the Fermi gas in response to any rapid change in potential and not just in x-ray absorption experiments. For example, the consequences of the FES are also seen in a tunnel junction. As the energy absorbed by the Fermi gas when switching is an important characteristic of the device, establishing how the FES changes in such tunneling devices is important for understanding fluctuations in energy transfer across such devices.

The Hamiltonian for the photon absorption experiment is⁷

$$\hat{H} = \boldsymbol{\epsilon}_0 \hat{b}^{\dagger} \hat{b} + \sum_{\boldsymbol{\epsilon}} \boldsymbol{\epsilon} \hat{\mathbf{a}}_{\boldsymbol{\epsilon}}^{\dagger} \hat{\mathbf{a}}_{\boldsymbol{\epsilon}} + \sum_{\boldsymbol{\epsilon}' \boldsymbol{\epsilon}} \hat{\mathbf{a}}_{\boldsymbol{\epsilon}}^{\dagger} V(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}') \hat{\mathbf{a}}_{\boldsymbol{\epsilon}'} \hat{b} \hat{b}^{\dagger} + \hat{H}_X, \quad (28)$$

with the operators \hat{a} as in Eq. (1) and $V(\epsilon, \epsilon')$ is an $N \times N$ matrix. The operator \hat{b}^{\dagger} is the creation operator corresponding to the core state and the coupling to the x-ray field is described semiclassically by

$$\hat{H}_{X} = \sum_{\epsilon} \mathbf{W}_{\epsilon} \cdot \hat{\mathbf{a}}_{\epsilon}^{\dagger} \hat{b} e^{i\omega t} + \text{H.c.} \equiv \hat{X} e^{i\omega t}$$
(29)

The absorption spectrum is proportional to the real part of the Fourier transform of the response function

$$S(t_f) = \langle 0 | T\{\hat{X}(t_f)\hat{X}(0)\} | 0 \rangle, \qquad (30)$$

with *T* the time-ordering operator. $S(t_f)$ can be computed from the core-hole Green's function⁷

$$G(t_f) = \langle 0 | T\{ \hat{b}^{\dagger}(t_f) \hat{b}(0) \} | 0 \rangle \tag{31}$$

and the function

$$F(t_f) = \sum_{\epsilon,\epsilon'} \langle 0 | T\{ \hat{b}^{\dagger}(t_f) [\mathbf{W}_{\epsilon'}^* \cdot \hat{\mathbf{a}}_{\epsilon'}(t_f)] \} [\mathbf{W}_{\epsilon'} \cdot \hat{\mathbf{a}}_{\epsilon}^{\dagger}(0)] \hat{b}(0) | 0 \rangle$$
(32)

Conventionally a minus sign is included in the definition of F and G. However, as we will only deal with the absorption case here and take $t_f > 0$, it is easier to work from these definitions. We have also left out the conventional factor of i in the definitions of these Green's functions as in Ref. 7.

The calculation of *F* and *G* reduces to a one-body scattering problem.^{7,17} As far as the Fermi gas is concerned the role of the core hole is to switch on the scattering potential $V(\epsilon, \epsilon')$ at time 0 and switch it off again at t_f . As such, the problem is clearly in the form of Eq. (1) with $M(t, \epsilon, \epsilon')=0$ for $t > t_f$ and t < 0 and $M(t, \epsilon, \epsilon') = V(\epsilon, \epsilon')$ for $0 < t < t_f$. The corresponding scattering matrix S(t, E) switches between the identity when the core hole is absent and some constant value $S^e(E)$ when it is present. The asymptotic behavior of the response at large t_f (when $\omega - \omega_0 \ll \xi_0^{-1}$) is determined by states with energies close to the Fermi surface. For these states we assume that the variation of $S^e(E)$ with E can be neglected so that the condition (5) is satisfied. (The limit $\xi_0 t_f \gg 1$ is the one considered in Ref. 7.)

The calculation of *G* is one of the simplest calculations within the RH approach. *G* is the expectation value of the operator \hat{R} in Eq. (4) with

$$\hat{R} = \hat{U}_{0}^{\dagger}(t_{f})\hat{U}(t_{f}).$$
 (33)

As the matrix elements of $\hat{U}(t_f)$ are just $e^{-i\epsilon t_f}\sigma_{\epsilon\epsilon'}$, it follows from Eq. (7) that¹⁰

$$G(t_f) = e^{i\epsilon_0 t_f} \det' |\sigma|, \qquad (34)$$

while from Eqs. (3), (15), and (16)

$$R(t) = S(t)$$
 and $R(\lambda, t) = \exp \lambda \ln S(t) = [S(t)]^{\lambda}$.
(35)

The RH problem, (22) and (23), reduces to

$$Y_{-}(t)Y_{+}^{-1}(t) = [S(t)]^{\lambda}, \quad Y \to 1 \text{ when } |z| \to \infty.$$
(36)

When the matrix *S* is constant between 0 and t_f , we will denote its value by S^e . In the single-channel case, $S^e = e^{2i\delta}$ and the RH problem is solved by¹⁶

$$Y(z) = \exp\left[\frac{1}{2\pi i}\ln\left(\frac{z}{z-t_f}\right)\lambda \ln S^e\right].$$
 (37)

(This solution was used implicitly in the original solution to the single-channel problem of Ref. 7.) In fact the result (37) solves the RH problem even where the problem is not separable provided that the matrices S(t) evaluated at different times t with $0 < t < t_f$ commute. [This can be checked by direct substitution into Eq. (36).] We insert Y(z) and $R(\lambda, t)$ into Eq. (26). The integral over t runs between 0 and t_f where ln $R(\lambda)$ is nonzero. Inserting into Eq. (13) and including the factor of $e^{i\epsilon_0 t_f}$ yield

$$\ln \chi_R = i\epsilon'_0 t_f - \ln i\xi_0 t_f \left(\frac{\delta}{\pi}\right)^2, \qquad (38)$$

where $\epsilon'_0 = \epsilon_0 + \sum_{\epsilon < 0} \delta(\epsilon) / \pi \nu(\epsilon)$, with $\nu(\epsilon)$ the density of states, is the shifted energy of the core-hole in the presence of the Fermi gas. (The form for the difference between ϵ_0 and ϵ'_0 is usually attributed to Fumi.^{18,19}) Close to the branch points of *Y* at 0 and t_f , we cut the integrals off at $i\xi_0^{-1}$ and $t_f + i\xi_0^{-1}$ where ξ_0 is an energy of order the bandwidth. Equation (38) gives the well-known result for the long-time asymptotic behavior of G:⁶

$$G(t_f) \sim (i\xi_0 t_f)^{-\alpha} e^{i\epsilon_0' t_f}, \quad \alpha = (\delta/\pi)^2.$$
(39)

To compute the function $F(t_f)$ in Eq. (32) is slightly more involved, although the underlying RH problem is the same.

As already mentioned, the role of the core hole is to switch on the potential at t=0 and switch it off again at t_f , so that $F(t_f)$ can be written (writing out the channel indices explicitly)

$$F(t_f) = \sum_{i \in i' \epsilon'} W_{i\epsilon}^* \langle 0 | \hat{r}(i\epsilon, i'\epsilon') | 0 \rangle W_{i'\epsilon'}, \qquad (40)$$

$$\hat{r}(i\boldsymbol{\epsilon},i'\boldsymbol{\epsilon}') = \hat{U}_0^{\dagger}(t_f)\hat{a}_{i\boldsymbol{\epsilon}}\hat{U}(t_f)\hat{a}_{i'\boldsymbol{\epsilon}'}^{\dagger}.$$
(41)

In the basis of the scattering states $\hat{a}_{j'a'}^{\dagger}|\rangle$ the matrix elements of this operator are easily shown to be given in terms of σ in Eq. (3) by

$$r(i\epsilon, i'\epsilon')_{j\alpha j'\alpha'} = e^{i(\epsilon_0 - e)t_f}(\sigma_{j\alpha j'\alpha'}\sigma_{i\epsilon i'\epsilon'} - \sigma_{j\alpha i'\epsilon'}\sigma_{i\epsilon j'\alpha'}).$$
(42)

Using Eqs. (7) and (40) we find

$$F(t_f) = e^{i\epsilon_0 t_f} \text{det}' | C\sigma - |h\rangle\langle g| |.$$
(43)

Here $C = C(t_f)$ is the number:

$$C = \sum_{i\epsilon,i'\epsilon'} e^{-i\epsilon t_f} W_{i\epsilon}^* \sigma_{i\epsilon i'\epsilon'} W_{i'\epsilon'}, \qquad (44)$$

while

$$|h\rangle = \sum_{j\alpha} \left(\sum_{i'\epsilon'} \sigma_{j\alpha i'\epsilon'} W_{i'\epsilon'} \right) a^{\dagger}_{j\alpha} |\rangle,$$

$$\langle g| = \sum_{j'\alpha'} \left(\sum_{i\epsilon} e^{-i\epsilon t_f} W^{*}_{i\epsilon} \sigma_{i\epsilon j'\alpha'} \right) \langle |a_{j'\alpha'}.$$
(45)

Expression (43) is now in the form (7). We could attempt to solve the corresponding RH problem (22) and (23) as before, although the relation between the corresponding operator $\hat{R}(t)$ and S is no longer simple. However, it is easier to simplify Eq. (46) by factoring out $G(t_f) = e^{i\epsilon_0 t_f} \det' |\sigma|$:

$$F(t_f) = CG(t_f) \det \left| 1 - C^{-1}O \right| h \rangle \langle g | \left| \right|$$
(46)

with

$$O = (1 - f + f\sigma)^{-1} f.$$
(47)

We have used Eq. (12) to put Eq. (46) in the form of the determinant over all states in the basis. Using the identity det $|1-C^{-1}O|h\rangle\langle g||=1-C^{-1}\langle g|O|h\rangle$, we obtain

$$F(t_f) = G(t_f)(C - \langle g | O | h \rangle).$$
(48)

As $C \rightarrow 0$ for large t_f (with a functional form which depends on assumptions about the density of states at the band edge), the response is determined by the second term.

The function Y(z) computed with $\lambda = 1$ in Eqs. (36) and (25) can be used to find $F(t_f)$. In the time representation

$$(1 - f + f\sigma)^{-1}f = Y_{+}fY_{-}^{-1}.$$
(49)

Writing $F(t_f) = L(t_f)G(t_f)$ (*L* is usually referred to as the open-line contribution), we find

$$L = -\frac{1}{2\pi} \sum_{ll'} \int d\epsilon \, d\epsilon' \, \int dt_1 dt_2 W_{l\epsilon}^* e^{i\epsilon(t_1 - t_f)} \\ \times \sqrt{v_1} [SY_+ fY_-^{-1}S]_{lt_1, l't_2} \sqrt{v_{l'}} e^{-i\epsilon' t_2} W_{l'\epsilon'}.$$
(50)

Taking W_i to be independent of ϵ (we are assuming that the long t_f behavior is determined by states with energies within $\sim 1/t_f$ of the Fermi surface), this simplifies to give

$$L \simeq \sum_{ii'} W_i \sqrt{\nu_i} \left[Y_{-}(t_f^{-}) \frac{1}{it_f} Y_{+}^{-1}(0^{-}) \right]_{ii'} \sqrt{\nu_{i'}} W_{i'}.$$
(51)

The functions Y_{-} and Y_{+} are evaluated at $t=0^{-}$ and $t=t_{f}^{-}$. This prescription is equivalent to the imaginary time cutoff used to derive Eq. (38) and used in Refs. 7 and 11. Strictly, the discontinuities in *S* at t=0 and $t=t_{f}$ should be thought of as the limit of a fast switching process, in which *S* starts to change at t=0 and reaches its new value S^{e} after a short time. Similarly at $t=t_{f}$, *S* starts to change back from S^{e} to its unperturbed value. (The corrections associated with a more realistic model of a noninstantaneous switching process were considered for a related problem in Ref. 20.) In the singlechannel case we can insert the explicit form for *Y* given by Eq. (37), and recover the standard results

$$L \sim \frac{1}{it_f} \frac{1}{(i\xi_0 t_f)^{-2\delta/\pi}}, \quad F \sim \frac{1}{it_f} \frac{1}{(i\xi_0 t_f)^{(\delta/\pi)^2 - 2\delta/\pi}}.$$
 (52)

When the potential $V(\epsilon, \epsilon')$ in Eq. (28) is strong enough for a bound state of the Fermi gas electrons to form below the bottom of the band, the results for $G(t_f)$ and $F(t_f)$ are no longer correct. The effect of the bound state can be taken into account explicitly as explained in the Appendix. The results for $G(t_f)$ given by Eq. (A2), and for $F(t_f)$ given by Eq. (A12), have two main contributions. After taking the Fourier transform to obtain the absorption spectrum, the first corresponds to having the bound state occupied and leads to the absolute threshold for absorption. The second term relates to scattering processes in which the bound state is always empty and leads to a subsidiary threshold at E_b above the first in the absorption spectrum.

The results (39), (52), and (A13) are of course very well known.^{7,8} However, none of the key formulas (37), (51), and (A12) require that the scattering matrix *S* should be diagonal in the channel indices. Provided that *S*(*t*) commutes with itself at different times, the results are valid for arbitrary channel number. We can therefore use the function *Y*(*z*) given by Eq. (37) to compute the corresponding results for the case of a nonseparable potential just as easily as in the separable case. In the absence of bound states, one obtains with $\epsilon'_0 = \epsilon_0 + \sum_{\epsilon < 0} \sum_{\epsilon} \delta_{\epsilon}(\epsilon) / \pi \nu_{\epsilon}(\epsilon)$:

$$G(t_f) = \exp(i\epsilon_0' t_f)(i\xi_0 t_f)^{-\beta},$$

$$L(t_f) = \sum_{\zeta} |\tau_{\zeta}|^2 \frac{1}{it_f} \exp\left(\frac{2}{\pi} \delta_{\zeta} \ln i\xi_0 t_f\right),$$
(53)

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$$\beta = \sum_{\zeta} \left(\frac{\delta_{\zeta}}{\pi}\right)^2$$

which are the results obtained perturbatively in Ref. 11. Here the eigenvalues of the matrix S^e [see after Eq. (36)] are written as $e^{2i\delta_{\zeta}}$. S^e has eigenvectors $f(\zeta)_i$ and $\tau_{\zeta} = \sum_i \sqrt{\nu_i} W_i^* f(\zeta)_i$.

The perturbing potential, characterized by scattering matrix S^e , can be strong enough to lead to a bound state with wave function given by Eq. (A4). In the presence of a bound state(s) we take the eigenvalues of S^e to be $e^{i2\tilde{\delta}_{\zeta}}$ with $\tilde{\delta}_{\zeta}$ defined as the phase shift modulo π in channel ζ on the interval $[-\pi/2, \pi/2]$ [see discussion after Eq. (A7)]. We then obtain the generalizations to the nonseparable case of the results of Ref. 10 for $G(t_f)$ and $F(t_f)$. We find

$$G(t_f) = \widetilde{G}(t_f)(1 + A_B), \qquad (54)$$

where $\tilde{G}(t_f)$ is the contribution of the scattering states given by the expression for *G* in Eq. (53) with phase shifts given by $\tilde{\delta}_{\ell}$, while

$$A_B \sim e^{-iE_B t_f} \sum_{\zeta} |\eta_{\zeta}|^2 e^{-2i\widetilde{\delta}_{\zeta}} \exp\left(-\frac{2}{\pi}\widetilde{\delta}_{\zeta} \ln i\xi_0 t_f\right).$$
(55)

Here $\eta_{\zeta} = \sum_i \sqrt{\nu_i} u_i^* f(\zeta)_i$ and the u_i are the bound state wavefunction coefficients given in Eq. (A4). In the presence of the bound state, the function $F(t_f) \sim F_0(t_f) + F_b(t_f)$ with

$$F_0(t_f) \sim \tilde{G}(t_f)\tilde{L}(t_f),$$

$$F_b(t_f) \sim e^{-iE_B t_f} \tilde{G}(t_f) |\mathbf{u} \cdot \mathbf{W}|^2,$$
(56)

where $\tilde{L}(t_f)$ is the scattering state contribution to $L(t_f)$ given by the expression in Eq. (53), using the phase shifts $\tilde{\delta}_{\zeta}$.

Formulas (56) and (53) are the natural generalizations of the single-channel result and have exactly the same interpretation as was given originally in Refs. 8 and 21. We repeat this briefly here as the results for the nonequilibrium case (given in the next section) can also be understood heuristically on a similar basis but with the phase shifts becoming complex. The exponents $(\delta_{\zeta}/\pi)^2$ and $(\delta_{\zeta}/\pi\pm 1)^2$ are, according to the Friedel sum rule, the square of the net charge that needs to move in to or away from the origin in order to screen the core hole potential. For $G(t_f)$ this is δ_{ζ}/π , while for $F(t_f)$ it is $(\delta_{\zeta} - \pi)/\pi$ if the photoelectron inserted at the origin is in the ζ channel and δ_{ζ}/π otherwise. If there is an occupied bound state after absorption of the photon, the respective values become $(\delta_{\zeta} + \pi)/\pi$ and δ_{ζ}/π , as now the Fermi gas has to provide the additional electron, which ends up in the bound state. The form t^{-n^2} is just the decay with time of the overlap of the wave function of the Fermi gas at $t=t_f$ and the one describing the system created at t=0 in which (with respect to the ground state in the presence of the core hole) there is an excess charge $n = -\delta/\pi$ at the origin. That it vanishes as $t \rightarrow \infty$ is the orthogonality catastrophe described by Anderson.²²



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.

B. Nonequilibrium effects

The experimental and technological interest in the out-ofequilibrium response of coupled Fermi systems has grown as electronic devices have shrunk. Examples include structured quantum dots, like the single-electron transistor or the singlephoton detector,²³ and quantum point contacts. The nonequilibrium Fermi edge singularity (NFES) will characterize the energy absorbed by the coupled Fermi gases in a rapid switching process in such devices. The NFES should help explain, for example, measurements of random telegraph signals (RTS). In these experiments, a two-level system (TLS) couples to the source-drain current flowing in the channel of a metal oxide semiconductor field effect transistor (MOS-FET) (the TLS resides in the insulating oxide layer²⁴). The RTS relates to the "random" switching of the TLS between its ground and excited states. The ratio between the times the TLS spends in the excited and ground states is measured experimentally. In equilibrium this ratio is fixed by detailed balance, and the deviations from this have been attributed to nonequilibrium effects.²⁵

As one of the simplest nontrivial many-body effects, the FES is also a natural point to start, when looking for a description of nonequilibrium effects in many-electron systems. Perhaps surprisingly, given its conceptual simplicity, the NFES has not attracted as much attention as more difficult nonequilibrium problems like the Kondo effect, to which it is known to be related. (The Kondo effect can be thought of as a sequence of FES's associated with each flipping of the localized moment.)²⁶

In Ref. 5 we reported results for $G(t_f)$ for a two-channel problem, which modeled a system with two electrodes separated by a barrier. The transmission of the barrier depends on the state of a two-level system inside the barrier, see Fig. 1, with the transition between the two levels assumed to be dipolar. The real part of the Fourier transform of the function

 $G(t_f)$ gives the absorption spectrum for the device. The nonequilibrium effects predicted in Ref. 5 should be visible in the voltage dependence of the absorption line shape of devices like the single-photon detector of Refs. 23 and 27. In Ref. 23 a quantum dot in the quantum Hall regime is 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. The absorption of the photon and the subsequent separation of the hole (which moves into the ν =1 ring on the outer part of the dot) and the particle (which "falls" into the center of the dot at $\nu = 2$) is rapid, while the response of the conduction electrons in the two electrodes is slow and will show effects characteristic of the FES. In the device of Ref. 27, an electron trapped in a dot underneath an electron channel gives rise to a potential that closes off a conducting channel. When a photon is absorbed, the photoexicted hole can recombine with the electron in the trap, the potential of the electron disappears and the channel opens. Again the conduction electrons on the two sides of the channel, 'see' the sudden reduction of a tunneling barrier on absorption of a photon.

The main result reported in Ref. 5 was that the formula of Nozières and de Dominicis⁷ (ND) describing the form of the FES and threshold shift (Fumi's theorem^{18,19}) generalized in a simple way to the nonequilibrium case. For time scales t_f $\ll 1/V$, the phase shifts that appear in $G(t_f)$ are real and are given by the logarithm of the eigenvalues of the scattering matrix $S^{e,9,11}$ This simply reflects the fact that, on these short time scales, the response of the Fermi gas involves excitations with energies $\epsilon \gg V$ that do not sense the nonequilibrium distribution function. On time scales $t_f \ge 1/V$, the equilibrium phase shifts in the two channels are replaced by "complex" phase shifts given by $\ln S_{11}^e$ and $\ln(1/S_{22}^e)^*$. The real part of these phase shifts describes the scattering within each electrode, while the imaginary part describes the effect of scattering processes in which particles cross the barrier. One effect of the nonequilibrium operation of the device is to make the scattering between the different electrodes effectively incoherent. Here, we find that this interpretation extends also for the function $F(t_f)$.

We show the key steps in the derivation of $G(t_f)$, emphasizing the relationship with the equilibrium results, and report the results for $F(t_f)$ including the role of possible bound states. Since the initial state involves a filled Fermi sea in both channels (left and right electrodes), the RH formulation of this nonequilibrium problem is the same as that for the equilibrium case. The bias across the tunnel junction means only that the chemical potentials are different in the two electrodes. One way of handling this difference is to introduce a gauge transformation acting only on the basis states in the left electrode:

$$\mathbf{a}(\boldsymbol{\epsilon}) \rightarrow \mathbf{a}(\boldsymbol{\epsilon},t) = \exp\left(+iP_l \int_0^t V(\tau)d\tau\right) \mathbf{a}(\boldsymbol{\epsilon}),$$
 (57)

$$S(t) \to S(t) = \exp\left(+iP_l \int_0^t V(\tau) d\tau\right) S(t)$$
$$\times \exp\left(-iP_l \int_0^t V(\tau) d\tau\right), \tag{58}$$

where P_l is the diagonal matrix projecting onto states in the first (left) electrode, i.e., $(P_l)_{11}=1$ and $(P_l)_{22}=0$. The effect of this transformation on states in the left electrode is to set $\epsilon \rightarrow \epsilon - V(t)$, so that the chemical potential in the left electrode becomes equal to that in the right electrode (taken to be zero as before). For the constant bias case, the transformation gives $\hat{\mathbf{a}}(t) \rightarrow \hat{\mathbf{a}}(t) = e^{+iP_lVt}\hat{\mathbf{a}}$.

The functions $\ln \chi_R^{(2)}$ and $L(t_f)$ for the NFES case are still given by Eqs. (26) and (50). However, the RH problem satisfied by the function Y(z) is different: In Eqs. (36) $S^{\lambda}(t)$ picks up an additional time dependence from the gauge transformation (58), which leads to two important differences to the equilibrium case. First, the function e^{iVt} introduces a new characteristic energy scale, *V*. If the function S(t) has Fourier components with freqencies $\omega \gg V$, the response will be dominated by states with energies $|\epsilon| \gg V$ and will be insensitive to the nonequilibrium nature of the distribution, which only becomes apparent on the energy scale *V*. If S(t) only varies at frequencies $\omega \ll V$ the response will come from states with energies $\epsilon \ll V$ and will normally be significantly different from what happens in equilibrium.

The second main difference following from the additional time dependence of S(t) relates to the case when between t =0 and $t=t_f$ the scattering matrix (before the gauge transformation) is constant and equal to S^{e} . In this case it is now no longer possible to solve the RH problem with a function of the form (37). Although this form satisfies formally the jump condition, $Y_{-}(t)Y_{+}^{-1}(t) = S^{\lambda}(t)$, the corresponding function Y(z) is not well-defined for large z if S^e is not diagonal. The off-diagonal elements of S^e contain factors $e^{\pm iVt}$ so that in the analytic continuation to complex z there is an essential singularity at $z \rightarrow \infty$ in Y(z) defined by Eq. (37), and Y(z) no longer satisfies the condition $Y \rightarrow 1$. This problem is clearly apparent in the RH formulation we have presented. It was much less clear in previous attempts to extend the ND method to the nonequilibrium case and may explain why these failed.²⁸ It is also interesting to note that for $t_f \ll 1/V$, we can expand the function e^{iVt} up to linear order in Vt. Then $S^e = S^e(V=0) + CVt$, there is no singularity at infinity for Y, and the form (37) still works.

In general there is no exact solution to the noncommuting RH problem.³ However, in the case relevant to the device shown in Fig 1, $S(t) = e^{iP_lVt}S^e e^{-iP_lVt}$ for $0 < t < t_f$, with S^e constant, we can find an asymptotically correct solution for the limit $t_f \ge 1/V$ relevant to the NFES.^{1,5} We will only consider the case where there is one channel in each electrode. As in the equilibrium case [cf. Eq. (35)]

$$R = \exp[\lambda \ln S(t)].$$
⁽⁵⁹⁾

In this case the solution for Y(z), valid for $|z| \ge V^{-1}$, is given for $\operatorname{Re}[z] < 0$ or $\operatorname{Re}[z] > t_f$ by

$$Y(z,\lambda) = \psi(z,\lambda), \tag{60}$$

while immediately above and below the cut, $[0, t_f]$,

$$Y_{+}(t,\lambda) = \begin{pmatrix} 1 & -\gamma(t,\lambda) \\ 0 & 1 \end{pmatrix} \psi_{+}(t,\lambda),$$

$$Y_{-}(t,\lambda) = \begin{pmatrix} 1 & 0 \\ + \eta(t,\lambda) & 1 \end{pmatrix} \psi_{-}(t,\lambda).$$
(61)

Here $\gamma(t,\lambda) = R_{12}/R_{11}$ and $\eta(t,\lambda) = R_{21}/R_{11}$. The functions $\psi_{\pm}(t,\lambda) = \psi(t\pm i0,\lambda)$, where $\psi(z,\lambda)$ is given by

$$\psi = \exp\left[\left(x_1 \tau_0 + x_2 \tau_3 \right) \ln \frac{z}{z - t_f} \right], \tag{62}$$

with

$$x_1(\lambda) = \frac{\ln R_{11}/R_{22}^*}{4\pi i}, \quad x_2(\lambda) = \frac{\ln(R_{11}R_{22}^*)}{4\pi i}.$$
 (63)

Here τ_3 is the third Pauli spin matrix and τ_0 is the identity matrix. The derivation of Eqs. (61) follows that given in Ref. 1. The idea, which was explained in detail in the context of inverse scattering problems in Ref. 3, is to solve for a function W(z), which satisfies the same jump condition as Y(z) but in a complex plane with additional cuts. For this problem, the additional cuts are parallel to the imaginary axis and run from the branch points at z=0 and $z=t_f$ to infinity. The discontinuities in W(z) across the vertical cuts scale as $e^{-|Vz|}$. If Y is approximated by W, the errors in $\ln \chi_R$ defined in ((13)) are only $O(1/Vt_f)$, and can, in principle, be computed order by order in powers of $(Vt_f)^{-1}$.

The form for $\log \chi_R$ for $t_f \ge V^{-1}$ is found by inserting Eqs. (61) into (26) and (13) and computing the integrals over *t* and λ as in the equilibrium case:⁵

$$\ln \chi(t_f, V) = -i [E_0 - \Delta(V)] t_f - \beta' \ln(iVt_f) + D, \quad (64)$$

where $\Delta(V)$ is given by the nonequilibrium generalization of Fumi's theorem^{18,19}

$$\Delta(V) = \int_{-\infty}^{0} \frac{\operatorname{tr}\ln[S^{e}(E)]}{2\pi i} dE + \int_{0}^{V} \frac{\ln[S^{e}_{11}(E)]}{2\pi i} dE.$$
 (65)

The constant β' is given by [cf. Eq. (53)]:

$$\beta' = \left(\frac{\ln(S_{11}^e)}{2\pi i}\right)^2 + \left(\frac{\ln(1/S_{22}^e)^*}{2\pi i}\right)^2.$$
 (66)

The constant term *D* can be estimated by requiring that the form for $\ln \chi$, Eq. (65), matches the equilibrium one at $t_f = V^{-1}$, Eq. (38), valid for $t_f \ll V^{-1}$. This constant gives the contribution from excitations with frequencies between *V* and ξ_0 . This gives

$$D = \beta \ln \xi_0 / V. \tag{67}$$

The result for $G(t_f)$ can be seen as an adaptation of the equilibrium result. The real phase shifts (given by -i times the logarithms of the eigenvalues of the scattering matrix S^e), which appear in the formulas (53), are replaced by complex phase shifts. In the forward bias case described by Eq. (53),



FIG. 2. Spectral function $\operatorname{Re}_{\chi G}(\omega)$ computed from Eq. (10) with ω in units of the bias voltage *V*. The spectra depend on $S_{11}^e = \sqrt{R}e^{i2\alpha_1}$ and $S_{22}^e = \sqrt{R}e^{i2\alpha_2}$, where *R* is the reflection probability. The curve marked + (-) refers to the case in which electrode 1 (2) is at the higher chemical potential. Also shown is the corresponding equilibrium result calculated from Eq. (53) using $\xi_0 = V$ (Ref. 29). In addition to the overall smoothing of the singularities, expected in a nonequilibrium system, there are two significant nonequilibrium features. First, the maximum in the spectral weight is shifted away from its equilibrium value by an amount proportional to the applied voltage. The shift, $\operatorname{Re}[\Delta(V) - \Delta(0)]$, which is given in the forward-biased case in Eq. (B4), depends on the polarity of the voltage. Second the form of the function changes on reversing the polarity of the device.

these are $-i \ln S_{11}^e$ and $-i \ln (1/S_{22}^e)^*$. The effect of the complex phase shifts is to smooth the singularity seen in equilibrium (this could be expected on quite general grounds) and to introduce a polarity dependence. This polarity dependence affects both the shape and the position of the spectrum and is evident in Fig. 2 where we show $\chi_G(\omega)$ for a particular choice of S^e. The dependence of the spectrum, $\chi_G(\omega)$, on the polarity of the device, when operating out of equilibrium, is governed by the difference $\alpha_{12} \equiv \alpha_1 - \alpha_2$ (with $\alpha_{1,2}$ as defined in the figure caption). The difference in the overall position of the spectrum on changing the polarity is given by the difference in the second term on the right hand side of Eq. (65) and is proportional to α_{12} . This origin of this shift of the spectrum is the change in the nature of the scattering across the barrier from fully coherent in the equilibrium case to incoherent for times $t_f \gg V^{-1}$ in the nonequilibrium case. The shape of the spectrum reflects the decay of charge from its initial distribution (the equilibrium distribution for S=1) to the steady-state distribution for $S = S^{e.8,21}$ In the nonequilibrium case, this decay can occur differently depending on the polarity. If more charge is needed in the left-hand electrode to screen the potential characterized by S^e than in the righthand one $(\alpha_{12} > 0)$, this charge can come from states within V of the Fermi energy of the right-hand electrode when the device is reverse-biased but not when it is forward-biased.

For the model device shown in Fig. 1 the absorption spectrum is given by the Fourier transform (see Appendix B) of $G(t_f)$ rather than $F(t_f)$, as the transition in the barrier is presumed to be dipolar. However, the corresponding function $F(t_f)$ is also important. In Refs. 30 and 31 Yuval and Anderson showed that the Kondo problem could be treated as an infinite sequence of spin flips or switching events, with the



FIG. 3. Spectral function $\operatorname{Re}\chi_F(\omega)$ computed from Eq. (B10) with ω in units of the bias voltage V for the case $(W_1, W_2) \sim (0, 1)$ in Eq. (51). The curve marked + (-) refers to the case in which electrode 1 (2) is at the higher chemical potential. Also shown is the corresponding equilibrium result (Ref. 29). For these relatively small phase shifts the singularity seen in equilibrium disappears completely, although there is still a polarity dependence of the spectrum even though the scattering matrix is symmetric.

response of the conduction electrons to each switching event characterized by $F(t_f)$. Given the long-standing interest in nonequilibrium effects in the Kondo effect,^{32,33} the correct nonequilibrium form for $F(t_f)$ would be the starting point for the study of the nonequilibrium Kondo effect using a generalization of the Yuval-Anderson mapping.

We must first write the function F and the open line function L in terms of the gauge-transformed basis:

$$L(t_f) \simeq W_i^* \sqrt{\nu_i} e^{-iP_l V t_f} \left[Y_-(t_f) \frac{1}{it_f} Y_+^{-1}(0) \right]_{ii'} W_{i'} \sqrt{\nu_{i'}}.$$
 (68)

We can now insert the solution for Y_+ (with $\lambda = 1$) from Eq. (61) into Eq. (51). The result can be written

$$L(t_f) \simeq \frac{1}{it_f} \mathbf{W}^* \begin{pmatrix} z_f (iVt_f)^{2x_+} & 0\\ \alpha z_f (iVt_f)^{2x_+} & (iVt_f)^{2x_-} \end{pmatrix} \mathbf{W},$$
(69)

where $x_{\pm} = x_1(1) \pm x_2(1)$ with $x_i(\lambda)$ defined in Eq. (63), $\alpha = S_{21}^e/S_{11}^e$ and $z_f = e^{-iVt_f.^{34}}$ The absence of a contribution proportional to $W_1^*W_2z_f$ is to be expected. This would involve a contribution to the open-line function from an electron initially placed in the right-hand electrode exciting the Fermi gas in the left electrode. Since we are assuming that the tunneling through the barrier by the electron is a slow process on the scale of 1/V, this does not lead to a singular contribution to F. [There is still a contribution to F proportional to $W_1^*W_2z_f$ from the direct scattering term $CG(t_f)$ in Eq. (48).]

The effect of the open line contribution on $F(t_f) = G(t_f)L(t_f)$ is the natural generalization of the equilibrium result that one might expect given the results for $G(t_f)$. The corresponding spectral functions is shown in Fig. 3 for a particular choice of S^e . For simplicity we only look at the case where the electron is added and removed from the same (i=2) electrode, i.e., $\mathbf{W} \sim (0, 1)$. The dependence of the spectrum on the polarity of the device is present even in the case where S^e is symmetric. When a particle is added to an electron

trode, the response of the system will depend on whether the electrode is at the higher or lower chemical potential. The form of the spectrum can also differ substantially from what happens in equilibrium. For the case $\alpha_1 = \alpha_2 = 0.4$ and R = 0.7 shown in Fig. 3, there is no real peak left over from the equilibrium result. This is because the phase shifts δ_{ζ} , corresponding to the eigenmodes of S^e , are small, and hence the exponents in Eq. (53) for the equilibrium function $\chi_F(\omega) \sim \omega^{-(\delta_{\zeta} - \pi)^2/\pi^2}$ are also small. The corresponding singularity is weak and easily smoothed out by the finite lifetimes of states close to the Fermi energy in the nonequilibrium case. This smoothing is enhanced because one of the phase shifts, δ_{ζ} , is always larger than α_1 and α_2 . This larger exponent gives the dominant singularity in equilibrium, but is then effectively replaced by α_1 out of equilibrium.

IV. CHARGE TRANSFER: CSAC

The existence of CSAC was predicted in Ref. 12. These consist of a sequence of pulses that propagate through a contact. When the bias across the contact is described a class of periodic (with period Ω) rational functions of the variable $z=e^{i\Omega t}$, then the shot noise is minimized and the noise distribution does not depend on the separation of the pulses. This result is still not well understood, nor is it possible, using the original derivation, to establish how robust these states are against deviations from zero temperature or from the ideal pulse shape.

Recent rapid experimental progress in the application of microwave radiation at low temperatures suggests that the experimental test of the existence of the CSAC is just about possible. Several experimental groups are pushing the technology in this direction,^{35–37} and it should only be a matter of time before experimental data become available. However, interpretation of these future experiments will not be easy using the analytical method used in Ref. 12 as this depends crucially on the particular shape of the pulses. There are no predictions about what happens when the shape of the pulses deviates slightly from the required one (something unavoidable in any real experiment), nor is the effect of nonzero temperature known.

Here we show that the results of Ref. 12 for the CSAC are easy to derive using the RH approach. When the pulses are periodic as in the case of the CSAC, the RH problem simplifies. It requires solving for functions that are analytic in two *disconnected* regions (inside and outside the unit circle) with the jump function specifying the discontinuity across the boundary between them. We show that the particular case of the CSAC corresponds to a RH problem that can be solved exactly using combinations of meromorphic functions in the plane—one of which is analytic inside and one outside the unit circle.

The model device considered in Refs. 1 and 12 consists of a tunnel junction driven by a bias voltage V(t), which is periodic in time with period $T=2\pi/\Omega$. It is equivalent to the device shown in Fig 1. We are interested in the change in physical quantities over one cycle of the pump in the limit $t_f \gg T$. In this limit, effects induced by the switching on and off of the periodic potential at t=0 and $t=t_f$ are irrelevant. The scattering matrix *S* is at some constant value S^e between 0 and t_f . Applying the time-dependent gauge transformation (58) leads to *S* becoming a periodic function of time, so that it no longer commutes with itself at different times.

The distribution function for any single-particle observable measured in this periodically pumped Fermi system will involve the solution of a noncommuting RH problem. In particular, the characteristic function or generating function for moments of the distribution of the net transfer of charge from electrode 1 (left electrode) to the electrode 2 (right electrode), $\chi(\lambda)$, is given by Eq. (4) with the operator *R* given by

$$\hat{R}(\lambda) = \hat{U}^{\dagger}(t_f) e^{-i\lambda\hat{Q}_1} \hat{U}(t_f) e^{i\lambda\hat{Q}_1}.$$
(70)

Here

$$\hat{Q}_1 = \sum_{\varepsilon} \hat{\mathbf{a}}_{\varepsilon}^{\dagger} P_l \hat{\mathbf{a}}_{\varepsilon}.$$
 (71)

For states close to the Fermi surface $(E = \varepsilon + \varepsilon' \simeq 0)$, the matrix *R* in the time representation can be written

$$R(t,\lambda) = S^{-1}(t)e^{-i\lambda P_l}S(t)e^{i\lambda P_l},$$
(72)

so that the characteristic function will be given by Eqs. (12), (13), and (25):

$$\ln \chi(\lambda) = \operatorname{Tr}[\ln(1 - f + fR)]. \tag{73}$$

If the inverse of the solution $Y_+(t)$ to the RH problem (22) and (23) with *R* given by Eq. (72), is analytic in the upper half-plane, we can write the characteristic function as

$$\ln \chi(\lambda) = \int_0^\lambda d\lambda' \int dt \, \mathrm{tr} \left\{ Y_+ f Y_+^{-1} R^{-1} \frac{dR}{d\lambda'} \right\}.$$
(74)

Using Eqs. (72) and (21), and computing explicitly the derivative with respect to λ , we obtain^{1,38}

$$\ln \chi(\lambda) = \int_0^\lambda \frac{d\lambda'}{2\pi} \int dt \operatorname{tr} \left\{ \frac{d(Se^{i\lambda' P_l}Y_+)}{dt} (Se^{i\lambda' P_l}Y_+)^{-1} P_l \right\}.$$
(75)

[If the eigenvalues of Y_+ have zeros in the upper half-plane, there are additional contributions to the right-hand side of the corresponding relations to Eq. (24) for Y_+^{-1} from its poles. In this case, $(1-f+fR)^{-1}$ is no longer given by Eq. (25) but can be found using methods described in Chap. 6 of Ref. 16.]

In the case of the periodically driven pump, the scattering matrix (after applying the gauge transformation) is periodic, S(t)=S(t+T). If we change variables to $z=e^{2\pi i t/T}$, we need to find a function $Y_+(z)$, which is analytic for |z| < 1, and Y_- , which is analytic for |z| > 1 and $Y_- \rightarrow \text{const}$ when $|z| \rightarrow \infty$. On the unit circle |z|=1,

$$Y_{-}Y_{+}^{-1} = S^{-1}(z)e^{-i\lambda P_{l}}S(z)e^{i\lambda P_{l}}.$$
(76)

The characteristic function for charge transmitted during one cycle of the periodic pump in the limit $t_f/T \ge 1$ is given by

$$\ln \chi = \int_0^\lambda \frac{d\lambda}{2\pi} \oint_{|z|=1} dz \operatorname{tr} \left\{ \frac{d(Se^{i\lambda P_l}Y_+)}{dz} (Se^{i\lambda P_l}Y_+)^{-1} P_l \right\}.$$
(77)

CSAC's were reported in Ref. 12 for the case when the phase factor in Eq. (58) can be written as a rational function, l(z), of the variable $z=e^{2\pi i t/T}$:

$$\exp\left(+iP_l\int_0^t V(\tau)d\tau\right) = \begin{pmatrix} l(z) & 0\\ 0 & 1 \end{pmatrix}$$
$$l(z) = \prod_{i=1}^N \frac{z-\alpha_i}{1-\alpha_i^* z},$$
(78)

where either all $|\alpha_i| > 1$ or all $|\alpha_i| < 1$. We can choose $|\alpha_i| > 1$ without loss of generality as $z \mapsto 1/z$ simply reverses the polarity of the device. In this case, we decompose $R(z,\lambda)$ (see Ref. 1) as follows:

$$R = \begin{pmatrix} 1 & 0 \\ \alpha/l(z) & 1 \end{pmatrix} \begin{pmatrix} a & 0 \\ 0 & 1/a \end{pmatrix} \begin{pmatrix} 1 & \beta l(z) \\ 0 & 1 \end{pmatrix},$$
(79)

where

$$a = |S_{12}|^2 e^{i\lambda} + |S_{11}|^2,$$

$$\alpha = -\frac{S_{21}^e(S_{22}^e)^*(1 - e^{i\lambda})}{a},$$

$$\beta = -\frac{S_{12}^e(S_{11}^e)^*(1 - e^{-i\lambda})}{a}.$$
(80)

The solution to the RH problem

$$Y_{-}Y_{+}^{-1} = \begin{pmatrix} 1 & 0 \\ \alpha/l(z) & 1 \end{pmatrix} \begin{pmatrix} a & 0 \\ 0 & 1/a \end{pmatrix} \begin{pmatrix} 1 & \beta l(z) \\ 0 & 1 \end{pmatrix}$$
(81)

is clearly

$$Y_{-} = \begin{pmatrix} 1 & 0 \\ \alpha/l(z) & 1 \end{pmatrix},$$
$$Y_{+} = \begin{pmatrix} 1 & -\beta l(z) \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1/a & 0 \\ 0 & a \end{pmatrix}.$$

Inserting this into Eq. (77) gives the result reported in Ref. 12:

$$\ln \chi(\lambda) = N \frac{t_f V}{2\pi} \ln a \tag{82}$$

with a given by Eq. (80).

The surprising feature of the result (82) is that it implies that the second moment of the shot noise $\langle n^2 \rangle$ achieves the absolute minimum for given charge transfer $\langle n \rangle$,¹² which is the value obtained in the constant bias case $\alpha_i \rightarrow \infty$ for all *i*. The feature of the phase factor l(z), which leads to the RH problem being so easy to solve, is that all its poles (zeros) are either inside or outside the unit circle |z|=1, which means that the decomposition of *R* in Eq. (79) automatically solves the RH problem. In the case of an arbitrary rational function for l(z) this is not the case as there can be points at which det $|Y_+(z)|$ vanishes inside the unit circle. The corresponding formulas to Eq. (24) Y_+^{-1} pick up additional terms on the right-hand side and $(1-f+fR)^{-1}$ is not given by Eq. (25), although, in principle, it can still be found given the solution to the RH problem Y(z).

V. CONCLUSIONS AND OUTLOOK

The RH approach is a general method for computing the response of a Fermi gas to a localized time-dependent perturbation. There are two key steps to the method. First, provided the condition (5) is met, the method works with the scattering matrix defined on the instantaneous value of the potential rather than with the Hamiltonian. This has the attractive feature of working directly with the physical quantities determining the long time response of the system to a perturbation, namely scattering amplitudes for particles close to the Fermi surface. Condition (5) is essentially the requirement that the perturbation varies more slowly than the delay time for a particle traversing the region in which the perturbation acts. The second key step is to relate the response of the Fermi gas to the solution of a noncommuting RH problem (22) and (23). The RH problem corresponding to any given experimental situation is usually easy to set up. Its solution and the interpretation of the results are a more delicate task that needs to be repeated for each new physical situation. While there is no analytical solution of the general non-Abelian RH problem, there is a powerful technique for finding asymptotic solutions valid for frequencies much smaller than those present in the jump function.³

Here we have emphasized the generality of the approach and applied it to two existing problems-the Fermi edge singularity and the shot noise in a periodically pumped tunnel junction. The calculations in the two cases are very similar. In the case of the FES we have rederived all the known results for the equilibrium case emphasizing, in particular, how the method is no more complicated in the case of the nonseparable potential than in the separable case. For the nonequilibrium device shown in Fig. 1, we have explained how the results for the core-hole Green's function of Ref. 5 were obtained and given the corresponding results for the open-line function $L(t_f)$ Eq. (69). For the case of the CSAC's, we have shown that the particular form of the periodically varying bias with the phase factor $l(e^{2\pi i t/T})$ given by Eq. (78) corresponds to a case in which the RH problem can be solved exactly.

It is possible within the RH approach to handle corrections to the asymptotic solution to the noncommunting RH problem we have been using in order to allow us to compute the response of systems in the intermediate regime (where one is interested in the response at frequencies comparable to those introduced by the perturbation). The RH problem lends itself naturally to a type of perturbative analysis. The corrections to the approximate solution valid for long times, Eqs. (60) and (61), can be described by multiplying the approximate solution by a function that is analytic except across the additional vertical cuts introduced to simplify the original problem. This function can be specified by a Cauchy integral around the cut. Preliminary work in this direction has been attempted in Ref. 39.

Finally, the RH method should generalize to nonzero temperatures. As was observed in Ref. 26, the singular integral equation appearing at finite temperatures in a related problem can be solved analytically. Also, the analytic treatment of the finite-temperature Fermi-edge singularity in Refs. 24 and 40 again suggests that the RH approach will generalize successfully to finite temperatures.

APPENDIX A: BOUND STATES

If the perturbing potential generates a bound state(s), then Eq. (6) is no longer correct. In the case where the potential [and hence S(t)] simply switches between its unperturbed value and a new but time-independent value at t=0 and back again at $t=t_f$, we can correct σ by including the effect of the bound state explicitly. The treatment follows closely that of Ref. 10, although only the case of a separable potential was treated there. We write

$$\sigma = \tilde{\sigma} + e^{iH_0 t} |b\rangle e^{-iE_b t} \langle b|.$$
 (A1)

Here $|b\rangle$ is the bound state wave function, while $\tilde{\sigma}$ describes the scattering of the states within the continuum, and is given by the Fourier transform of the scattering matrix S(t), Eq. (6), as before. (H_0 is the matrix of \hat{H}_0 taken between singleparticle basis states.)

For the case of the function $G(t_f) = \det |1 - f + f\sigma|$ [see Eq. (31)] we have

$$G(t_f) = \tilde{G}(t_f) \det |1 + A|b\rangle \langle b|| = \tilde{G}(t_f)(1 + A_B), \quad (A2)$$

where $A_B = \langle b | A | b \rangle$ with

$$A = (1 - f + f\widetilde{\sigma})^{-1} f e^{iH_0 t} e^{-iE_b t}, \tag{A3}$$

and where $\tilde{G}(t_f) = \det |1 - f + f\tilde{\sigma}|$. We write the bound state as an expansion over the basis vectors

$$|b\rangle = \sum_{\epsilon} \mathbf{u}_{\epsilon} \cdot \hat{\mathbf{a}}_{\epsilon}^{\dagger}|\rangle. \tag{A4}$$

For long times t_f the response is dominated by states within $1/t_f$ of the Fermi energy and it is a reasonable approximation to neglect the energy dependence of the coefficients \mathbf{u}_{ϵ} . After switching to the time representation, and using Eq. (49) with $\tilde{\sigma}$ in place of σ , we obtain (ν_l is the density of states in channel l)

$$\langle b|A|b\rangle = \frac{1}{2\pi} e^{-iE_b t_f} \sum_{ll'} \int d\epsilon d\epsilon' \int dt_1 dt_2 u_{l'}^* u_l \times \sqrt{\nu_l \nu_l'} e^{i\epsilon' t_1} [Y_+ f Y_-^{-1}]_{lt_1, l't_2} e^{i\epsilon(t_f - t_2)}.$$
 (A5)

Integrating over energies and times gives

$$A_B \sim e^{-iE_b t_f} u_l \sqrt{\nu_l} \left[Y_+(0) \frac{1}{-it_f} Y_-^{-1}(t_f) \right]_{ll'} u_{l'}^* \sqrt{\nu_{l'}}.$$
 (A6)

Provided S(t) commutes with itself at all times between 0 and t_f , Y is given by Eq. (37). For the single-channel case with $S = e^{2i\tilde{\delta}}$, we obtain

$$\langle b|A|b\rangle \sim \frac{\nu}{it_f} \frac{1}{(i\xi_0 t_f)^{2\tilde{\delta}/\pi}}.$$
 (A7)

Here we introduce the quantity $\tilde{\delta}$, which is the phase shift modulo π and takes values on the interval $[-\pi/2,\pi/2]$. Normally the phase shift δ is defined with a jump of π at a bound state, thereby ensuring compliance with the Friedel sum rule.¹⁹ However, when writing the scattering matrix as in Eq. (A1), the contribution from the bound state to the scattering matrix is explicitly included in the second term on the right-hand side and is not in the scattering matrix *S*. At the bottom of the band, the value of the phase shift that enters the threshold shift is clearly $\tilde{\delta}$ as emphasized in Ref. 10.

Although the calculation is longer, the function $F(t_f)$ can be obtained in a similar manner by replacing σ in Eq. (46) by the form (A1). One needs only to keep track of terms up to first order in $e^{-iE_b t_f}$. [Higher-order terms must give zero as they correspond to double or higher occupancy of the bound state. They can be seen to make no contribution by subsituting the formula (A1) in Eq. (42)].) As for the case of the function $G(t_f)$ considered above, we neglect the energy dependence of \mathbf{W}_{ϵ} and \mathbf{u}_{ϵ} [see Eqs. (29) and (A4)]. We define

$$C_b = (\mathbf{W}^* \cdot \mathbf{u})(\mathbf{u}^* \cdot \mathbf{W})e^{-iE_b t_f}, \qquad (A8)$$

$$\widetilde{O} = (1 - f + f\widetilde{\sigma})^{-1}f.$$
(A9)

Here \tilde{O} is just the scattering state contribution to O [see Eq. (47)]:

$$O \simeq \tilde{O} - \tilde{O}e^{iH_0 t_f} |b\rangle e^{-iE_b t_f} \langle b|\tilde{O}.$$
 (A10)

We obtain [from Eq. (48)]

$$F(t_f) = G(t_f) [C - \langle g | O | h \rangle] \simeq \tilde{G}(t_f) C_b - \tilde{G}(t_f) [1 + A_B] \langle g | O | h \rangle.$$
(A11)

Retaining the dominant terms and ignoring the possibility that there is an unexpected cancellation between terms proportional to $e^{-iE_b t_f}$,

$$F(t_f) = \tilde{G}(t_f)\tilde{L}(t_f) + aC_b\tilde{G}(t_f), \qquad (A12)$$

where $\alpha \sim 1$ is some constant and $\tilde{L}(t_f)$ is the scattering state contribution to the open-line function. For the single-channel case with $S = e^{i2\delta}$, we again assume that the exponent in $\tilde{G}(t_f)$ is $\delta = \delta - \pi$ and obtain $F(t_f) \sim F_b(t_f) + F_0(t_f)$ with

$$F_b(t_f) \sim e^{-iE_b t_f} \frac{1}{(i\xi_0 t_f)^{(\tilde{\delta}/\pi)^2}}, \quad F_0(t_f) \sim \frac{1}{(i\xi_0 t_f)^{(\tilde{\delta}/\pi - 1)^2}}.$$
(A13)

APPENDIX B: COMPUTING SPECTRAL FUNCTIONS

Given $G(t_f)$ or $F(t_f)$ we would like to compute the corresponding spectral functions given by a Fourier integral over t_f . Assume that scattering matrix, S^e , has diagonal elements

 $\sqrt{R}e^{i2\alpha_{1,2}}$. Using the complex cutoff ζV (normally $\zeta = i$), we have from Eq. (64)

$$\ln G(t_f,V) = -i[E_0 - \Delta(V)]t_f - \beta_G \ln(\zeta V t_f) + D. \quad (B1)$$

The exponent $\beta_G = x_+^2 + x_-^2$, where

$$x_{+} = \frac{\ln S_{11}^{e}}{2\pi i} = \frac{\alpha_{1}}{\pi} - i\frac{\ln R}{4\pi}$$
(B2)

and

$$x_{-} = \frac{\ln(1/S_{22}^{e^*})}{2\pi i} = \frac{\alpha_2}{\pi} + i\frac{\ln R}{4\pi}.$$
 (B3)

The modified threshold shift is given by Eq. (65)

$$\Delta(V) = \left(\Delta(0) + V \frac{\alpha_1 - (\ln S^e)_{11}}{\pi}\right) - iV \left(\frac{\ln R}{4\pi}\right).$$
(B4)

The real part of $\Delta(V)$ fixes the threshold. We will absorb this into the definition of frequency when computing Fourier transforms.

We write $\beta_G = \beta_{G1} + i\beta_{G2}$ with

$$\beta_{G1} = \left(\frac{\alpha_1}{\pi}\right)^2 + \left(\frac{\alpha_2}{\pi}\right)^2 - \frac{1}{2}\left(\frac{\ln R}{2\pi}\right)^2 \tag{B5}$$

and

$$\beta_{G2} = -\frac{(\alpha_1 - \alpha_2)}{\pi} \frac{\ln R}{2\pi}.$$
(B6)

For the function $F(t_f)$, the exponent becomes $\beta_F = (x_--1)^2 + x_+^2$ or $\beta_F = x_-^2 + (x_+-1)^2$ depending on whether the electron is added to the electrode with lower or higher chemical potential. This gives $\beta_F = \beta_G - 2x_{\pm} + 1$ and

$$\beta_{F1} = \beta_{G1} - \frac{2\alpha_{1,2}}{\pi} + 1, \quad \beta_{F2} = \beta_{G2} \pm \frac{\ln R}{2\pi}.$$
 (B7)

Introducing

$$\omega_2 = -\ln R/4\pi, \tag{B8}$$

the spectral functions of *G* or *F* are proportional to the real part of the Fourier integral, $\chi_{F,G}(\epsilon)$, where:

$$\chi(\epsilon) = \int_0^\infty dt_f (\zeta V t_f)^{-\beta} e^{(i\epsilon - \omega_2 V) t_f},$$
 (B9)

with $\beta = \beta_F$ for χ_F and β_G for χ_G . Here the lower limit of the integral is taken to be 0, which is only valid when $\beta_1 < 1$. When $\beta_1 > 1$, contributions from the lower limit of the integral dominate and the response is dominated by high-frequency contributions that are not changed from the equilibrium case. These are not described by formula (64) and depend on details relating to the band edge. If the phase shifts x_{\pm} are small, which can be the case for the spectral function of F [or $\tilde{G}A_B$ in the presence of a bound state; see Eqs. (A2) and (A7)], then β_1 will be close to 1. In this case $\chi(\epsilon)$ given in Eq. (B9) contains a significant contribution for $F(t_f)$ (or $\tilde{G}A_B$) is incorrect. We can correct for this by noting that when $1-\beta \ll 1$ the contribution from times with $Vt_f < 1$ gives just a constant offset that can be subtracted from χ . To see this, we expand the exponential term $e^{(i\epsilon-\omega_2 V)t}$ in the integrand and integrate term by term from $Vt_f=0$ to $Vt_f=1$. The first term in the expansion is independent of ϵ and much larger than subsequent terms provided $(\epsilon/V) \ll 1/|1-\beta|$. In practice we subtract from the real part of χ its value at ω $\approx -V$. (When $1-\beta$ is not small the contribution from the times $Vt_f < 1$ to the real part of χ is negligible anyway.)

Equation (B9) is in the form of a standard integral and [see Eq. (8.312.2) in Ref. 41] is given by

$$\chi(\omega_1) = (i\zeta)^{-\beta} \frac{i}{V} \left(\frac{1}{\omega_1 + i\omega_2}\right)^{1-\beta} \Gamma(1-\beta).$$
 (B10)

If we define $\Omega = |\omega_1 + i\omega_2| e^{i\phi_\Omega}$ and write

$$\Gamma(1-\beta) = |\Gamma(1-\beta)|e^{i\phi_{\Gamma}}, \text{ and } i\zeta = e^{i\phi_{\zeta}}, (B11)$$

then

$$\chi(\omega_{1}) = e^{-i\beta_{1}\phi_{\zeta}+\beta_{2}\phi_{\zeta}} \frac{i}{V} \frac{e^{i\beta_{2}\ln\Omega}}{\Omega^{1-\beta_{1}}}$$
$$\times e^{i(\beta_{1}-1)\phi_{\Omega}-\beta_{2}\phi_{\Omega}} |\Gamma(1-\beta)| e^{i\phi_{\Gamma}}. \tag{B12}$$

. . . .

The real part of $\chi(\omega_1)$ can then be written²⁹

$$\operatorname{Re}_{\chi}(\omega_{1}) = \frac{|\Gamma(1-\beta)|}{V} \frac{1}{\Omega^{1-\beta_{1}}} e^{-\beta_{2}(\phi_{\Omega}-\phi_{\zeta})} \\ \times \sin[\beta_{1}(\phi_{\zeta}-\phi_{\Omega}) + (\phi_{\Omega}-\phi_{\Gamma}) - \beta_{2}\ln\Omega].$$
(B13)

For both functions *F* and *G*, the cutoff parameter $\zeta = i$, so $\phi_{\zeta} = \pi$.

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