

# Response of a Fermi gas to time-dependent perturbations: Riemann-Hilbert approach at nonzero temperatures

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We provide an exact finite temperature extension to the recently developed Riemann-Hilbert approach for the calculation of response functions in nonadiabatically perturbed (multichannel) Fermi gases. We give a precise definition of the finite temperature Riemann-Hilbert problem and show that it is equivalent to a zero temperature problem. Using this equivalence, we discuss the solution of the nonequilibrium Fermi-edge singularity problem at finite temperatures.

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## I. INTRODUCTION

The response of a Fermi gas to an external, time-dependent perturbation is a well-known hard problem. It has repeatedly been studied in various contexts, mostly on systems exhibiting the orthogonality catastrophe, Fermi-edge singularities, or the Kondo effect.<sup>1</sup> The technical difficulties are connected to the necessity of summing an infinite number of logarithmically divergent diagrams, and has led to the development of a multitude of methods to tackle this task, including diagram summations, singular integral equation approaches, bosonization, and summation schemes based on Slater determinants.<sup>1</sup> Many of these approaches are technically involved or require assumptions such as, for instance, the separability of the external potential. In addition, the recent controversies concerning nonequilibrium Fermi systems<sup>2</sup> have shown that extensions of these methods are problematic and hard to achieve. A unified approach, depending on a minimum of assumptions is, therefore, desirable.

Very recently, a major step in this direction has been made in the form of the *Riemann-Hilbert approach*,<sup>3,4</sup> and applied to the calculation of Fermi-edge singularities at  $T=0$  in Fermi gases under nonequilibrium constraints.<sup>5</sup> In this approach, the calculation of general response functions in the perturbed Fermi gas is transformed into the problem of solving a (generally non-Abelian) Riemann-Hilbert (RH) boundary value problem: The response functions are rewritten in terms of complex matrix functions  $Y(t)$  that satisfy boundary conditions, for  $\text{Im } t \rightarrow \pm 0$ , expressed by a matrix function  $R(t)$ . In most cases of interest,  $R(t)$  is directly related to the scattering matrix of the time-dependent potential.

In this paper, we extend the RH technique to finite temperatures. We first give a precise definition of the finite temperature RH problem. We then show that the finite temperature problem is equivalent to a different zero temperature RH problem through the bijective mapping of the time variable  $t \rightarrow \tanh[(\pi/\beta)t]$ , with  $\beta=1/k_B T$ . In simple (i.e., Abelian) cases, this allows us to construct the explicit solution, but generally the resulting RH problem remains highly non-trivial. We show, however, on the concrete example of the nonequilibrium problem of Refs. 3–5 how the equivalence between finite and zero temperature solutions can be ex-

plored to construct approximate solutions to the corresponding RH problem in the high and low temperature limits.

The paper is organized as follows: In Sec. II, we summarize the essential steps in the zero temperature RH approach. In Sec. III, the finite temperature RH problem is defined, and the equivalence to the zero temperature case is shown. Finally, in Sec. IV, we discuss the finite temperature extensions for some simpler examples and for the nonequilibrium Fermi-edge singularity problem discussed in Refs. 3–5.

## II. ZERO TEMPERATURE CASE

We start with the introduction of the required concepts and notations for the zero temperature RH approach, following Ref. 4.

The approach has been developed for the calculation of response functions in a nonadiabatically perturbed system of fermions. We consider a gas of noninteracting fermions that is exposed to a time-dependent potential  $M$ . The Hamiltonian is assumed to take the form

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

$$\hat{H}_0 = \sum_{\epsilon} \epsilon \mathbf{a}_\epsilon^\dagger \mathbf{a}_\epsilon, \quad (1)$$

where  $\epsilon$  labels the single-particle energies of the electrons, and  $\mathbf{a}_\epsilon^\dagger$  is a vector of the electron operators  $a_{\epsilon,j}^\dagger$ , where  $j=1, \dots, N$  is a channel index labeling any further classification of the single particle states. The potential  $M(t, \epsilon, \epsilon')$  is a  $N \times N$  matrix in channel space, which we assume to be non-zero only for some finite time interval  $0 < t < t_f$ , during which the external perturbation is switched on.

The quantities of interest are response functions of the type

$$\chi_R = \langle \hat{R} \rangle. \quad (2)$$

At zero temperature,  $\langle \dots \rangle$  denotes the average over the ground state  $|0\rangle$ ; at finite temperatures, as considered in Sec. III, it represents the thermal average over the noninteracting system states at  $t=0$ . The operator  $\hat{R}$  is related to the time-

evolution operators  $\hat{U}(t_f)$  and  $\hat{U}_0(t_f)$  of  $\hat{H}(t)$  and  $\hat{H}_0$ , respectively, or equivalently to the scattering matrix  $S$  for the potential  $M$ . For the present discussion, the precise form of  $\hat{R}$  is unimportant. A summary of necessary conditions on  $\hat{R}$  is given in Appendix A, while a detailed discussion can be found in Refs. 3, 4, and 6; some examples are given at the end of this paper.

Since the Hamiltonian is quadratic in the electron operators, the action of the many-body operator  $\hat{R}$  is fully specified by its action on single-particle states (see the Appendices). Let  $R = \{R_{j,j'}(\epsilon, \epsilon')\}$  be the matrix formed of the matrix elements of  $\hat{R}$  between the single-particle states  $(j, \epsilon)$ ,  $R_{j,j'}(\epsilon, \epsilon') = \langle a_{\epsilon,j} \hat{R} a_{\epsilon',j'} | \rangle$ , with  $| \rangle$  the true vacuum. For the following treatment, it is essential to assume that  $R$  is diagonal in the time representation,  $R = R(t)$  (with  $t$  the variable conjugated to the energy representation  $\epsilon$ ). For the response functions relevant for Fermi-edge singularity problems, it can be shown<sup>3,4,6</sup> (see Appendix A) that this assumption is valid as long as the variation of the scattering matrix is slow compared to the delay time of the scattering process itself.

For the noninteracting system,  $|0\rangle$  is a Slater determinant in the single particle states. As shown in Appendix B, we can write

$$\chi_R = \det[(1-f) + fR], \quad (3)$$

where  $R$  represents the matrix elements of  $\hat{R}$  taken between the single-particle states, and  $f$  is the Fermi function, which has the matrix elements

$$f_{j,j'}(\epsilon, \epsilon') = \delta_{\epsilon\epsilon'} \delta_{j,j'} \theta(-\epsilon). \quad (4)$$

In this expression, we have set the chemical potential  $\mu$  to zero. This is possible without loss of generality even in the nonequilibrium case of several Fermi seas  $j$  with different chemical potentials  $\mu_j$ , such as for biased tunneling barriers. For the unperturbed system with uncoupled Fermi seas, we can shift the single-particle energies by  $\epsilon \rightarrow \epsilon - \mu_j$  and set all chemical potentials to zero. In other words, the fermion operators are replaced by  $a_{\epsilon,j} \rightarrow e^{i\mu_j t} a_{\epsilon,j}$ . The Hamiltonian keeps the same form except that the potential  $M(t)$ , and thus  $R(t)$ , acquires an additional dependence on time,<sup>3</sup>  $R_{j,j'}(t) \rightarrow R_{j,j'}(t) e^{i(\mu_j - \mu_{j'})t}$ .

The logarithm of the determinant in Eq. (3) can be written in the form

$$\ln \chi_R = \text{Tr}[f \ln R] + \text{Tr}[\ln(1-f+fR) - f \ln R] \equiv \ln \chi_R^{(1)} + \ln \chi_R^{(2)}, \quad (5)$$

with  $\text{Tr}$  being the trace over channel indices  $j$  and energy.  $\ln \chi_R^{(1)} = \text{Tr}[f \ln R]$  consists of the diagonal terms of  $\ln R$  summed over the occupied states of the unperturbed system. Depending on the system under investigation, it expresses, for instance, a shift of the ground state or threshold energy (Fumi's theorem<sup>7</sup> if  $R$  is the scattering matrix) together with an imaginary correction for nonequilibrium conditions,<sup>5</sup> or the average transfer of charge across a barrier.<sup>3</sup> The second term,  $\ln \chi_R^{(2)}$ , contains the nontrivial effects close to the Fermi surface which are, for instance, associated with Fermi-edge

singularities. In the following, we will focus on  $\ln \chi_R^{(2)}$  only.

It is convenient to switch from the energy representation to the time representation of the trace, in which  $R$  is diagonal. The Fermi function, however, becomes nondiagonal in time and reads

$$f_{j,j'}(t, t') = \frac{i/2\pi}{t-t'+i0} \delta_{j,j'}. \quad (6)$$

(Here and henceforth we set  $\hbar=1$ .) The logarithm of an infinite matrix is represented by introducing a dependence on a parameter  $\lambda$  as

$$R \rightarrow R(\lambda) = \exp(\lambda \ln R), \quad (7)$$

and by writing

$$\ln \chi_R^{(2)} = \int_0^1 d\lambda \int dt \text{tr} \left[ [(1-f+fR)^{-1} f - fR^{-1}] \frac{dR}{d\lambda} \right], \quad (8)$$

where  $\text{tr}$  denotes the trace over the channel index  $j$  only.

The difficult task is to find the inverse of  $(1-f+fR)$ . For this, a complex  $N \times N$  matrix function  $Y(t)$  is introduced, which solves an auxiliary *RH problem*, defined by:

(a)  $Y(t)$  is a nonsingular  $N \times N$  matrix function, which is analytic and nonzero in the complex plane, except on the interval  $(0, t_f)$ , where it satisfies the boundary condition

$$Y_-(t) Y_+^{-1}(t) = R(t), \quad (9)$$

for  $Y_{\pm}(t) = Y(t \pm i0)$ , and except at the end points  $t_e=0, t_f$ , where  $Y(t)$  may vanish or be weakly singular as  $|Y(t)| \sim |t - t_e|^{\epsilon}$  for  $-1 < \epsilon < 1$ ,  $\epsilon \neq 0$ .

(b)  $Y(t)$  has the asymptotic condition

$$Y(t) \rightarrow 1 \quad \text{when } |t| \rightarrow \infty. \quad (10)$$

From these two properties, two important identities follow:

$$f Y_+ f = Y_+ f, \quad (11)$$

$$f Y_- f = f Y_-, \quad (12)$$

which equally hold if  $Y$  is replaced by  $Y^{-1}$ . In the time representation, Eq. (11) reads

$$\int dt \frac{i/2\pi}{t_1 - t + i0} Y_+(t) \frac{i/2\pi}{t - t_2 + i0} = Y_+(t_1) \frac{i/2\pi}{t_1 - t_2 + i0}, \quad (13)$$

which is proved by closing the contour in the upper half-plane. A similar contour in the lower half-plane proves Eq. (12).

In terms of the functions  $Y_{\pm}$ , the inverse of  $(1-f+fR)$  is expressed by

$$(1-f+fR)^{-1} = Y_+ [(1-f) Y_+^{-1} + f Y_-^{-1}], \quad (14)$$

which can be verified by multiplication by  $(1-f+fR)$  from the right or left, and by making use of the identities (11) and (12).

Finally, the following result

$$\begin{aligned} \int dt \operatorname{tr}\{[A, f]B\} &= \int dt \lim_{t' \rightarrow t} \operatorname{tr} \frac{i}{2\pi} \left[ \frac{A(t) - A(t')}{t - t' + i0} \right] B(t') \\ &= \frac{i}{2\pi} \int dt \operatorname{tr} \left\{ \frac{dA(t)}{dt} B(t) \right\} \end{aligned} \quad (15)$$

for any differentiable matrix functions  $A$  and  $B$ , allows us to write Eq. (8) in the compact form

$$\ln \chi_R^{(2)} = \frac{i}{2\pi} \int_0^1 d\lambda \int dt \operatorname{tr} \left\{ \frac{dY_+}{dt} Y_+^{-1} R^{-1} \frac{dR}{d\lambda} \right\}. \quad (16)$$

The response function  $\chi_R^{(2)}$ , therefore, is fully expressed in terms of the solution  $Y(t)$  of the RH problem.

### III. FINITE TEMPERATURE CASE

We show in this section that we can define a finite temperature version of the RH problem such that the important formula (14) [and, therefore, Eq. (16)] remains valid. Subsequently, we show that this new RH problem is equivalent to a zero temperature RH problem.

#### A. Finite temperature RH problem

Note that Eq. (14) remains valid if we generalize the identities (11) and (12) to

$$fY_+f = Y_+f + F, \quad (17)$$

$$fY_-f = fY_- + F, \quad (18)$$

with the same  $F = F(t, t')$ , a (finite) matrix function, appearing in both identities.

At finite temperatures  $T$ , the Fermi function becomes

$$f(t, t') = \frac{i/2\pi}{\frac{\beta}{\pi} \sinh\left(\frac{\pi}{\beta}(t - t') + i0\right)}, \quad (19)$$

with  $\beta = 1/k_B T$ . With this function, Eq. (17) reads explicitly

$$\begin{aligned} \int_{-\infty}^{\infty} dt \frac{i/2\beta}{\sinh\left(\frac{\pi}{\beta}(t_1 - t + i0)\right)} Y_+(t) \frac{i/2\beta}{\sinh\left(\frac{\pi}{\beta}(t - t_2 + i0)\right)} \\ = Y_+(t_1) \frac{i/2\beta}{\sinh\left(\frac{\pi}{\beta}(t_1 - t_2 + i0)\right)} + F(t_1, t_2). \end{aligned} \quad (20)$$

The Fermi function is antiperiodic in the imaginary time direction,  $f(t + i\beta, t') = -f(t, t')$ . If we impose that Eqs. (17) and (18) are invariant under such transformations,  $Y(t)$  and  $F(t, t')$  must be (anti)periodic in the imaginary time direction as  $Y(t + i\beta) = Y(t)$  and  $F(t + i\beta, t') = F(t, t' + i\beta) = -F(t, t')$ . This allows us to restrict the analysis to the strip  $-\beta/2 < \operatorname{Im} t < \beta/2$ .

The *finite temperature RH problem* can then be formulated as follows:

(i)  $Y(t)$  is a nonsingular  $N \times N$  matrix function, which is analytic in the strip  $\mathcal{S}_\beta = \{t \in \mathbb{C} | -\beta/2 < \operatorname{Im} t < \beta/2\}$ , except

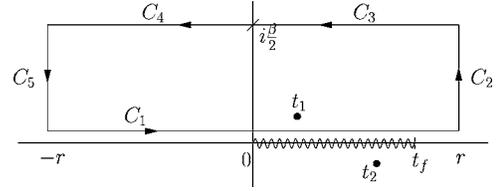


FIG. 1. Integration contour in the  $t$  plane. The wiggled line indicates the branch cut for  $Y(t)$ , the isolated dots the poles of the integrand. The limit  $r \rightarrow \infty$  is assumed.

on the interval  $(0, t_f)$ , where it satisfies Eq. (9), and except at the end points  $t_e = 0, t_f$ , where it may vanish or be weakly singular as  $|Y(t)| \sim |t - t_e|^\varepsilon$  with  $-1 < \varepsilon < 1$ ,  $\varepsilon \neq 0$ .

(ii)  $Y(t)$  tends to definite finite values as  $|t| \rightarrow \infty$  in  $\mathcal{S}_\beta$  (the values on the far right or far left, however, are generally different).

(iii)  $Y(t)$  can be analytically continued through  $t \pm i\beta/\pi$ , for real  $t$ , such that  $Y(t + i\beta/2) = Y(t - i\beta/2)$ . For convenience, we normalize  $Y(t)$  (by multiplication by a constant matrix from the right) such that  $Y(\pm i\beta/2) = 1$ .

Condition (iii) is absent in the zero temperature case, but is essential for the validity of Eqs. (17) and (18).

Indeed, let us first focus on Eq. (17). We integrate  $fY_+f$  over the contour  $C = C_1 + \dots + C_5$  shown in Fig. 1. In the figure,  $r$  is a large number, which we eventually send to infinity. Since  $Y(t)$  remains bounded as  $|t| \rightarrow \infty$ , the integrals over the vertical lines  $C_2$  and  $C_5$  vanish in this limit, and we obtain Eq. (17) with  $F$  given by the integral of  $fY_+f$  over the line through  $i\beta/2$ , parallel to the real axis.

A similar contour in the lower part of  $\mathcal{S}_\beta$  leads to Eq. (18), with  $F$  given by the integral over the line through  $-i\beta/2$ , parallel to the real axis. Both integrals for  $F$  are identical due to the periodicity and analyticity of  $Y(t)$ , and Eqs. (17) and (18) are fulfilled.

The solution of the finite temperature RH problem, together with Eqs. (17) and (18), immediately leads to the solution for the response function  $\chi_R$  by means of Eq. (16). [Note that Eq. (15) remains true when replacing  $(t - t')^{-1}$  by  $\{(\beta/\pi) \sinh[\pi(t - t')/\beta]\}^{-1}$ .]

#### B. Equivalence to zero temperature case

The finite temperature RH problem, defined by conditions (i)–(iii), is equivalent to the RH problem at zero temperature, defined by conditions (a) and (b), upon a redefinition of the boundary condition (9).

The equivalence is shown by means of the mapping

$$t \mapsto w = \tanh\left(\frac{\pi}{\beta}t\right), \quad (21)$$

which is often used to switch between zero and finite temperatures, and which describes a bijection between the strip  $\mathcal{S}_\beta$  and the slit plane  $\mathcal{S} = \{w \in \mathbb{C} | w \notin (-\infty, -1], w \notin [1, \infty)\}$ . Let us set  $\tilde{Y}(w) = Y(t)$  for  $w = \tanh[(\pi/\beta)t]$ .

(1) The boundary condition (9) for  $Y(t)$  and  $t \in (0, t_f)$  becomes a boundary condition of the same type (9) for  $\tilde{Y}(w)$

and  $w \in (0, w_f)$ ,  $0 < w_f = \tanh[(\pi/\beta)t_f] < 1$ , and the matrix  $\tilde{R}(w) = R(t)$ .

(2) The analyticity of  $Y(t)$  in  $\mathcal{S}_\beta \setminus [0, t_f]$  ensures the analyticity of  $\tilde{Y}(w)$  in  $\mathcal{S} \setminus [0, w_f]$ . The periodicity  $Y(t + i\beta/2) = Y(t - i\beta/2)$  for real  $t$  is nothing but the condition of analyticity of  $\tilde{Y}(w)$  through the real axis at  $|w| > 1$ .

(3)  $t = \pm i\beta/2$  maps onto infinity in the  $w$  plane. With the normalization  $Y(\pm i\beta/2) = 1$ , we have  $\tilde{Y}(w) \rightarrow 1$  as  $|w| \rightarrow \infty$ . On the other hand, the boundedness of  $Y(t)$  as  $|t| \rightarrow \infty$  in  $\mathcal{S}_\beta$  implies that  $\tilde{Y}(w)$  is finite at  $w = \pm 1$ .

This proves that the zero and finite temperature versions of the RH problem are equivalent, upon the change of boundary condition  $R(t) \rightarrow \tilde{R}(w) = R(t)$ .

With the mapping, the identities (17) and (18) are mapped onto (11) and (12), too. The infinite  $t$  integrals over the real axis map onto  $(-1, 1)$  in the  $w$  plane (including the cut  $[0, w_f]$ ), while the integrals over the contours  $C_3$  and  $C_4$  provide the remaining parts of the real axis in the  $w$  plane,  $(1, \infty)$  and  $(-\infty, -1)$ , respectively, at which  $\tilde{Y}(w)$  is analytic. The integrands can be identified through the formula

$$\sinh\left(\frac{\pi}{\beta}(t - t')\right) = \cosh\left(\frac{\pi}{\beta}t\right) \cosh\left(\frac{\pi}{\beta}t'\right) (w - w'). \quad (22)$$

The dependence on  $\cosh[(\pi/\beta)t]$  in the integrand cancels with  $dw/dt = (\pi/\beta)/\cosh^2[(\pi/\beta)t]$ . After factorization of  $(\pi/\beta)\cosh[(\pi/\beta)t_1]\cosh[(\pi/\beta)t_2]$ , we see that Eqs. (17) and (18) are identical to (11) and (12).

#### IV. EXAMPLES

A solution to the finite temperature RH problem allows the calculation of the response function (16). We illustrate this with a few simpler examples of how the equivalence to the zero temperature RH problem can be used to construct explicit finite temperature solutions. We then discuss approximate finite temperature solutions for the nonequilibrium RH problem of Ref. 5.

##### A. Some simpler examples

The RH problem appeared early in the study of Fermi-edge singularities. It is part of the solution of the Dyson equation for the Green's function, formulated by Nozières and De Dominicis as a singular integral equation,<sup>8</sup> for which the standard method of solution consists in the transformation into a RH problem.<sup>9</sup> In Nozières and De Dominicis' case, the boundary condition  $R$  is a constant, for  $t \in (0, t_f)$ , given by the single-particle single-channel scattering matrix  $R = S = e^{-2i\delta}$ , where  $\delta$  is the scattering phase shift ( $|\delta| < \pi/2$ ). The solution is given by

$$Y(t) = [(t - t_f)/t]^{\delta/\pi}. \quad (23)$$

The finite temperature extension to this expression was achieved by Yuval and Anderson<sup>10</sup> in their application of the Nozières-De Dominicis approach to the Kondo problem. It resulted from writing  $1/\sinh(\pi t/\beta)$ , the free Green's func-

tion in the kernel of the integral equation, as the sum of  $(-1)^n/(t + in\beta)$  over integer  $n$  in the kernel of the integral equation. The corresponding RH problem becomes the product of zero-temperature RH problems with branch cuts shifted by  $in\beta$ . Hence, the finite temperature solution found by Yuval and Anderson reads

$$Y(t) = \prod_n \left( \frac{t - t_f + in\beta}{t + in\beta} \right)^{\delta/\pi} = \left[ \frac{\sinh\left(\frac{\pi}{\beta}(t - t_f)\right)}{\sinh\left(\frac{\pi}{\beta}t\right)} \right]^{\delta/\pi}. \quad (24)$$

With the replacement  $t \rightarrow \tanh[(\pi/\beta)t]$  in Eq. (23) and the use of Eq. (22), this solution can immediately be verified, as constant matrices  $R$  and  $\tilde{R}$  coincide. Note that with the mapping we obtain an additional constant factor  $\cosh[(\pi/\beta)t_f]^{\delta/\pi}$ , reflecting the fact that a solution of the RH problem remains a solution upon multiplication by a constant matrix from the right. With our normalization (iii) this factor is suppressed. Such constants are unimportant since they drop out in the physical solution (16).

Equations (23) and (24) remain valid if  $R$  is a time-independent diagonalizable matrix. In this case,  $\delta$  becomes a matrix with eigenvalues representing the phase shifts of the multichannel scattering matrix  $R$ .

For scalar, but time-dependent  $R(t)$ , the solution of the RH problem can be constructed in a standard way,<sup>9</sup> and is given by

$$Y(t) = \exp\left(\frac{1}{2\pi i} \int_0^{t_f} dt' \frac{\ln R(t')}{t' - t}\right). \quad (25)$$

At finite temperatures, the mapping allows here the explicit solution, too, which has the same form as the previous equation, with  $R$  replaced by  $\tilde{R}$ ,

$$Y(t) = \exp\left(\frac{1}{2\pi i} \int_0^{\tanh[(\pi/\beta)t_f]} dw' \frac{\ln \tilde{R}(w')}{w' - \tanh\left(\frac{\pi}{\beta}t\right)}\right) = \exp\left(\frac{1}{2\beta i} \int_0^{t_f} dt' \frac{\cosh\left(\frac{\pi}{\beta}t\right)}{\cosh\left(\frac{\pi}{\beta}t'\right)} \frac{\ln R(t')}{\sinh\left(\frac{\pi}{\beta}(t' - t)\right)}\right). \quad (26)$$

Notice that all these expressions become singular at  $t \rightarrow 0$  or  $t \rightarrow t_f$ . These divergences are spurious and due to the approximation of an infinite bandwidth (given by the form of the Fermi function), and have a natural cutoff in the true inverse bandwidth,<sup>8</sup>  $1/\xi$ .

In these simple examples, the response function (16) can explicitly be calculated. Let us, for instance, consider Eq. (24). Since  $S^{-1}(dS/d\lambda) = -2i\delta$ , we obtain

$$\begin{aligned} \ln \chi_R^{(2)}(t_f) &= \frac{\text{tr}\{\delta^2\}}{2\pi^2} \int_0^{t_f} dt \frac{d}{dt} \ln \left[ \frac{\sinh\left(\frac{\pi}{\beta}(t-t_f+i0)\right)}{\sinh\left(\frac{\pi}{\beta}t+i0\right)} \right] \\ &= -\frac{\text{tr}\{\delta^2\}}{\pi^2} \ln \left[ \frac{\sinh(\pi t_f/\beta)}{\sinh(\pi/\beta\xi)} \right], \end{aligned} \quad (27)$$

again with the cutoff at the inverse bandwidth  $1/\xi$ . For short times  $t_f \ll \beta$ , we obtain a power-law similar to the well known zero temperature result  $\chi_R^{(2)}(t_f) \sim t_f^{-\delta^2/\pi^2}$ , which, however, crosses over into an exponential decay as  $t_f \gg \beta$ ,  $\chi_R^{(2)}(t_f) \sim e^{-(\delta^2/\pi\beta)t_f}$ .

### B. Biased tunneling barriers

As a more involved example, let us consider the non-Abelian RH problem, in which  $R(t)$  is a time-dependent matrix that does not allow a time-independent diagonalization. Such situations naturally arise in nonequilibrium systems, and have recently been studied with the RH approach:<sup>4,5</sup> Consider, for instance, the coupling between a defect state in a tunneling barrier and the connecting electrodes that are kept at a voltage bias  $V$ . The defect is assumed to be either in its ground state  $g$  or in an excited state  $e$ . We further assume that in the ground state the defect is fully screened and does not interact with the conduction electrons, whereas in the excited state it acts on the conduction electrons through the potential  $M$ . The diagonal matrix elements of this potential describe the scattering of the electrons in the electrodes, while the nondiagonal matrix elements represent a modification of the tunneling rate. The matrix  $R=S$  is the scattering matrix for  $M$ . The response function  $\chi_R(t=t_f-0)$  is related to the transition rate of the defect into the excited state,  $p_{g \rightarrow e}(\Delta E)$ , by

$$p_{g \rightarrow e}(\Delta E) = |u|^2 \int_0^\infty dt \chi_R(t) e^{i\Delta E t}, \quad (28)$$

which is the Golden Rule expression rewritten as a time integral.  $\Delta E$  is the bare energy difference between ground state and excited state of the defect, and  $u$  is the bare amplitude in the Hamiltonian for the transition  $g \rightarrow e$ .

A closed solution to the resulting time-dependent RH problem is not known. In the short time limit  $t \ll 1/V$  and in the long time limit  $t \gg 1/V$ , however, it is possible to construct approximate solutions.<sup>3-5</sup> We first give an example for such an approximation at zero temperature, and then discuss how it extends to finite temperatures.

#### 1. Zero temperature case

In the nonequilibrium Fermi-edge singularity problem,<sup>4,5</sup>  $R(t)$  is a unitary time-dependent scattering matrix coupling two Fermi liquids,  $j=1$  and  $j=2$ , at the left and at the right of a tunneling barrier. The nonequilibrium constraint is introduced by a finite voltage bias  $V$ , keeping the left and right chemical potentials at the values  $\mu_1=V+\mu$  and  $\mu_2=\mu$ , respectively (the electronic charge  $e$  is set to unity). As noted

in Sec. II, we can shift  $\mu_{1,2}$  to 0 in the unperturbed system by passing to the interaction representation  $\hat{H}_0 \rightarrow \tilde{H}_0 = \hat{H}_0 - \mu_1 \hat{N}_1 - \mu_2 \hat{N}_2$ , where  $\hat{N}_{1,2}$  are the number operators for the electrons in the electrodes 1 and 2. This is equivalent to a gauge transformation, transforming the electron operators as  $a_{\epsilon,j} \rightarrow \tilde{a}_{\epsilon,j} = e^{i\mu_j t} a_{\epsilon,j}$ . The voltage difference now appears only as an additional time-dependent phase factor in the matrix elements of  $R(t)$  that couple electrodes 1 and 2

$$R(t) = \begin{pmatrix} R_{11} & e^{iVt} R_{12} \\ e^{-iVt} R_{21} & R_{22} \end{pmatrix}, \quad (29)$$

where  $R_{11}$  and  $R_{22}$  are the backscattering matrix elements, and  $R_{12}$  and  $R_{21}$  describe transmission through the barrier. For  $V=0$ , the scattering matrix  $R$  is time-independent during  $(0, t_f)$ , and the explicit solution of the RH problem is given by Eq. (23), with  $\delta$  the matrix of phase shifts,  $R = \exp(-2i\delta)$ .

If  $V \neq 0$ , an explicit solution to the RH problem is not known. The naive solution, obtained by multiplication of Eq. (23) by  $V$ -dependent phase factors  $\exp(\pm iVt)$  would solve Eq. (9) but violate condition (b), expressed by Eq. (10), because of the divergence of  $\exp(\pm iVt)$  for large complex-valued arguments  $t$ . Such a divergence cannot be compensated by multiplication by  $t$ -dependent analytic matrix functions from the right. The solution (16) would become invalid. An approximate solution, however, can be constructed as follows:<sup>3-5</sup> For  $V > 0$ , we decompose  $R(t)$  into the product

$$R(t) = \begin{pmatrix} 1 & 0 \\ \alpha/z & 1 \end{pmatrix} \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \begin{pmatrix} 1 & \alpha'z \\ 0 & 1 \end{pmatrix}, \quad (30)$$

with  $z = \exp(iVt)$ ,  $a = R_{11}$ ,  $b = \det R / R_{11} = 1/R_{22}^*$ ,  $\alpha = R_{21}/R_{11}$ , and  $\alpha' = R_{12}/R_{11}$ . Now define the function

$$\psi(t) = \exp\left(\frac{\ln D}{2\pi i} \ln \left[ \frac{t}{t-t_f} \right]\right), \quad (31)$$

where  $D = \text{diag}(a, b)$ . This function satisfies the boundary condition

$$\psi_-(t) \psi_+^{-1}(t) = D \quad (32)$$

at  $t \in (0, t_f)$ . To approximate the unknown solution  $Y(t)$ , we consider the following function  $W(t)$ :

$$W_1(t) = \psi(t), \quad W_2(t) = \begin{pmatrix} 1 & -\alpha'z \\ 0 & 1 \end{pmatrix} \psi(t),$$

$$W_3(t) = \begin{pmatrix} 1 & 0 \\ \alpha/z & 1 \end{pmatrix} \psi(t), \quad W_4(t) = \psi(t), \quad (33)$$

where the functions  $W_s$  are defined in the regions  $s = 1, \dots, 4$  indicated in Fig. 2(a).  $W$  has branch cuts between the boundaries of all four regions  $s$ . Most importantly, between regions  $s=2$  and  $s=3$ , it satisfies

$$W_3(t) W_2^{-1}(t) = W_-(t) W_+^{-1}(t) = R(t). \quad (34)$$

Furthermore,  $W(t) \rightarrow 1$  as  $|t| \rightarrow \infty$ . Hence  $W(t)$  satisfies the conditions (a) and (b) of the RH problem, at the price of the

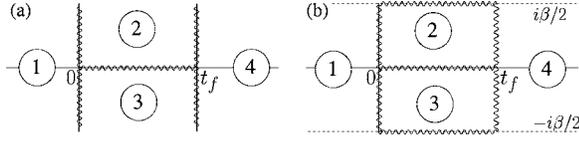


FIG. 2. Regions  $s=1, \dots, 4$  of definition of the functions  $W_j$  [Eq. (33)]. Branch cuts are indicated by the wiggled lines. (a) Zero temperature case. (b) Modification for finite temperatures with additional branch cuts at  $\text{Im } t = \pm \beta/2$ .

additional vertical branch cuts through 0 and  $t_f$ . These branch cuts, however, become exponentially small,  $\propto e^{-V|t|}$ , with increasing distance to the real time axis. For instance, consider the vertical cut at  $\text{Re } t=0$  in the upper half-plane. We have

$$W_2(t)W_1^{-1}(t) = \begin{pmatrix} 1 & -\alpha' e^{-V|t|} \\ 0 & 1 \end{pmatrix} \psi(t)\psi^{-1}(t) = 1 + O(e^{-V|t|}). \quad (35)$$

Similar exponential suppressions hold for the remaining vertical cuts. Therefore,  $Y(t) \equiv W(t)$  is a good approximation to the solution of the RH problem if we consider times  $t$  such that  $|t|, |t-t_f| \gg 1/V$ . Notice that in the boundary condition (32) only  $a=R_{11}$  and  $b=1/R_{22}^*$  are involved, the matrix elements of backscattering into the left electrode at  $\mu_1=V+\mu$  and into the right electrode at  $\mu_2=\mu$ . This reduction of the full scattering matrix can be explained in a simple picture based on the uncertainty relation: For long times  $t \gg 1/V$ , the energy uncertainty  $\Delta\epsilon$  of the scattered particles is smaller than the voltage,  $\Delta\epsilon \ll V$ . The Fermi surface of the other electrode, therefore, is not seen by the scattered particle, and only the backscattering part of the scattering matrix is of importance. For the left electrode, this is  $R_{11}$ , while for the right electrode, the Pauli principle forbids virtual trajectories into the left electrode. After removal of these, the scattering amplitude becomes  $R_{22} - R_{21}R_{11}^{-1}R_{12} = 1/R_{22}^*$ .

Since  $R_{11}$  and  $R_{22}$  alone are not unitary the real phase shifts  $\delta$  are replaced by complex numbers. The implications, mainly, a broadening of the Fermi-edge singularity, are shortly discussed below. For more details we refer to Refs. 4 and 5.

In the limit  $|t|$  or  $|t-t_f| \ll 1/V$ , on the other hand, nonequilibrium constraints play no major role, and the equilibrium expression (23) is expected to become appropriate. This indeed is confirmed by the same argument of the uncertainty relation: For small times,  $t \ll 1/V$ , the energy uncertainty  $\Delta\epsilon$  of the scattered particles becomes large,  $\Delta\epsilon \gg V$ , and both Fermi surfaces at  $\mu_1$  and  $\mu_2$  are coupled. The full scattering matrix is involved.

## 2. Low temperatures: $k_B T \ll V$

Let us focus now on low temperatures,  $k_B T \ll V$ . An approximate solution to  $Y(t)$  to the RH problem can be constructed in the same way as for the zero temperature case: We decompose  $R(t)$  according to Eq. (30), and consider the RH problem for  $\psi(t)$ , described by Eq. (32). Since this problem is diagonal with a time-independent boundary condition, it can be exactly solved by the mapping on the zero-

temperature problem. Its solution is given by Eq. (24) with  $-\delta/\pi$  replaced by  $\ln D/2i\pi$ ,

$$\psi(t) = \exp \left( \frac{\ln D}{2\pi i} \ln \left[ \frac{\sinh\left(\frac{\pi}{\beta}t\right)}{\sinh\left(\frac{\pi}{\beta}(t-t_f)\right)} \right] \right). \quad (36)$$

The function  $W(t)$  is given by the same conditions (33) as before, but where the regions  $s=1, \dots, 4$  now are defined in the strip  $\mathcal{S}_\beta$ , with additional branch cuts at  $\text{Im } t = \pm \beta/2$  [see Fig. 2(b)]. The validity of the approximation on the vertical branch cuts remains unchanged from the zero temperature case, and corresponds to  $|t|, |t-t_f| \gg 1/V$ . On the additional horizontal cut,  $W_2(t+i\beta/2)$  and  $W_3(t-i\beta/2)$  differ in their nondiagonal parts, which are of the order of  $e^{-\beta V/2}$ . This leads to corrections for the identities (11) and (12) of the form

$$\begin{aligned} fW_+f &= W_+f + F_0 + e^{-\beta V/2}F_+, \\ fW_-f &= fW_- + F_0 + e^{-\beta V/2}F_-, \end{aligned} \quad (37)$$

where  $F_0$  is the integral over all coinciding parts of  $fWf$  along  $\text{Im } t = \pm \beta/2$ .  $F_+ \neq F_-$  are the contributions due to the mismatch of  $W_2$  and  $W_3$ . Both  $F_+$  and  $F_-$  are finite quantities of the order of unity. Since  $\beta \gg 1/V$ , their contribution is negligible compared with the error arising from the vertical cuts.

On the other hand, for  $|t-t_f|, |t| \ll 1/V \ll \beta$ , the voltage (i.e., the nonequilibrium situation) as well as the temperature become unimportant. The solution to the RH problem, therefore, is that of a zero temperature equilibrium system, expressed by Eq. (23).

## 3. High temperatures: $k_B T \gg V$

At high temperatures,  $k_B T \gg V$ , we expect that  $V$  plays no longer an important role. Indeed, since  $\beta V \ll 1$ , the naive solution of the RH problem

$$Y(t) = \begin{pmatrix} 1 & e^{iVt} \\ e^{-iVt} & 1 \end{pmatrix} \left( \frac{\sinh\left(\frac{\pi}{\beta}t\right)}{\sinh\left(\frac{\pi}{\beta}(t-t_f)\right)} \right)^{\delta/\pi} \quad (38)$$

now becomes accurate. Because of the restriction of  $t$  to the strip  $\mathcal{S}_\beta$ ,  $Y(t)$  cannot diverge exponentially, so that  $|Y(t)|$  remains bounded as  $|t| \rightarrow \infty$  in  $\mathcal{S}_\beta$ . Yet, Eq. (38) violates the condition of periodicity,  $Y(t+i\beta/2) \neq Y(t-i\beta/2)$  due to the exponentials  $e^{\pm iVt}$ . Again, this leads to different integrals  $F$  from the integration along  $t+i\beta/2$  and  $t-i\beta/2$ , respectively. Since  $\beta V \ll 1$ , however, we can expand the exponential functions, and we are led to similar identities as before

$$\begin{aligned} fY_+f &= Y_+f + \tilde{F}_0 + \beta V \tilde{F}_+, \\ fY_-f &= fY_- + \tilde{F}_0 + \beta V \tilde{F}_-, \end{aligned} \quad (39)$$

with  $\tilde{F}_\pm$  of the order of unity. The solution  $Y$ , and hence the inverse of the matrix, which is solved by the RH problem, as

well as the logarithm of the response function are accurate within corrections of the order of  $\beta V$ .

#### 4. Nonequilibrium Fermi-edge singularities

The results above allow us to extend the nonequilibrium Fermi-edge singularity problem to finite temperatures. We consider the case where  $R(t)$  has the form given in Eq. (29) with  $R=S=e^{-2i\delta}$ .

The high temperature limit leads to an expression, which is unchanged from the equilibrium result (27). At lower temperatures  $k_B T \ll V$ , on the other hand, we can use the approximation  $Y(t) \approx W(t)$  for  $|t|, |t-t_f| \gg 1/V$ . With these functions and the decomposition of  $R$  in Eq. (30), the matrix products in Eq. (16) can be evaluated to

$$\text{tr} \left\{ \frac{dY_+}{dt} Y_+^{-1} R^{-1} \frac{dR}{d\lambda} \right\} = g(t) \frac{d}{d\lambda} \frac{\text{tr}\{(\ln D)^2\}}{2\pi i} - iVC(\lambda), \quad (40)$$

where

$$g(t) = \frac{d}{dt} \ln \left[ \frac{\sinh\left(\frac{\pi}{\beta}(t+i0)\right)}{\sinh\left(\frac{\pi}{\beta}(t-t_f+i0)\right)} \right], \quad (41)$$

and  $C(\lambda)$  is a time-independent function of  $\lambda$ . The term proportional to  $C(\lambda)$  leads to a contribution to  $\ln \chi_R^{(2)}$  that is linear in  $Vt_f$ , and hence consists in a voltage dependent (generally complex) shift of the ground state energy, similar to that of  $\ln \chi_R^{(1)}$ . The time integration over  $g(t)$  has to be cutoff at  $t=1/V$  and  $t_f-t=1/V$ , where the solution  $Y(t)$  crosses over into the equilibrium solution. The remaining integral can be estimated by integrating the equilibrium solution from  $t=1/\xi$  to  $1/V$ . This leads to

$$\begin{aligned} \ln \chi_R^{(2)}(t_f) = & -it_f VC - \frac{\text{tr}\{(\ln D)^2\}}{(2\pi)^2} \ln \left[ \frac{\sinh(\pi t_f/\beta)}{\sinh(\pi/\beta V)} \right] \\ & - \frac{\text{tr}\{\delta^2\}}{\pi^2} \ln \left[ \frac{\sinh(\pi/\beta V)}{\sinh(\pi/\beta \xi)} \right], \end{aligned} \quad (42)$$

where we recall that  $t_f \gg 1/V$ . Since  $1/\xi \ll 1/V \ll \beta$ , this can be rewritten as

$$\begin{aligned} \ln \chi_R^{(2)}(t_f) = & -it_f VC - \frac{\text{tr}\{(\ln D)^2\}}{(2\pi)^2} \ln \left[ \frac{\sinh(\pi t_f/\beta)}{\pi/\beta V} \right] \\ & - \frac{\text{tr}\{\delta^2\}}{\pi^2} \ln(\xi/V). \end{aligned} \quad (43)$$

For  $1/\xi \ll t_f \ll 1/V$ , this function crosses over into the equilibrium solution (27).

Since both  $\delta$  and  $\ln D$  are time-independent [for  $t \in (0, t_f)$ ] we see that, in this limit  $k_B T \ll V$ , the extension from zero to finite temperatures, originally achieved by the mapping  $t \rightarrow \tanh(\pi t/\beta)$ , can here be obtained by a rule of thumb of replacing  $t_f$  by  $(\beta/\pi) \sinh(\pi t_f/\beta)$  in the logarithms. For  $\chi_R(t)$  this means that the zero temperature power laws of the form  $t_f^\alpha$  are replaced by  $[\sinh(\pi t_f/\beta)]^\alpha$ .

Therefore, finite temperatures replace the power-law tails by an exponential decay with a decay time proportional to the inverse temperature  $\beta$ . In other words, while the system at zero temperature keeps a long-term memory to the initial perturbation, finite temperature fluctuations suppress it within a characteristic time set by  $\beta/\alpha$ .

The transition rate  $p_{g \rightarrow e}(\Delta E)$  is determined by the Fourier integral (28). An explicit calculation of the integral is possible and leads to a Beta function, yet the following estimates are physically more instructive:

At zero temperature both the singularity at  $t \rightarrow 0$  as well as the power-law tails for  $t \rightarrow \infty$  contribute equally to the integral. In the equilibrium situation, we obtain the well-known Fermi-edge singularity, a power-law dependence on energy,  $p_{g \rightarrow e} \sim \Delta E^{\text{tr}\{\delta^2\}/\pi^2 - 1}$ . For  $V \neq 0$ ,  $\Delta E$  and the exponent acquire an imaginary correction. The nonequilibrium effects dominate for small energies  $\Delta E < V$ , and the imaginary corrections to  $\Delta E$  lead to a broadening of the Fermi-edge singularity. The high energy tails,  $\Delta E \gg V$ , coincide with the equilibrium solution.

At finite but small temperatures,  $k_B T \ll V$ , the exponential decay of the response functions for  $t \gg 1/k_B T$  causes an additional, Lorentzian, broadening of the singularity for  $\Delta E < k_B T$ . At high temperatures,  $k_B T \gg V$ , the nonequilibrium effects are completely washed out. For small energies,  $\Delta E \ll k_B T$ , the exponential decay then dominates the integral, and the singularity is broadened to a Lorentzian with a width proportional to  $k_B T$ . On the other hand, for high energies  $\Delta E \gg k_B T$ , the exponential decay is slow compared to the quickly oscillating phase factor. The behavior of the integral can be estimated through a saddle point approximation, leading to  $p_{g \rightarrow e}(\Delta E) \sim \exp(-\Delta E/k_B T)$ , corresponding to an activated transition such as for a noninteracting system.

In summary, nonequilibrium constraints and temperature have the similar effect of a broadening of the Fermi-edge singularity with two different shapes: A Lorentzian broadening from the temperature with a width given by  $k_B T$ , and a Lorentzian to the power of an expression depending on  $\ln D$  from the nonequilibrium constraints with a width determined, to first order, by  $V$ . Away from the resonance, but still for  $\Delta E \ll k_B T$ , the transition rate has a power-law dependence on energy, which eventually turns into an activated behavior for  $\Delta E > k_B T$ .

## V. CONCLUSIONS

We have shown that the RH approach developed in Refs. 3 and 4 has an exact finite temperature extension. This finite temperature case can be mapped onto a different zero temperature problem, for which much is mathematically known,<sup>9</sup> and which allows, in some simpler cases, an exact solution. Based on this equivalence we have constructed approximate solutions for the nonequilibrium RH problem at finite temperatures. These results provide a necessary tool for a general application as well as for further developments of the RH approach and the study of Fermi-edge singularities or related phenomena in nonequilibrium or nonadiabatic situations.

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APPENDIX A: TIME REPRESENTATION OF  $R$ 

The presented method requires that the time representation of  $R$ , the matrix elements of the many-body operator  $\hat{R}$  between single-particle states, is diagonal,  $R=R(t)$ . For clarity and completeness, we here shortly state the conditions necessary for this, summarizing the arguments of Ref. 4 (see also Ref. 3 and, in particular, Ref. 6). For a more extended discussion we refer to the cited references.

In most cases of interest,  $\hat{R}$  is connected to the evolution operators  $\hat{U}(t_f)$  and  $\hat{U}_0(t_f)$  for the Hamiltonians  $H$  and  $H_0$ , respectively. For instance, in the case of the Fermi-edge singularities,  $\hat{R}$  represents the overlap between perturbed and unperturbed states,  $\hat{R}=\hat{U}_0^\dagger(t_f)\hat{U}(t_f)$ . On the other hand, for the shot noise spectrum of a tunneling barrier,  $\hat{R}$  can be the moment generating function for the distribution of charge transferred out of electrode  $j=1$  during the time  $t=0$  to  $t_f$ . If  $\hat{Q}_1$  measures the charge of this electrode,  $\hat{R}(\lambda)=\hat{U}^\dagger(t_f)e^{-i\lambda\hat{Q}_1}\hat{U}(t_f)e^{i\lambda\hat{Q}_1}$ .

Since the Hamiltonian is quadratic, the action of  $\hat{U}(t_f)$  on the many-body states can fully be described by its action on the single-particle states (see also Appendix B),

$$\hat{U}(t_f)\mathbf{a}_{\epsilon'}^\dagger|\rangle = \sum_{\epsilon} e^{-i\epsilon t_f} \sigma(\epsilon, \epsilon') \mathbf{a}_{\epsilon}^\dagger|\rangle, \quad (\text{A1})$$

where  $\sigma(\epsilon, \epsilon')$  is a  $N \times N$  matrix in channel space, and  $|\rangle$  the true vacuum. The matrix  $\sigma$  can be related to the single-particle scattering matrix  $S(t, E)$  for a particle of energy  $E$  calculated for the instantaneous value of the potential  $M(t)$ . In general, this relation is complicated, but becomes simple when the following condition of adiabaticity is met:

$$\frac{\partial S^{-1}}{\partial t} \frac{\partial S}{\partial E} \ll 1. \quad (\text{A2})$$

This equation encodes nothing than the condition that the scattering matrix has to vary slowly during the characteristic scattering time of a particle (the Wigner delay time). In this case, the connection to the matrix  $\sigma$  is simple

$$\sigma_{j,j'}(\epsilon, \epsilon') = S_{j,j'}(\epsilon, \epsilon'), \quad (\text{A3})$$

where

$$S_{j,j'}(\epsilon, \epsilon') = \frac{1}{2\pi\sqrt{v_j v_{j'}}} \int dt S_{j,j'}(t, E) e^{i(\epsilon - \epsilon')t}, \quad (\text{A4})$$

with  $E=(\epsilon + \epsilon')/2$  and  $v_j$  the density of states in channel  $j$ .

The time representation  $R(t)$  is obtained by a similar Fourier transform of  $R_{j,j'}(\epsilon, \epsilon') = \langle a_{\epsilon_j} \hat{R} a_{\epsilon'_j}^\dagger | \rangle$ .

$$R_{j,j'}(\epsilon, \epsilon') = \frac{1}{2\pi\sqrt{v_j v_{j'}}} \int dt R_{j,j'}(t, E) e^{i(\epsilon - \epsilon')t}. \quad (\text{A5})$$

As noted above, the definition of  $R$  involves  $\sigma$  or simple combinations of  $\sigma$ , so that the same condition of adiabaticity applies. The transformations in the RH method do not involve the dependence of these matrices on  $E$ . At low temperatures and in equilibrium, the relevant physics is restricted to energies close to the chemical potential  $\mu$ , so that we can fix  $E=\mu$ . For nonequilibrium situations, the treatment remains valid as long as the dependence of  $R$  on  $E$  is weak.

## APPENDIX B: DERIVATION OF EQ. (3)

In this appendix, we demonstrate the equality

$$\text{Tr}[\hat{\rho}\hat{R}] = \det[fR + (1-f)], \quad (\text{B1})$$

stated in Eq. (3) that connects a many-body description on the left-hand side to a single-body representation on the right-hand side.  $\hat{R}$  is the many-body operator of interest,  $\hat{\rho}$  the initial many-body density matrix at  $t=0$ ,  $\hat{\rho} \propto e^{-\beta\hat{H}_0}$ , and  $\text{Tr}$  the trace over all many-body states. On the other hand,  $R = \{R_{ij}\}$  is the  $N_s \times N_s$  matrix between the  $N_s$  possible single-particle states in the system,  $R_{ij} = \langle a_i \hat{R} a_j^\dagger | \rangle$  (for simplicity of notation, we here label single-particle states by a single index  $i$  only—in the main text this is split into energy  $\epsilon$  and channel indices  $j$ ).  $|\rangle$  is the true vacuum, not the ground state,  $f$  the corresponding Fermi function, and  $\det$  the determinant over the  $N_s \times N_s$  matrices.

The Hamiltonian  $\hat{H}$  is quadratic in the single-particle operators for all times  $t$ . At time  $t=0$  and at zero temperature, the density matrix projects on the ground state  $|0\rangle$ , which is a Slater determinant in the single-particle states  $|\psi_i\rangle = a_i^\dagger|\rangle$ . If the many-body operator  $\hat{R}$  conserves particle numbers, it is, therefore, fully described by its action on the single-particle constituents of the ground state, represented by the matrix  $R$ . Explicitly, for a system of  $N \leq N_s$  particles, the ground state is  $|0\rangle = (N!)^{-1/2} \sum_{\pi} (-1)^{\pi} |\psi_{\pi(1)}\rangle \otimes \cdots \otimes |\psi_{\pi(N)}\rangle$ , where the sum runs over all permutations  $\pi$ ,  $(-1)^{\pi}$  is the sign of the permutation, and where we assume that  $i=1, \dots, N$  labels the  $N$  single-particle states of lowest energy. We have  $\hat{R}|\psi_i\rangle = \hat{R}_i|\psi_i\rangle = \sum_{j=1}^{N_s} R_{ji}|\psi_j\rangle$ , where  $\hat{R}_i$  is the restriction of  $\hat{R}$  to the single-particle state  $i$ . Further  $\hat{R}(|\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots) = \hat{R}_1|\psi_1\rangle \otimes \hat{R}_2|\psi_2\rangle \otimes \cdots$ , from which follows that

$$\begin{aligned} \langle 0 | \hat{R} | 0 \rangle &= \frac{1}{N!} \sum_{\pi\pi'} (-1)^{\pi+\pi'} [\langle \psi_{\pi'(1)} | \otimes \cdots \otimes \langle \psi_{\pi'(N)} |] \\ &\quad \times \hat{R} [|\psi_{\pi(1)}\rangle \otimes \cdots \otimes |\psi_{\pi(N)}\rangle] \\ &= \frac{1}{N!} \sum_{\pi\pi'} (-1)^{\pi+\pi'} [\langle \psi_{\pi'(1)} | \otimes \cdots \otimes \langle \psi_{\pi'(N)} |] \\ &\quad \times \left[ \sum_{j_1, \dots, j_N=1}^{N_s} R_{j_1 \pi(1)} |\psi_{j_1}\rangle \otimes \cdots \otimes R_{j_N \pi(N)} |\psi_{j_N}\rangle \right] \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{N!} \sum_{\pi\pi'} (-1)^{\pi+\pi'} R_{\pi'(1)\pi(1)} \cdots R_{\pi'(N)\pi(N)} \\
&= \sum_{\pi} (-1)^{\pi} R_{1\pi(1)} \cdots R_{N\pi(N)}. \tag{B2}
\end{aligned}$$

This is the determinant of  $R$ , taken over the occupied states only, and thus corresponds to the right-hand side of Eq. (B1).

The generalization to nonzero temperatures is immediate: Every excited state of  $N$  particles yields a similar determinant of  $R$  for a different selection of  $N$  particles  $\psi_j$ . The density matrix  $\hat{\rho}$  weights these states with the Boltzmann factors  $\propto e^{-\beta\hat{H}_0}$ . Since these are exponentials of single-particle operators, they just provide the weights  $e^{-\beta\epsilon_j}$  for the occupied single-particle states that sum up to the Fermi function when summing over all excited states. Therefore, Eq. (B1) remains valid at nonzero temperatures.

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