Generalized Nozières–De Dominicis approach to transport through nano–junctions

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Abstract

We investigate the transport properties of a model of an interacting electronic resonant level system. The hybridization of the localized resonant level is treated in perturbation and the contributions to all orders are computed. This includes an exact treatment of the electron scattering from the localized level. The renormalization of the direct tunneling between the electrodes arising from the Coulomb repulsion of trapped particles is taken into account. Further, we provide a detailed solution of the system of coupled singular integral equations which determine the propagator in the interacting system.

1 Introduction

Over 30 years ago, Nozières and De Dominicis (ND) [1] proposed an ingenious solution of the x-ray absorption/emission edge singularity problem in metals. Their solution, being non-perturbative, allowed to circumvent the difficulties arising from the Anderson orthogonality catastrophe [2], and revealed the singular behavior of the absorption/emission resonance. Soon thereafter, Yuval and Anderson [3] used the formal resemblance between the x-ray problem and the Kondo spin 1/2 model to extend the method to describe the vacuum-to-vacuum amplitude (or the partition function in the finite temperature case). They showed that the latter is formally equivalent to the partition function of a classical one-dimensional gas of particles with logarithmic interactions. In a subsequent work, Anderson, Yuval and Hamann [4] introduced renormalization group methods to solve this partition function. Another formal correspondence to the x-ray problem can be found in the description of the tunneling of an electron through a localized state in a junction. For such a system, Matveev and Larkin [5] applied ND’s technique to express the resonant behavior of the tunneling current.
The common property shared among these examples is a time-dependent interaction between conduction electrons in certain quantum channels with a localized structureless scatterer (a hole, an impurity spin, or a trapped electron). Since the interaction does not change the internal state of the scatterer, a reduction of the many-body problem into one-body problems is possible. The latter can then be solved by the methods devised by ND.

In the examples above it was assumed that electrons in different quantum channels (such as angular momentum, spin, pseudo spin, or indexing spatially separated electrodes) do not interact. Generally this results from symmetry arguments and a partial diagonalization of the Hamiltonian. In the present paper, however, we focus on the case in which such a decoupling is not possible, and in which particles can be scattered onto different channels due to the interaction with the localized scatterer. We choose as an example the physical system considered by Matveev and Larkin of two electrodes connected to a barrier containing one localized state. However, in contrast to Matveev and Larkin, we assume a direct coupling of the conduction electrons in both electrodes. The method is illustrated through the computation of the tunneling current, expressed in the form of an infinite series (see Eqs. (59) and (60) which are the results of this paper), although a large part of the derivations is performed in the most general case accessible by this approach.

This is a technical paper and we focus mainly on the formal aspects of the problem. We expect to come back in the future to physical applications of the generic problem solved below. On the other hand, the physical nature of the system considered below has already been discussed thoroughly in [5]. For pedagogical reasons details of the computation are written down explicitly. In particular, we present in the Appendix A a full solution of the singular integral equations determining the one-particle propagators. In this respect, we also restrict ourselves to an equilibrium description of the system. An extension to the non-equilibrium case will be performed in a subsequent work.

In Sec. 2 and 3 we define the model and derive the Dyson series for the tunneling current. Sec. 4 and 5 contain the central part of the paper in which first ND’s method is adapted to the present problem, and then extended to all orders in the Dyson series following Yuval’s and Anderson’s ideas. The application to some simpler problems is discussed in Sec. 6.

2 Model

The Hamiltonian of the system reads

\[ H = H_0 + H_W + H_V, \] (1)
with
\[ H_0 = \sum_{k\alpha} \varepsilon_{k\alpha} C_{k\alpha}^\dagger C_{k\alpha} + E_d d^\dagger d, \]  
\[ H_W = \sum_{kk'\alpha'\alpha} W_{kk'}^{\alpha\alpha'} C_{k\alpha}^\dagger C_{k'\alpha'} d^\dagger d, \]  
\[ H_V = \sum_{k\alpha} \left( V_{k\alpha} C_{k\alpha} d^\dagger + \text{h.c.} \right), \]

where \( C_{k\alpha}^\dagger \) and \( C_{k\alpha} \) are the creation and annihilation operators of spinless fermions with momentum \( k \) which are characterized by an additional quantum number \( \alpha = 1, \ldots, N \) for some integer \( N \). These particles are assumed to form for every \( \alpha \) a Fermi liquid with chemical potential \( \mu_{\alpha} \), described by \( H_0 \).

The Hamiltonian \( H_W \) describes the interaction of the particles \((k,\alpha)\) with a localized state, \( \phi_d \), which is characterized by the operators \( d^\dagger, d \) and the energy \( E_d \). The hermiticity of \( H_W \) imposes that \((W_{kk'}^{\alpha\alpha'})^* = W_{k'k}^{\alpha'\alpha} \). Finally, \( H_V \) denotes the hybridization term with the localized state.

It is essential for the following to assume that this localized state is completely structureless and that the interaction with the Fermi liquid is short-ranged. Under these assumptions the short-ranged potentials can be considered to be separable as
\[ W_{kk'}^{\alpha\alpha'} = W^{\alpha\alpha'} (u_k^\alpha)^* u_{k'}^{\alpha'}, \]  
\[ V_k^{\alpha} = V^{\alpha} u_k^{\alpha}, \]

with \( u_k^\alpha \) some normalized functions that are peaked at the chemical potentials \( \mu_{\alpha} \) where they take the value \( u_k^{\alpha_{\mu_{\alpha}}} = 1 \). It is convenient to define the operators
\[ C_{\alpha} = \sum_k C_{k\alpha} u_k^\alpha \quad \text{and} \quad C_{\alpha}^\dagger = \sum_k C_{k\alpha}^\dagger (u_k^\alpha)^* \]

that annihilate and create a particle localized near \( \phi_d \). The Hamiltonians \( H_W \) and \( H_V \) become
\[ H_W = \sum_{\alpha\alpha'} W^{\alpha\alpha'} C_{\alpha}^\dagger C_{\alpha'} d^\dagger d, \]  
\[ H_V = \sum_{\alpha} \left( V_{\alpha} C_{\alpha} d^\dagger + \text{h.c.} \right). \]

As an example for such a system we consider the situation depicted in Fig. 1. An insulating barrier is assumed to be connected on two sides to electrodes containing spinless Fermi liquids. The index \( \alpha \) labels here the left or right electrode, \( \alpha = L, R \). The localized state \( \phi_d \) corresponds to an impurity trap inside the barrier. Both electrodes are considered as particle reservoirs that are kept at the chemical potentials \( \mu_L \) and \( \mu_R \) (with generally \( \mu_L \neq \mu_R \)), respectively. It is assumed that in absence of a particle in the impurity trap the two Fermi gases are completely independent (we neglect the direct tunneling
which can be regarded as a constant background current). However, if an electron is trapped at the impurity site, it interacts with the particles near the junction in the electrodes since the potential created by its charge is not screened in the insulator. We denote this scattering potential by $W_{kk'}^{\alpha \alpha'}$ where the diagonal terms with respect to $\alpha, \alpha = \alpha'$, describe the backscattering of electrons and the non-diagonal terms, $\alpha \neq \alpha'$, the renormalization of the background tunneling current.

We intend to calculate the current through the junction, which can be expressed as the time variation of the number of particles in the electrodes,

$$J(t) = e \left\langle \frac{d}{dt} \left( N^R(t) - N^L(t) \right) \right\rangle,$$

(10)

where $N^\alpha(t) = \sum_k C^\dagger_{\alpha k}(t) C_{\alpha k}(t)$ is the electron number operator in the electrode $\alpha$. Its time derivative is determined by the Heisenberg equation

$$i \frac{d}{dt} N^\alpha(t) = \left[ N^\alpha(t) , H \right] = i\hat{N}^\alpha_W(t) + i\hat{N}^\alpha_V(t),$$

(11)

where we have defined

$$\hat{N}^\alpha_W(t) = (-i) \left[ N^\alpha(t) , H_W(t) \right] = (-i) \sum_{\alpha'} \left\{ W^{\alpha \alpha'} C^\dagger_{\alpha}(t) C_{\alpha'}(t) - W^{\alpha' \alpha} C^\dagger_{\alpha'}(t) C_{\alpha}(t) \right\} \ d^\dagger(t) d(t)$$

(12)

$$\hat{N}^\alpha_V(t) = (-i) \left[ N^\alpha(t) , H_V(t) \right] = (-i) \left\{ V^\alpha C^\dagger_{\alpha}(t) d(t) - (V^\alpha)^* C_{\alpha}(t) d^\dagger(t) \right\}. $$

(13)

Therefore the computation of the averages

$$\langle \hat{N}^\alpha_W(t) \rangle = 2 \Im \left[ \sum_{\alpha'} W^{\alpha \alpha'} \langle C^\dagger_{\alpha'}(t) C_{\alpha'}(t) d^\dagger(t) d(t) \rangle \right],$$

(14)

$$\langle \hat{N}^\alpha_V(t) \rangle = 2 \Im \left[ V^\alpha \langle C^\dagger_{\alpha}(t) d(t) \rangle \right],$$

(15)
which can be expressed by the response functions,
\[
F_W^{\alpha \alpha'}(t) = \langle C_\alpha^\dagger(t) C_{\alpha'}(t) d^\dagger(t) d(t) \rangle, \quad (16)
\]
\[
F_V^\alpha(t) = \langle C_\alpha^\dagger(t) d(t) \rangle, \quad (17)
\]
is required.

3 Dyson series

We expand the functions \(F_W^{\alpha \alpha'}(t)\) and \(F_V^\alpha(t)\) in a zero-temperature perturbation series in powers of \(H_V\). The interactions due to \(H_W\) will be treated in the exact way indicated by ND. For this purpose, we define an interaction picture with respect to \(H_1 = H_0 + H_W\) by
\[
i \frac{d}{dt} \hat{A}(t) = \left[ \hat{A}(t), H_1 \right] \quad (18)
\]
for an arbitrary Schrödinger operator \(A\). In order to take averages over operators we impose artificially to the system to be in the same state \(|i\rangle\) at an initial time \(t_0\), as well as at the final time \(t_1\). We choose \(|i\rangle\) to be an eigenstate of \(H_1\) in which the state \(\phi_d\) is unoccupied, \(d|i\rangle = 0\). This choice of the average is definitely wrong because the occupancy of \(\phi_d\) in the final state is not well-defined due to the hybridization term \(H_V\). A more subtle investigation of the problem would involve Keldysh’s formulation of perturbation theory for non-equilibrium processes \[6\] in which only the initial, but no final state appears. An extension to the Keldysh formulation of the methods described below will be the subject of a future publication. In the present paper, however, we choose for pedagogical reasons to restrict ourselves to the case in which the system comes back to the state \(|i\rangle\) at the time \(t_1\).

The standard perturbation theory tells us that in this case the average value over the operator \(A(t)\), for \(t_0 < t < t_1\), can be expressed by the relation
\[
\langle A(t) \rangle = \langle i | T \{ S(t_0, t_1) \hat{A}(t) \} | i \rangle
\]
where \(T\) denotes the time-order operator, and where
\[
S(t_0, t_1) = \exp \left( -i \int_{t_0}^{t_1} d\tau \hat{H}_V(\tau) \right) \quad (19)
\]
is the \(S\)-matrix. In this representation, the functions \(F_W^{\alpha \alpha'}(t)\) and \(F_V^\alpha(t)\) read
\[
F_W^{\alpha \alpha'}(t) = \langle i | T \{ S(t_0, t_1) \hat{C}_\alpha^\dagger(t) \hat{C}_{\alpha'}(t) d^\dagger(t) d(t) \} | i \rangle,
\]
\[
F_V^\alpha(t) = \langle i | T \{ S(t_0, t_1) \hat{C}_\alpha^\dagger(t) d(t) \} | i \rangle,
\]
or, explicitly,

\[
F_{W}^{\alpha\alpha'}(t) = \sum_{n=0}^{\infty} \left( \frac{(-i)^{2n}}{(2n)!} \int_{t_0}^{t_1} \int_{t_0}^{t_2} \cdots \int_{t_0}^{t_{2n}} \right) d\tau_1 \cdots d\tau_{2n}
\]

\[\langle i | T \left\{ \hat{H}_V(\tau_1) \cdots \hat{H}_V(\tau_{2n}) \hat{C}_\alpha^\dagger(t) \hat{C}_{\alpha'}(t) \hat{d}^\dagger(t) \hat{d}(t) \right\} | i \rangle, \tag{20}
\]

\[
F_{V}^{\alpha}(t) = \sum_{n=1}^{\infty} \left( \frac{(-i)^{2n-1}}{(2n-1)!} \int_{t_0}^{t_1} \int_{t_0}^{t_2} \cdots \int_{t_0}^{t_{2n-1}} \right) d\tau_1 \cdots d\tau_{2n-1}
\]

\[\langle i | T \left\{ \hat{H}_V(\tau_1) \cdots \hat{H}_V(\tau_{2n-1}) \hat{C}_\alpha^\dagger(t) \hat{d}^\dagger(t) \right\} | i \rangle. \tag{21}
\]

4 Illustration of the method at lowest order

In order to illustrate the method of calculation, let us consider the first non-trivial term \((n = 1)\) in the expansion (21) of \(F_{W}^{\alpha\alpha'}\). This approximation, quadratic in \(H_V\), is formally equivalent to a direct generalization of ND’s solution of the x-ray problem to several interacting quantum channels \(\alpha\). For conceptual details we refer to ND’s article [1].

The central assumption in this approach consist in considering the localized state \(\phi_d\) to be structureless. The scattering of conduction electrons described by \(H_W\) therefore depends on the occupancy of the \(\phi_d\) state only, but on no other internal structure of \(\phi_d\). This allows us to consider the scattering potential \(W_{kk'}^{\alpha\alpha'}\) as a time-dependent external potential acting on the conduction electrons during the times of occupancy of \(\phi_d\).

At the order \(n = 1\), for fixed times \(\tau_1\) and \(\tau_2\) with, for instance, \(\tau_1 < \tau_2\), the hybridization term \(H_V\) at the time \(\tau_1\) describes the tunneling of an electron into \(\phi_d\), whereas the hybridization term at \(\tau_2\) transfers this particle back to one of the electrodes. The potential \(W_{kk'}^{\alpha\alpha'}\) applies therefore during the interval \((\tau_1, \tau_2)\) and is zero for all other times. The time \(t\) must lie between \(\tau_1\) and \(\tau_2\) because of the operators \(d^\dagger(t) d(t)\) in the definition of \(F_{W}^{\alpha\alpha'}(t)\). The only contribution of the localized state to the amplitude is its free propagation factor

\[\exp\left( -iE_d(\tau_2 - \tau_1) \right)\].

If we expand the amplitude \(\langle i | T \left\{ \hat{H}_V(\tau_1) \hat{H}_V(\tau_2) \hat{C}_\alpha^\dagger(t) \hat{C}_{\alpha'}(t) \hat{d}^\dagger(t) \hat{d}(t) \right\} | i \rangle\) in the external potential, the Feynman diagrams arising from the different contractions factorize into two groups: the diagrams that are connected to at least one of the points \(\tau_1, \tau_2\) and \(t\), and the closed loops where no vertex coincides with one of these points (see Fig. 2 for an example). If we denote by \(L^{\alpha\alpha'}(\tau_1, \tau_2, t)\) the former group of diagrams, and by \(e^{\mathcal{C}(\tau_1, \tau_2)}\) the latter, where by the linked cluster theorem the complete closed loop sum can be expressed by the exponential
Fig. 2. Example of the factorization of the many-body problem. The plain lines represent free conduction electron propagators (evolving under $H_0$) and the dashed line the propagator of the particle in $\phi_d$. The full dots are interaction vertices due to $W^{\alpha\alpha'}$ and the open dots at $\tau_1$ and $\tau_2$ due to $V^\alpha$.

of the sum $C(\tau_1, \tau_2)$ of all single closed loops, the amplitude at $n = 1$ in (21) becomes

$$\langle i | T \left\{ \hat{H}_V(\tau_1) \hat{H}_V(\tau_2) \hat{C}_\alpha(t) \hat{C}_{\alpha'}(t) \right\} | i \rangle = L^{\alpha \alpha'}(\tau_1, \tau_2, t) e^{C(\tau_1, \tau_2)} e^{-i E_d(\tau_2 - \tau_1)}$$

(24)

As we will see below, both quantities, $L^{\alpha \alpha'}(\tau_1, \tau_2, t)$ and $C(\tau_1, \tau_2)$, can be expressed by one-body propagators $G^{\alpha \alpha'}(\tau, \tau')$ describing a particle which is created at the time $\tau'$ in the electrode $\alpha'$ and annihilated at the time $\tau$ in the electrode $\alpha$, and which propagates under the external potential $W$ during the time interval $(\tau_1, \tau_2)$.

$$G^{\alpha \alpha'}(\tau, \tau') = \langle i | T \left\{ \hat{C}_\alpha(\tau) \hat{C}_{\alpha'}(\tau') \right\} | i \rangle.$$  

(25)

This propagator is determined by the Dyson equation

$$G^{\alpha \alpha'}(\tau, \tau') = G^\alpha_0(\tau, \tau') \delta_{\alpha \alpha'} - i \sum_{\alpha''} \int_{\tau_1}^{\tau_2} d\tau'' G^\alpha_0(\tau, \tau'') W^{\alpha \alpha''} G^{\alpha'' \alpha'}(\tau'', \tau')$$

(26)

where $G^\alpha_0(\tau, \tau')$ is the free propagator. The factor $(-i)$ in front of the integral in (26) arises from the unusual definition (25) of the Green’s functions. The Dyson equation will be calculated using the asymptotic expressions for large $|\tau - \tau'|$ developed by ND. Since for the free propagators, the electrodes $\alpha$ are assumed to be independent, ND’s development can be carried out for each $G^\alpha_0$ separately, and is given by (see [1], Eq. (38))

$$G^\alpha_0(\tau - \tau') = (-i \nu_\alpha) \left[ P\left( \frac{1}{\tau - \tau'} \right) + \pi \tan \vartheta_\alpha \delta(\tau - \tau') \right] e^{-i \mu_\alpha(\tau - \tau')}$$

(27)
where the $P$ indicates a principal value distribution. The angle $\tan \vartheta_{\alpha}$ contains the short-time corrections to the asymptotic form in $1/(\tau - \tau')$ and depends on the form of the conduction band. For a completely symmetric band around the Fermi surface it vanishes. If we introduce the propagators (27) into the Dyson equation (26) and integrate over the delta functions, we find the following system of singular integral equations

$$\tilde{A}(\tau) G(\tau, \tau') - \frac{1}{\pi i} \int_{t_0}^{t_1} d\tau'' \mathcal{P} \left( \frac{1}{\tau'' - \tau} \right) \tilde{B}(\tau'') G(\tau'', \tau') = \tilde{f}(\tau, \tau'). \quad (28)$$

where the coefficients $\tilde{A}$ and $\tilde{B}$ are $2 \times 2$ matrix functions of the form

$$\tilde{A}(\tau) \equiv e^{i\mu \tau} A = e^{i\mu \tau} (\mathbb{1} + \pi \tan \vartheta g), \quad (29)$$

$$\tilde{B}(\tau) \equiv e^{i\mu \tau} B = e^{i\mu \tau} (i\pi g), \quad (30)$$

for the $2 \times 2$ matrices $\mu = \{\mu_\alpha \delta_{\alpha\alpha'}\}$, $\tan \vartheta = \{\tan \vartheta_\alpha \delta_{\alpha\alpha'}\}$, and $g \equiv \nu W = \{\nu_\alpha W^{\alpha\alpha'}\}$, and where $\mathbb{1}$ is the $2 \times 2$ unit matrix. The inhomogeneous term $\tilde{f}(\tau, \tau')$ is given by

$$\tilde{f}(\tau, \tau') = e^{i\mu \tau} G_0(\tau - \tau'). \quad (31)$$

The system of singular integral equations (28) turns out to be exactly solvable. We provide the solution in the Appendix A. Let us define the constant matrices

$$S = A + B = \mathbb{1} + \pi (\tan \vartheta + i\mathbb{1}) g, \quad (32)$$

$$D = A - B = \mathbb{1} + \pi (\tan \vartheta - i\mathbb{1}) g. \quad (33)$$

As shown in Appendix B, the matrix

$$\mathcal{S} = SD^{-1} = \left( \mathbb{1} - \pi (\tan \vartheta + i\mathbb{1}) g \right) \left[ \mathbb{1} - \pi (\tan \vartheta - i\mathbb{1}) g \right]^{-1} \quad (34)$$

is the inverse of the (unitary) scattering matrix due to $W^{\alpha\alpha'}$ evaluated on the chemical potentials $\mu_\alpha$. Thus, if we write

$$\mathcal{S} = e^{2i\Delta}, \quad (35)$$

the solution of the Dyson equation (26), for $\tau, \tau' \in (\tau_1, \tau_2)$ is given by Eq. (A.34), and reads

$$G(\tau, \tau') = (-i) S^{-1}(\tau) e^{-i\Delta(\tau)} \left[ \frac{\tau - \tau_2}{\tau - \tau_1} \mathcal{P} e^{-i\mu(\tau - \tau')} \left| \frac{\tau' - \tau_1}{\tau' - \tau_2} \right| e^{i\Delta(\tau)} \right] \mathcal{P} \left( \frac{1}{\tau - \tau'} \right) + \pi \Theta(\tau') \delta(\tau - \tau') \right] M(\tau') \nu, \quad (36)$$
In the limit where the non-diagonal entries of $W^{\alpha \alpha'}$ vanish and the electrodes are decoupled, we recover for $\tilde{G}^{\alpha \alpha'}(\tau, \tau')$ ND’s result ([1], Eq. (51)).

Let us now calculate the factor $L^{\alpha \alpha'}(\tau_1, \tau_2, t)$. Since we know the propagator $G(\tau, \tau')$ in the presence of $W$, we will use Wick’s theorem to contract the four conduction electron operators at the points $\tau_1, \tau_2$ and $t$. Every contraction is associated to a propagator $G(\tau, \tau')$. As we see in Fig. 3, there are only two possible diagrams. The first diagram, Fig. 3(a), contributes

$$-(-1)^2 \sum_{\alpha_1 \alpha_2} G^{\alpha_1 \alpha}(\tau_1, t) G^{\alpha' \alpha_2}(t, \tau_2)$$

where a contraction of the operators $\hat{C}^\dagger(\tau')\hat{C}(\tau)$ equals $-G(\tau, \tau')$ and where the third minus sign arises from the commutation of $\hat{C}_{\alpha}^\dagger(t)$ and $\hat{C}_{\alpha'}(t)$ to separate the contractions. The second diagram, Fig. 3(b) gives, accordingly,

$$( -1 )^2 \sum_{\alpha_1 \alpha_2} G^{\alpha_1 \alpha_2}(\tau_1, \tau_2) G^{\alpha' \alpha}(t, t).$$

For convenience, we introduce the auxiliary times $\tau_3 = \tau_4 = t$, and the indices $\alpha_3 = \alpha'$ and $\alpha_4 = \alpha$. With these notations we find that

$$L^{\alpha \alpha'}(\tau_1, \tau_2, t) = \sum_{\alpha_1 \alpha_2} V^{\alpha_1}(V^{\alpha_2})^* \det G^{\alpha_2j-1 \alpha_2k}(\tau_{2j-1}, \tau_{2k})$$

Fig. 3. The two possible contractions contributing to $L(\tau_1, \tau_2, t)$. The bold lines represent the propagator $G$, given in (36).
where the determinant is taken over the indices $j, k = 1, 2$.

If we introduce the explicit form (36) of the propagator into the latter equation, we are lead to divergences in both propagators $G(\tau_2, \tau_1)$ and $G(t, t)$. According to ND, these divergences are due to the asymptotic approximation of the propagators and must be cured by a (pure imaginary) cutoff $i\xi_0$ of the order of the bandwidth, such that

$$G(\tau_1, \tau_2) = (-i) \frac{1}{\tau_1 - \tau_2} S^{-1} e^{-i\Delta \left(i\xi_0|\tau_2 - \tau_1|\right)} - \hat{\phi} e^{-i\mu(\tau_1 - \tau_2)} e^{+i\Delta \left(i\xi_0|\tau_2 - \tau_1|\right)} - \hat{\phi} BD^{-1} B^{-1} \nu,$$  \hspace{1cm} (42)

and, if we interpret $G(t, t)$ as $G(t - i\xi_0^{-1}, t)$,

$$G(t, t) = (-i) S^{-1} BD^{-1} B^{-1} \nu (i\xi_0).$$  \hspace{1cm} (43)

Notice that in this form, $G(t, t)$ does not depend explicitly on the boundaries $\tau_1$ and $\tau_2$. This might be an acceptable approximation for the Green’s function in the determinant of $L^{\alpha\alpha'}$, but it is not sufficient if we consider the closed loop sum.

The sum over all simple closed loops can be calculated by use of the equation ([1], Eq. (22))

$$\lambda \frac{\partial C(\tau_1, \tau_2)}{\partial \lambda} \bigg|_{\lambda=1} = i \sum_{\alpha\alpha'} \int_{\tau_1}^{\tau_2} d\tau W^{\alpha\alpha'} G^{\alpha'\alpha}(\tau, \tau) = i \int_{\tau_1}^{\tau_2} d\tau \ Tr [W G(\tau, \tau)]$$  \hspace{1cm} (44)

where in $C(\tau_1, \tau_2)$ all potentials $W$ have been multiplied by the parameter $\lambda$.

Again $G(\tau, \tau)$ is singular, but if we develop $G(\tau, \tau')$ in powers of $\Delta \tau = \tau - \tau'$, we can separate out the singular term which diverges like $1/\Delta \tau$. Namely, since

$$X(\tau) e^{-i\mu \Delta \tau} X^{-1}(\tau') = \left[ \frac{\tau - \tau_2}{\tau - \tau_1} \right] \hat{\phi} e^{-i\mu \Delta \tau}$$

$$\left\{ \frac{\tau - \tau_1}{\tau - \tau_2} \hat{\phi} + \frac{\Delta \tau}{\pi} \left[ \frac{1}{\tau - \tau_1} - \frac{1}{\tau - \tau_2} \right] \frac{1}{(\tau - \tau_2)^2} + \frac{1}{(\tau - \tau_1)^2} \right\} \Delta \tau + O(\Delta \tau)^2$$  \hspace{1cm} (45)

we have in the limit $\Delta \tau \rightarrow 0$

$$G(\tau, \tau') \xrightarrow{\Delta \tau \rightarrow 0} (\text{Sing.}) - (-i) \left[ \frac{1}{\tau_2 - \tau} + \frac{1}{\tau - \tau_1} \right] S^{-1}(\tau) \frac{\Delta \tau}{\pi} M(\tau) \nu$$  \hspace{1cm} (46)

where the singular part (Sing.) is due only to the approximation on the propagators. The important point is that it does not depend on $\tau_1$ and $\tau_2$. As shown in ND, its contribution to the exponential is proportional to the first
correction in energy (for a static potential \( W \) extending in time from \(-\infty\) to \(+\infty\)) which will be denoted by \( \Delta E_1 \).

The integration of \( \tau \) over the interval \((\tau_1, \tau_2)\) leads to a logarithmic divergence at the boundaries and requires again the introduction of the cutoff \( \xi_0 \), so that (considering only the regular parts of \( G(\tau, \tau) \))

\[
\frac{\lambda}{\pi} \partial C \bigg|_{\lambda=1} = \frac{2}{\pi} \log \left[ i |\tau_2 - \tau_1| \xi_0 \right] \text{Tr} \left[ WS^{-1} \Delta BD^{-1} B^{-1} \nu \right] \\
= \frac{2i}{\pi^2} \log \left[ i |\tau_2 - \tau_1| \xi_0 \right] \text{Tr} \left[ \Delta BD^{-1} S^{-1} \right] \\
= -\frac{1}{\pi^2} \log \left[ i |\tau_2 - \tau_1| \xi_0 \right] \lambda \frac{d}{d\lambda} \text{Tr} \left[ \Delta^2 \right].
\] (47)

The last equality can be shown as follows: If \( M(\lambda) \) is an invertible matrix depending on the parameter \( \lambda \), we have

\[
\frac{d}{d\lambda} M^{-1}(\lambda) = -M^{-1}(\lambda) \left( \frac{d}{d\lambda} M(\lambda) \right) M^{-1}(\lambda), \tag{48}
\]

as can easily be verified by deriving the matrix product \( M(\lambda) M^{-1}(\lambda) = \mathbb{1} \) with respect to \( \lambda \). Therefore, if we replace the potential \( W \) by \( \lambda W \) in the definition of the matrix \( \mathcal{G} \) in Eq. (34), and derive \( \mathcal{G}^{-1} \) with respect to \( \lambda \) by using (48), we find after some algebra

\[
\lambda \mathcal{G} \frac{d\mathcal{G}^{-1}}{d\lambda} = -2BD^{-1} S^{-1}.
\]

Furthermore, since \( \Delta \) is defined by \( \mathcal{G} = e^{2i\Delta} \), we have

\[
(-2) \text{Tr} \left[ \Delta BD^{-1} S^{-1} \right] = \lambda \text{Tr} \left[ \Delta \mathcal{G} \frac{d\mathcal{G}^{-1}}{d\lambda} \right] \\
= \lambda \text{Tr} \left[ \Delta e^{2i\Delta} \frac{d}{d\lambda} e^{-2i\Delta} \right] = -i \lambda \frac{d}{d\lambda} \text{Tr} \left[ \Delta^2 \right]
\]

where we have used the invariance of the trace under cyclic permutations. With help of the latter expression we can integrate the simple closed loop sum. This yields, reintroducing the contribution in \( \Delta E_1 \),

\[
C = \int_0^1 d\lambda \frac{dC}{d\lambda} = -\frac{1}{\pi^2} \log \left[ i |\tau_2 - \tau_1| \xi_0 \right] \text{Tr} \left[ \Delta^2 \right] - i \Delta E_1 (\tau_2 - \tau_1) \tag{49}
\]

and the closed loops contribute

\[
e^{C(\tau_1, \tau_2)} = \left[ i |\tau_2 - \tau_1| \xi_0 \right]^{-\frac{\lambda \Delta^2}{2\pi^2}} e^{-i \Delta E_1 (\tau_2 - \tau_1)}. \tag{50}
\]
Putting together Eqs. (41) and (50), the contribution to $F_{W}^{'\alpha\alpha'}(t)$ in the series (21) takes the form

$$\left[F_{W}^{'\alpha\alpha'}(t)\right]_{(2)}(-i)^2 = \int_{t_0<\tau_1<\tau_2<t_1} d\tau_1 d\tau_2 L^{\alpha\alpha'}(\tau_1, \tau_2, t) e^{C(\tau_1, \tau_2)} e^{-iE_d(\tau_2-\tau_1)} = (-i)^2 \int_{t_0<\tau_1<\tau_2<t_1} d\tau_1 d\tau_2 \sum_{\alpha_1\alpha_2} (V^{\alpha_1})^* V^{\alpha_2} \det G^{\alpha_2j-\alpha_1k}(\tau_{2j-1}, \tau_{2k})$$

$$\left[i\xi_0|\tau_2-\tau_1|\right] \frac{\Delta^2}{4} e^{-i(E_d+\Delta E_1)(\tau_2-\tau_1)}$$

(51)

where $\tau_3 = \tau_4 = t$, $\alpha_3 = \alpha'$, $\alpha_4 = \alpha$, and $j, k = 1, 2$. The factor $1/2!$ occurring in (21) has been eliminated by the restriction of the domain of integration.

5 Extension to higher orders

An extension to higher orders in perturbation of ND’s ideas was carried out already a long time ago by Yuval and Anderson [3] who derived in this way an expression for the partition function of the single spin 1/2 impurity Kondo problem. In this section we show how their method can be generalized to the present problem. Consider an amplitude at order $n \geq 2$ in the Dyson series (21) for $F_{W}^{'\alpha\alpha'}$. If the intermediate times $\tau_j$ are fixed and chosen such that $\tau_1 < \tau_2 < \cdots < \tau_{2n}$, an electron tunnels into the localized state at odd times $\tau_{2j-1}$, and leaves it at even times $\tau_{2j}$ ($j = 1, \ldots, n$). As before, these times have to be chosen such that the state $\phi_d$ is occupied at the time $t$. The many-body problem can be factorized into one-body problems as in the previous section, and the amplitude in the expansion (21) can be written in a form similar to Eq. (24),

$$\langle i|T\{\hat{H}_V(\tau_1) \cdots \hat{H}_V(\tau_{2n}) \hat{C}^\dagger_\alpha(t) \hat{C}_{\alpha'}(t)\}|i\rangle = L^{\alpha\alpha'}(\tau_1, \ldots, \tau_{2n}, t) e^{C(\tau_1, \ldots, \tau_{2n})} e^{-iE_d \sum_{j=1}^n (\tau_{2j-1}-\tau_{2j})},$$

(52)

where $L^{\alpha\alpha'}(\tau_1, \ldots, \tau_{2n}, t)$ contains all diagrams that are connected to at least one of the times $\tau_1, \ldots, \tau_{2n}$ or $t$, and $e^{C(\tau_1, \ldots, \tau_{2n})}$ is the closed loop sum. Both quantities are evaluated in the external potential $W(\tau)$ which equals $W$ for $\tau$ in the intervals $(\tau_{2j-1}, \tau_{2j}), j = 1, \ldots, n$, and is zero for all other times. The one-particle propagator in this potential obeys the Dyson equation

$$G(\tau, \tau') = G_0(\tau - \tau') - i \int_{t_0}^{t_1} d\tau'' G_0(\tau - \tau'') W(\tau'') G(\tau'', \tau').$$

(53)
The solution of the latter equation is given in Eq. (A.40) and reads

\[ G(\tau, \tau') = (-i) S^{-1}(\tau) e^{-i\Delta(\tau)} \left| \prod_{j=1}^{n} \frac{\tau - \tau_{2j}}{\tau - \tau_{2j-1}} \right| \frac{\pi}{e^{-i\mu(\tau-\tau')}} \left| \prod_{j=1}^{n} \frac{\tau' - \tau_{2j-1}}{\tau' - \tau_{2j}} \right| \frac{\pi}{e^{i\Delta(\tau)}} \left[ \mathcal{P}\left(\frac{1}{\tau - \tau'}\right) + \pi \Theta(\tau') \delta(\tau - \tau') \right] M(\tau')\nu. \] (54)

for the same definitions of the matrices as in Eqs. (37)–(39) in which the conditions \( \tau \in (\tau_1, \tau_2) \) are replaced by \( \tau \in (\tau_{2j-1}, \tau_{2j}), j = 1, \ldots, n. \)

In order to determine the factor \( L^{\alpha\alpha'}(\tau_1, \ldots, \tau_{2n}, t) \) we take advantage from the fact that the \( \tau_j \) are time ordered, \( \tau_1 < \cdots < \tau_{2n} \). A full contraction of the operators at the times \( \tau_1, \ldots, \tau_{2n}, \tau_{2n+1} = t, \tau_{2n+2} = t \) can be regarded as a permutation \( \pi \) of \( n + 1 \) elements, where the creator \( \hat{C}^\dagger(\tau_{2j}) \) is contracted with the annihilator \( \hat{C}(\tau_{2\pi(j)-1}) \). By Wick’s theorem, the whole amplitude must be multiplied by the signature of the permutation that brings all contracted operators together. Since the operators at the times \( \tau_1, \ldots, \tau_{2n} \) are explicitly time ordered and since the operators at \( t \) occur as a pair of creation and annihilation operators (for which their relative position with respect to the \( \tau_j \) is of no importance) this separation is performed by \( \pi^{-1} \). Every contraction is expressed by the factor \(-G_{\alpha 2\pi(j)-1, \alpha 2j}(\tau_{2\pi(j)-1}, \tau_{2j})\) as was seen in the previous section. Therefore, the sum over all contractions equals the sum over all permutation \( \pi \) and is given by \( \tau_{2n+1} = \tau_{2n+2} = t, \alpha_{2n+1} = \alpha', \alpha_{2n+2} = \alpha \)

\[ L^{\alpha\alpha'}(\tau_1, \ldots, \tau_{2n}, t) = \]

\[ (-1)^n \sum_{\alpha_1 \ldots \alpha_{2n}} (V^{\alpha_1})^* V^{\alpha_2} \cdots V^{\alpha_{2n}} \sum_{\pi} \text{sign}(\pi^{-1}) \prod_{j=1}^{n} G_{\alpha^{2\pi(j)-1}\alpha 2j}(\tau_{2\pi(j)-1}, \tau_{2j}) = \]

\[ (-1)^n \sum_{\alpha_1 \ldots \alpha_{2n}} (V^{\alpha_1})^* V^{\alpha_2} \cdots V^{\alpha_{2n}} \det_{n+1} G_{\alpha 2j-1\alpha 2k}(\tau_{2j-1}, \tau_{2k}) \] (55)

where we used Leibniz’ definition of the determinant. The subscript \( n+1 \) in the determinant indicates that it must be taken over the indices \( j, k = 1, \ldots, n+1. \) Again the Green’s functions \( G(\tau_{2j-1}, \tau_{2k}) \) and \( G(t, t) \) are singular and must be cured by the cutoff \( \xi_0 \) as in Eqs. (42) and (43). The closed loops are determined by the equation

\[ \lambda \frac{\partial C(\tau_1, \ldots, \tau_{2n})}{\partial \lambda} \bigg|_{\lambda=1} = i \int_{t_0}^{t_1} d\tau \ Tr [W(\tau) G(\tau, \tau)] . \] (56)

A similar kind of investigation of the singular and nonsingular behavior of
Discussion and limiting cases

In order to obtain the full expression at order 2 for \( F_W(t) \), we must integrate over the times \( \tau_1, \ldots, \tau_{2n} \) with the constraint of \( t \) lying on a time interval in which the localized state is occupied. This can be taken into account if we multiply the integrand by the expression \( \sum_{m=1}^{n+1} \delta_{\alpha_2m, \alpha'} \delta(t-\tau_{2m}) \delta(t-\tau_{2m+1}) \) and integrate over the \( 2n + 2 \) time variables \( \tau_1 < \cdots < \tau_{2n+2} \) and sum over the indices \( \alpha_1, \ldots, \alpha_{2n+2} \). The time order of the integration variables drops the factor \( 1/(2n)! \) in the Dyson series, and the full amplitude reads

\[
\left[ F_W^{\alpha\alpha'}(t) \right]_{(2n)} = (-i)^n \int_{t_0<\tau_1<\cdots<\tau_{2n+2}<t_1} d\tau_1 \cdots d\tau_{2n+2} \sum_{\alpha_1 \cdots \alpha_{2n}} (V^{\alpha_1})^* V^{\alpha_2} \cdots V^{\alpha_{2n+2}} \frac{1}{(V^\alpha)^* V^{\alpha'}} \sum_{m=1}^{n+1} \delta_{\alpha_2m, \alpha'} \delta(t-\tau_{2m}) \delta(t-\tau_{2m+1}) \right] \det_n G^{\alpha_{2j-1}, \alpha_{2k}}(\tau_{2j-1}, \tau_{2k}) e^{-i(E_d+\Delta E_1) \sum_{j=1}^{n} (\tau_{2j}-\tau_{2j-1})} \exp \left[ \frac{Tr\Delta^2}{\pi^2} \sum_{i,j=1}^{2n} (-1)^{i+j} \ln \left( i\xi_{0}(\tau_{2j-\tau_i}) \right) \right].
\]

In order to obtain the full expression at order 2 for \( F_W^{\alpha\alpha'}(t) \), we must integrate over the times \( \tau_1, \ldots, \tau_{2n} \) with the constraint of \( t \) lying on a time interval in which the localized state is occupied. This can be taken into account if we multiply the integrand by the expression \( \sum_{m=1}^{n+1} \delta_{\alpha_2m, \alpha'} \delta(t-\tau_{2m}) \delta(t-\tau_{2m+1}) \) and integrate over the \( 2n + 2 \) time variables \( \tau_1 < \cdots < \tau_{2n+2} \) and sum over the indices \( \alpha_1, \ldots, \alpha_{2n+2} \). The time order of the integration variables drops the factor \( 1/(2n)! \) in the Dyson series, and the full amplitude reads

\[
\left[ F_W^{\alpha\alpha'}(t) \right]_{(2n)} = (-i)^n \int_{t_0<\tau_1<\cdots<\tau_{2n+2}<t_1} d\tau_1 \cdots d\tau_{2n+2} \sum_{\alpha_1 \cdots \alpha_{2n}} (V^{\alpha_1})^* V^{\alpha_2} \cdots V^{\alpha_{2n+2}} \frac{1}{(V^\alpha)^* V^{\alpha'}} \sum_{m=1}^{n+1} \delta_{\alpha_2m, \alpha'} \delta(t-\tau_{2m}) \delta(t-\tau_{2m+1}) \right] \det_n G^{\alpha_{2j-1}, \alpha_{2k}}(\tau_{2j-1}, \tau_{2k}) e^{-i(E_d+\Delta E_1) \sum_{j=1}^{n} (\tau_{2j}-\tau_{2j-1})} \exp \left[ \frac{Tr\Delta^2}{\pi^2} \sum_{i,j=1}^{2n} (-1)^{i+j} \ln \left( i\xi_{0}(\tau_{2j-\tau_i}) \right) \right].
\]

6 Discussion and limiting cases

If we introduce the expressions (51) and (58) into the Dyson series (21) for \( F_W^{\alpha\alpha'} \), we obtain

\[
(V^\alpha)^* V^{\alpha'} F_W^{\alpha\alpha'}(t) = \sum_{n=2}^{\infty} (-i)^{2n} \int_{t_0<\tau_1<\cdots<\tau_{2n}<t_1} d\tau_1 \cdots d\tau_{2n} \sum_{\alpha_1 \cdots \alpha_{2n}} (V^{\alpha_1})^* V^{\alpha_2} \cdots V^{\alpha_{2n}} \sum_{m=1}^{n} \delta_{\alpha_{2m-1}, \alpha} \delta_{\alpha_{2m}, \alpha'} \delta(\tau_{2m-1}-t) \delta(t-\tau_{2m}) \right] \det_n G^{\alpha_{2j-1}, \alpha_{2k}}(\tau_{2j-1}, \tau_{2k}) e^{-i(E_d+\Delta E_1) \sum_{j=1}^{n} (\tau_{2j}-\tau_{2j-1})} \exp \left[ \frac{Tr\Delta^2}{\pi^2} \sum_{i,j=1}^{2n} (-1)^{i+j} \ln \left( i\xi_{0}(\tau_{2j-\tau_i}) \right) \right].
\]

A similar derivation holds for \( F_V^{\alpha}(t) \). The main difference lies in the fact that one single creation operator is fixed at the time \( t \). Its relative position with respect to the times of integration is important to determine the signature of the permutation separating the contractions. We express this property by multiplying the integrand by \( \sum_{m=1}^{n} \delta_{\alpha, \alpha_{2m}} \delta(t-\tau_{2m}) \). The integration is performed
over \( \tau_1 < \cdots < \tau_{2n} \), and the sum over \( \alpha_1, \ldots, \alpha_{2n} \). This yields

\[
V^\alpha F^\alpha_V(t) = \sum_{n=1}^{\infty} (-i)^{2n-1} \int_{t_0 < \tau_1 < \cdots < \tau_{2n} < t_1} d\tau_1 \cdots d\tau_{2n} \left[ \sum_{m=1}^{n} \delta_{\alpha, \alpha_{2m}} \delta(t - \tau_{2m}) \right] 
\]

\[
\begin{aligned}
&\left( V^{\alpha_1} \right)^* V^{\alpha_2} \cdots V^{\alpha_{2n}} \det_n G^{\alpha_{2j-1} \alpha_{2k}}(\tau_{2j-1}, \tau_{2k}) \\
&\exp \left[ \frac{T \Delta^2}{\pi^2} \sum_{i,j=1}^{2n} (-1)^{i+j} \ln \left( i \xi_0 (\tau_j - \tau_i) \right) \right] \\
&\quad \quad \quad \quad \quad \exp \left[ i \beta \sum_{j=1}^{n} (\tau_{2j} - \tau_{2j-1}) \right] e^{-i(E_d + \Delta E_1) \sum_{j=1}^{n} (\tau_{2j} - \tau_{2j-1})}. \tag{60}
\end{aligned}
\]

The latter two equations represent the central result of this article. Since they are by far too complex for a direct interpretation, we discuss here two limiting cases. The first one consists in the scalar problem with only one channel \( \alpha \). In the second one we suppress the off-diagonal terms, \( \alpha \neq \alpha' \), in the matrix \( W^{\alpha \alpha'} \).

If we assume that the number \( N \) of quantum channels \( \alpha \) is equal to 1, the present model can be interpreted as an extension to all orders of perturbation of ND’s x-ray absorption model [1], or as the spin 1/2 Kondo problem investigated by Yuval and Anderson [3] where the occupancy of the localized state \( \phi_d \) corresponds to the directions of the impurity spin. The propagator at the \( n \)-th order of perturbation simplifies to

\[
G(\tau, \tau') = \frac{-i\nu}{\beta} \prod_{j=1}^{n} \left[ \frac{\tau - \tau_{2j}}{\tau - \tau_{2j-1}} \frac{\tau' - \tau_{2j}}{\tau' - \tau_{2j-1}} \right] \frac{\beta}{\pi} e^{-i\mu(\tau - \tau')} \\
\left[ P \left( \frac{1}{\tau - \tau'} \right) + \pi \tan \vartheta' \delta(\tau - \tau') \right], \tag{61}
\]

for \( \tau, \tau' \) lying on an interval where \( W \neq 0 \). The constants \( \beta \) and \( \tan \vartheta' \) are given by (see [1], Eq. (42))

\[
\beta = 1 - 2\pi g \tan \vartheta + \pi^2 g^2 / \cos^2 \vartheta,
\]

\[
\tan \vartheta' = \tan \vartheta - \pi g / \cos^2 \vartheta,
\]

and \( \delta \) is the phase shift. Since all \( G(\tau_{2j-1}, \tau_{2k}) \) commute and the exponent \( \delta/\pi \) is the same for all factors in the determinant, the latter can be expressed in terms of Cauchy determinants, which are defined as (see [7], Chap. 7, 3.)

\[
(Cauchy)_n = \det_n \left[ \frac{1}{\tau_{2j-1} - \tau_{2k}} \right] = \frac{\prod_{1 \leq j < k \leq n} (\tau_{2j-1} - \tau_{2k-1})(\tau_{2k} - \tau_{2j})}{\prod_{j,k=1,\ldots,n} (\tau_{2j-1} - \tau_{2k})}. \tag{62}
\]
If \( \tau_1 < \cdots < \tau_{2n} \), we have

\[
(Cauchy)_n = (-1)^n \exp \left( \sum_{i,j=1 \atop i<j}^{2n} (-1)^{i+j} \ln |\tau_j - \tau_i| \right). \tag{63}
\]

The determinant in \( L(\tau_1, \ldots, \tau_{2n}, t) \) reads \( (\tau_{2n+1} = \tau_{2n} = t) \)

\[
\det_{n+1} G(\tau_{j-1}, \tau_k) = \left( \frac{-i \nu}{\beta} \right)^{n+1} e^{+i \mu \sum_{j=1}^{n}(\tau_j - \tau_{j-1})} \prod_{j=1}^{n+1} \prod_{k=1}^{n} \frac{\tau_{2j-1} - \tau_{2k} - \tau_{2j-2} - \tau_{2k-1}}{\tau_{2j-1} - \tau_{2k}} \frac{\tau_{2j} - \tau_{2k}}{\tau_{2j} - \tau_{2k}} \int_{1}^{+1} \det_{n+1} \left[ 1 \frac{1}{\tau_{2j-1} - \tau_{2k}} \right],
\]

where all singularities must be replaced by the cutoff \( i \xi_0 \). The last factor is a Cauchy determinant in which all factors depending on \( t \) cancel out, except the singular contribution \( 1/(t-t) \) for which we introduce a cutoff, too. Similarly, the double product in front of the determinant does not depend on \( t \), and is nothing else than \( (i \xi_0^2/(Cauchy)_n)^2 \). Hence

\[
\det_{n+1} G(\tau_{j-1}, \tau_k) = \left( \frac{-i \nu}{\beta} \right)^{n+1} \xi_0^{1+2n} e^{+i \mu \sum_{j=1}^{n}(\tau_j - \tau_{j-1})} (-1)^n \exp \left[ (1 - 2 \frac{\Delta}{\pi}) \sum_{i,j=1 \atop i<j}^{2n} (-1)^{i+j} \ln (i \xi_0(\tau_j - \tau_i)) \right],
\]

where we have used the identity \( \sum_{1 \leq i < j \leq 2n} (-1)^{i+j} = -n \). If we define \( \Omega_m = \{(i,j) | 1 \leq i < j \leq 2n, (i,j) \neq (2m-1, 2m)\} \), we obtain for \( F_W(t) \) a result similar to that of Yuval and Anderson [3].

\[
F_W(t) = \frac{1}{|V|^2} \frac{1}{i \xi_0} \sum_{n=2}^{\infty} \left( \frac{-i \nu}{\beta} \right)^{n} (i \xi |V|)^{2n} \int_{t_0 < \tau_1 < \cdots < \tau_{2n} < t_1} d\tau_1 \ldots d\tau_{2n}
\]

\[
\sum_{m=1}^{n} \delta(\tau_{2m-1} - t) \delta(t - \tau_{2m}) \exp \left[ -i(E_0 + \Delta E_1 - \mu) \sum_{j=1}^{n}(\tau_{2j} - \tau_{2j-1}) \right.
\]

\[
+ \left. (1 - 2 \frac{\Delta}{\pi} + \frac{\delta^2}{\pi^2}) \sum_{(i,j) \in \Omega_m} (-1)^{i+j} \ln (i \xi_0(\tau_j - \tau_i)) \right]. \tag{64}
\]

The function \( F_W(t) \) does no longer express a current but a joint probability amplitude of the presence of a particle in the localized state \( \phi_d \) as well as of a particle in the conduction band described by the operator \( C(t) \). If we pass to imaginary times, \( \tau_j \rightarrow -i \tau_j \), the latter equation becomes formally equivalent to a grand canonical correlation function of a classical one-dimensional gas with two different types of particles: a type \( A \) situated at the (space) positions \( \tau_{2j-1} \), and a type \( B \) at the positions \( \tau_{2j} \). All particles are subject to external potentials, \(- (E_d + \Delta_1 - \mu) \tau \) for the type \( A \) and \( + (E_d + \Delta_1 - \mu) \tau \) for the
type \( B \), as well as to logarithmic two-body interactions which are repulsive between particles of the same type and attractive otherwise. There is no kinetic energy. The cutoff \( \xi_0 \) enters as the (hard-core) volume of the particles. In this context, the positions \( \tau_{2m-1} \) and \( \tau_{2m} \) that are fixed to the value \( t \) by the delta functions must be regarded as having the distance \( \xi_0 \) between each other. The correlation function \( F_W(t) \) can therefore be interpreted as the (unnormalized) average density of a couple \( AB \) at the point \( t \) (with \( A \) to the left of \( B \)).

We can derive an analogous result for the function \( F_V(t) \) which represents now the transition rate of an electron into the localized state. In the same way as above, we find

\[
F_V(t) = \frac{i}{V} \sum_{n=1}^{\infty} \left( -\frac{i\nu}{\beta} \right)^n \left( i\xi_0 |V| \right)^{2n} \int_{t_0<\tau_1<\ldots<\tau_{2n}<t_1} d\tau_1 \ldots d\tau_{2n} \\
\sum_{m=1}^{n} \delta(t - \tau_{2m}) \exp \left[ -i(E_d + \Delta E_1 - \mu) \sum_{j=1}^{n} (\tau_{2j} - \tau_{2j-1}) \right] \\
+ (1 - 2\frac{\delta}{\pi} + \frac{\delta^2}{\pi^2}) \sum_{(i,j)\in\Omega_m} (-1)^{i+j} \ln \left( i\xi_0 (\tau_j - \tau_i) \right) \right]. \tag{65}
\]

Analogously, this expresses the average number of particles of the type \( B \) at the position \( t \).

A investigation of the partition function of the one-dimensional gas was performed by Anderson, Yuval and Hamann [4] by renormalization group methods, a route we will not pursue here. For the general case with the number of channels \( N \geq 2 \), a similar mapping onto a classical gas is not possible in the same way because the determinants of propagators do not form Cauchy determinants. Within the scope of the present work a similar, but different mapping has not been found.

Let us now consider the case in which the left and right electrodes are not coupled via \( H_W \). If we assume further that each electrode contains some number of different non-interacting quantum channels, we recover a simplified version of the system considered by Matveev and Larkin [5]. The latter authors computed the phase shifts for different geometries of the electrodes and determined the current through the resonant level in the barrier in first nontrivial order in perturbation, corresponding to \( [F^R_V(t)]_2 \) in our notation. If there is only one quantum channel in each electrode, we have

\[
\left[ F^R_V(t) \right]_2 = (V^R)^s \frac{\mu_R}{\beta_R} \int_{t_0}^{t} \frac{e^{-i(E_d + \Delta E_1 - \mu_\beta)(t-\tau)}}{t - \tau} \left( i\xi_0 (t - \tau) \right)^{-2\frac{\delta}{\pi} + \frac{\delta^2}{\pi^2}} \left( \frac{\beta}{\pi} \right)^{\frac{\delta^2}{\pi^2}},
\]

with a similar definition of \( \beta_R \) as for \( \beta \) above. We see that the influence of the left electrode enters through the closed loop spreading only. In the limit \( t_0 \to -\infty \), this expression becomes time-independent (it is a Gamma function),
whereas scaling arguments reveal the resonant behavior of the current

\[
\left[ F^R \right]_{(2)} \sim (E_d + \Delta E_1 - \mu_R)^2 \delta_R - \frac{\delta^2}{\pi} - \frac{\delta^2}{\pi^2}.
\]

Following [3] the sign of the exponent depends on whether the impurity state is localized near the left or near the right electrode.

7 Conclusions

In this paper we studied the tunneling of interacting spinless electrons through an insulating barrier. It was assumed that the interaction was restricted to scattering of conduction electrons with a single trapped particle in a structureless localized state in the barrier. Our central result is given in Eqs. (59) and (60) in which we express the tunneling current as an infinite perturbation series with respect to the hybridization term of the Hamiltonian. An extension of the method of Nozières and De Dominicis [1] allowed an exact computation of each term in this series, including the effects of transient interaction between the conduction electrons and the localized state. The renormalization of the tunneling amplitude due to the additional charge in the barrier was taken into account.

The calculations were based on two essential assumptions: a separable potential, and a completely structureless localized state. Since the uncoupled systems were assumed to be Fermi liquids, the model does not apply to one-dimensional systems. With these limitations, extensions of the model may be considered, such as to include electron-phonon interactions, many traps, or disorder in the barrier as well as in the electrodes. Because of the nanometric size of the system, disorder in the electrodes situates us in the regime of the universal conductance fluctuations (UCF) which have been intensively investigated in the last two decades [12]. It is believed that further developments of the present work will yield a microscopic description of the stochastic time behavior of these fluctuations.

A Solution of the singular integral equation

In this appendix we solve the system of coupled singular integral equations obtained from the Dyson equations (28) and (53) for the one-body matrix propagator \( G^{\alpha\alpha'}(\tau, \tau') \) which we denote in this section as \( \varphi^{\alpha\alpha'}(\tau, \tau') \). Generally,
these systems of integral equations can be written in the form

\[ A(\tau) \varphi(\tau, \tau') - \frac{1}{\pi i} \int_L B(\tau'') \frac{\varphi(\tau'', \tau')}{\tau'' - \tau} \, d\tau'' = f(\tau, \tau'). \]  

(A.1)

Here \( A, B \) and \( f \) are given \( N \times N \) matrix functions, \( \varphi \) is the unknown propagator with the entries \( \varphi^{\alpha \alpha'} \), and \( L \) is a contour in the complex plane with the end points \( t \) and \( t' \) which may take finite values or lie at infinity (we do not consider the case where \( L \) is a closed contour, i.e. \( t = t' \)). The positive direction on \( L \) is chosen to run from \( t \) to \( t' \).

The technique to solve such integral equations was developed by Muskhelishvili [8] and Vekua [9] and consists normally in a transformation to a system of ordinary coupled Fredholm equations. However, the particular form of the coefficients \( A \) and \( B \) as given in Eqs. (29) and (30) and their generalization to higher orders in perturbation allows us to develop a compact, closed solution by a method similar to that used by Yuval and Anderson [3] for the scalar problem. This method is in fact nothing else than Vekua’s technique to regularize discontinuities in the coefficients \( A \) and \( B \), and we formulate it for arbitrary smooth contours \( L \) in the complex plane. In Sec. A.3 this solution will be carried out in detail. Furthermore, we will show its limitation in the solution of more general problems.

A.1 Transformation to a Hilbert problem

The first step in the solution of Eq. (A.1) consists in a transformation of the integral equation to a Hilbert boundary value problem. We follow the lines of Muskhelishvili and Vekua (see e.g. [9] §16), which we expose briefly in the sequel.

From now on it is assumed that the functions \( A(\tau) \) and \( B(\tau) \) are \( N \times N \) matrices, which are - for the theory to be valid - required to be such that

\[ S(\tau) \equiv A(\tau) + B(\tau), \quad D(\tau) \equiv A(\tau) - B(\tau), \]

are regular, i.e. \( \det S(\tau) \neq 0 \) and \( \det D(\tau) \neq 0 \) for all \( \tau \in L \). Furthermore we assume that all entries of \( A(\tau) \) and \( B(\tau) \) satisfy a Hölder condition on the line \( L \) except at some points \( \tau_1, \ldots, \tau_d \in L \) where they have finite discontinuities, but where they still are assumed to be such that \( S(\tau) \) and \( D(\tau) \) remain regular when considering the left and right limits \( \tau \to \tau_k \pm 0 \) (\( k = 1, \ldots, d \)) on \( L \).

The Hilbert problem is formulated by means of the function \( \Psi(z) \), which is holomorphic in the whole plane, except on the line \( L \) where it is continuous from the left and the right side with respect to the positive direction of \( L \).
(except possibly at the points $\tau_k$),

$$\Psi(z) = \frac{1}{\pi i} \int_L \frac{B(\tau'') \varphi(\tau'')}{\tau'' - z} \, d\tau''.$$ 

In the terminology of Muskhelishvili and Vekua, such a function is called a \textit{sectionally holomorphic function}.

The connection between the functions $\Psi$ and $\varphi$ is given by the Plemelj formulae (see e.g. [8], §17 or [9], §3)

$$\frac{1}{2} \left[ \Psi^+(\tau) - \Psi^-(\tau) \right] = B(\tau) \varphi(\tau, \tau'),$$

$$\frac{1}{2} \left[ \Psi^+(\tau) + \Psi^-(\tau) \right] = \frac{1}{\pi i} \int_L \frac{B(\tau'') \varphi(\tau'', \tau')}{\tau'' - \tau} \, d\tau''$$

for $\tau \in L$, not a point of discontinuity $\tau_k$. The functions $\Psi^+(\tau)$ and $\Psi^-(\tau)$ denote respectively the limiting values of $\Psi(z)$ when $z$ approaches the point $\tau \in L$ from the left or the right side of $L$ with respect to the positive direction on $L$. By replacing the integral in equation (A.1) by the second Plemelj formula (A.2) we obtain

$$A(\tau) \varphi(\tau) = \frac{1}{2} \left[ \Psi^+(\tau) + \Psi^-(\tau) \right] + f(\tau).$$

Adding and subtracting the first Plemelj formula (A.2) from this last expression leads to

$$\varphi(\tau) = [S(\tau)]^{-1} \Psi^+(\tau) + [S(\tau)]^{-1} f(\tau),$$

$$\varphi(\tau) = [D(\tau)]^{-1} \Psi^-(\tau) + [D(\tau)]^{-1} f(\tau).$$

(A.3)

From these two expressions we obtain the following Hilbert boundary value problem, equivalent to the integral equation (A.1),

$$\Psi^+(\tau) = \mathfrak{S}(\tau) \Psi^-(\tau) + b(\tau)$$

(A.4)

where we have defined

$$\mathfrak{S}(\tau) = S(\tau) [D(\tau)]^{-1} = [A(\tau) + B(\tau)] [A(\tau) - B(\tau)]^{-1},$$

$$b(\tau) = \left( \mathfrak{S}(\tau) - \mathbb{1} \right) f(\tau, \tau').$$

(A.5)

The matrix $\mathfrak{S}$ is called the \textit{coefficient} of the Hilbert problem. Once we have found the solution of the Hilbert problem (A.4) the function $\varphi(\tau, \tau')$ can be recovered by any of the equations (A.3).

As will be shown below, this matrix $\mathfrak{S}$ is equal to the inverse scattering matrix at the Fermi levels, and is therefore unitary.
The Hilbert problem (A.4) is solved by means of a particular solution (the so-called fundamental solution) of the homogeneous Hilbert problem obtained by putting $b(\tau) \equiv 0$ in (A.4). This fundamental solution will be computed in Sec. A.3 and is given by a $N \times N$ matrix function $X(z)$, where $z$ is a point in the plane, not on $L$. The limits of $X(z)$ on $L$ from the left and from the right with respect to the positive direction on $L$ will be denoted by $X^+(\tau)$ and $X^-(\tau)$, respectively, for $\tau \in L\backslash\{\tau_1, \ldots, \tau_d\}$.

Since $X(z)$ is a solution of the homogeneous Hilbert problem corresponding to (A.4), we have

$$\mathcal{S}(\tau) = X^+(\tau) [X^-(\tau)]^{-1}.$$  

By Vekua [9, §6], the general solution of the non homogeneous problem (A.4), having at most polynomial divergence at infinity, is then given by the expression

$$\Psi(z) = \frac{X(z)}{2\pi i} \int_L \frac{[X^+(\tau'')]^{-1} b(\tau'')}{\tau'' - z} \, d\tau'' + X(z) p(z)$$

with $p(z)$ a matrix of size $N \times N$ with arbitrary polynomials as entries which must be determined by the boundary conditions. In the physical applications to follow, it is sufficient to notice that the function $\varphi(\tau, \tau')$ is a Green’s function which must vanish as its arguments go to infinity. Since the function $X(z)$ remains bounded at infinity (as we will see later) these polynomials must identically vanish, which allows us to drop the term $X(z) p(z)$ in the sequel.

The boundary values $\Psi^+(\tau)$ and $\Psi^-(\tau)$ follow again from the Plemelj formulae and are given by

$$\Psi^+(\tau) = X^+(\tau) \left\{ + \frac{1}{2} [X^+(\tau)]^{-1} b(\tau) \right. + \frac{1}{2\pi i} \int_L \frac{[X^+(\tau'')]^{-1} b(\tau'')}{\tau'' - \tau} \, d\tau'' \left. \right\},$$

$$\Psi^-(\tau) = X^-(\tau) \left\{ - \frac{1}{2} [X^+(\tau)]^{-1} b(\tau) \right. + \frac{1}{2\pi i} \int_L \frac{[X^+(\tau'')]^{-1} b(\tau'')}{\tau'' - \tau} \, d\tau'' \left. \right\}.$$  

The solution of the original integral equation (A.1) can then be computed by any of the equations (A.3) and takes the form

$$\varphi(\tau, \tau') = A(\tau) f(\tau) - \frac{1}{\pi i} \mathcal{Z}(\tau) \int_L \frac{B(\tau'') f(\tau'')}{\tau'' - \tau} \, d\tau'' \quad (A.7)$$
where we have defined

\[ A(\tau) = \frac{1}{2} \left\{ [S(\tau)]^{-1} + [D(\tau)]^{-1} \right\}, \quad (A.8) \]

\[ B(\tau) = \frac{1}{2} \left\{ [X^+(\tau)]^{-1} - [X^-(\tau)]^{-1} \right\}, \quad (A.9) \]

\[ Z(\tau) = [S(\tau)]^{-1} X^+(\tau) = [D(\tau)]^{-1} X^-(\tau). \quad (A.10) \]

The fact that the inhomogeneous term \( f(\tau, \tau') \) is proportional to the free propagator and that \( B(\tau) \) is the difference between the limiting values of the inverse fundamental solution allows us to evaluation the remaining integral in (A.7),

\[ I = \int_L B(\tau'') \frac{f(\tau'')}{\tau'' - \tau} \, d\tau''. \quad (A.11) \]

Let us write

\[ f(\tau) = a \mathcal{P}\left(\frac{1}{\tau - \tau'}\right) + b \delta(\tau - \tau') \quad (A.12) \]

where \( a \) and \( b \) are \( N \times N \) matrices that may depend on \( \tau' \) but not on \( \tau \). Such \( f \) can be continued analytically to the remaining complex plane, and vanish at \( |z| \to \infty \). Considering the term proportional to \( a \) only and assuming that \( \tau \neq \tau' \), the integral (A.11) can be calculated explicitly by the integration of \( [X(z)]^{-1} a / (z - \tau)(z - \tau') \) over the contour \( C \) indicated in Fig. A.1. In fact, by the theorem of residues, we have on the one hand

\[ \oint_C \frac{[X(z)]^{-1} a \, dz}{(z - \tau)(z - \tau')} = 0. \]

Since \( X(z) \) is the fundamental solution, we will see in Sec. A.3 that its entries are non-vanishing, analytic functions everywhere in \( \mathbb{C} \) except on \( L \setminus \{ \tau_1, \ldots, \tau_d \} \) where it is continuous from the left and the right. At the points \( \tau_1, \ldots, \tau_d \) it either has integrable poles or vanishes. Moreover, we will see that \( X(z) \) remains bounded at infinity, and hence there is no residue at infinity. On the
other hand, the integral on the contour $C$ can be split as follows

\[
\oint_C \frac{[X(z)]^{-1} a \, dz}{(z - \tau)(z - \tau')} = \int_L \frac{[X^+(\tau'')]^{-1} a \, d\tau''}{(\tau'' - \tau)(\tau'' - \tau')} - \int_L \frac{[X^-(\tau'')]^{-1} a \, d\tau''}{(\tau'' - \tau)(\tau'' - \tau')}
\]

\[-\pi i \left[ \frac{[X^+(\tau)]^{-1} + [X^-(\tau)]^{-1}}{\tau - \tau'} a - \pi i \left[ \frac{[X^+(\tau')]^{-1} + [X^-(\tau')]^{-1}}{\tau' - \tau} a \right] \right].
\]

Notice that the singularities at the points of discontinuity (if there are any) are of order $z^{-\varepsilon}$ for certain $0 < \varepsilon < 1$ and do not contribute. When combining the last two equations, we obtain the integral,

\[
I = \frac{\pi i}{2} P \left( \frac{1}{\tau - \tau'} \right) \left\{ \left( [X^+(\tau)]^{-1} + [X^-(\tau)]^{-1} \right) a 
- \left( [X^+(\tau')]^{-1} + [X^-(\tau')]^{-1} \right) a 
+ \frac{1}{\pi i} \left( [X^+(\tau')]^{-1} - [X^-(\tau')]^{-1} \right) b \right\}.
\]

where we have now added the contribution arising from the integration over the delta function. Since we assumed explicitly that $\tau \neq \tau'$ the last expression has to be considered as being a Cauchy principal value distribution. The singular contribution for $\tau = \tau'$ can be computed from the Poincaré-Bertrand formula

\[
P \left( \frac{1}{\tau'' - \tau} \right) P \left( \frac{1}{\tau'' - \tau'} \right) = P \left( \frac{1}{\tau - \tau} \right) \left\{ P \left( \frac{1}{\tau'' - \tau} \right) - P \left( \frac{1}{\tau'' - \tau'} \right) \right\}
+ \pi^2 \delta(\tau'' - \tau) \delta(\tau'' - \tau')
\]

and is given by

\[
\frac{\pi^2}{2} \left( [X^+(\tau)]^{-1} - [X^-(\tau)]^{-1} \right) a \delta(\tau - \tau').
\]

These results are introduced into the expression (A.7) which leads to the solution of the integral equation (A.1),

\[
\varphi(\tau, \tau') = Z(\tau) [Z(\tau')]^{-1} \left( A(\tau') a + \frac{1}{\pi i} C(\tau') b \right) P \left( \frac{1}{\tau - \tau'} \right)
+ (A(\tau') b + \pi i C(\tau') a) \delta(\tau - \tau')
\]

(A.13)

where $A(\tau)$ and $Z(\tau)$ are defined by (A.8) and (A.10), where

\[
C(\tau) = \frac{1}{2} \left\{ [S(\tau)]^{-1} - [D(\tau)]^{-1} \right\}.
\]

(A.14)
A.3 Fundamental solution of the homogeneous Hilbert problem obtained from the integral equation

In this section we determine the fundamental solution of the homogeneous Hilbert problem

$$\Phi^+ (\tau) = \mathcal{S}(\tau) \Phi^- (\tau)$$  \hspace{1cm} (A.15)

for $\tau \in L \setminus \{\tau_1, \ldots, \tau_d\}$. The matrix $\mathcal{S}(\tau)$ is defined by Eq. (A.5) for the different cases imposed by the underlying physical problems.

A.3.1 Characterization of the fundamental matrix

Following Vekua [9], §5, a fundamental solution of (A.15) is a matrix, $X(z)$, characterized by the following two properties:

(a) If $X(z)$ is a fundamental matrix, then its determinant, $\det X(z)$, does not vanish anywhere in the finite part of the complex plane.

(b) Let $\zeta(z)$ be the vector formed from the column $\beta$ ($\beta = 1, \ldots, N$) of $X(z)$, $\zeta_{\alpha}(z) = X_{\alpha\beta}(z)$ for $\alpha = 1, \ldots, N$, and $(-\kappa_{\beta})$ its degree at infinity (i.e. $\zeta_{\alpha}(z) = \mathcal{O}(z^{-\kappa_{\beta}})$ for $z \to \infty$). Then the determinant $\det Y(z)$ of the matrix $Y_{\alpha\beta}(z) = z^{\kappa_{\beta}} \zeta_{\alpha}(z)$ has a finite non-zero value at infinity.

Any system of solutions (represented by such a matrix $X$) satisfying these two properties will be called fundamental, and it can be shown ([9], §5) that the set of degrees at infinity $\{\kappa_1, \ldots, \kappa_N\}$ is the same for all fundamental systems.

A.3.2 Regularization of the discontinuities

Consider the homogeneous Hilbert problem (A.15). We assume first that the matrix $\mathcal{S}(\tau)$ is a constant, unitary matrix $\mathcal{S}$ on the whole line $L$, $\mathcal{S}(\tau) = \mathcal{S}, \forall \tau \in L$.

We choose an auxiliary line $L'$ in the complex plane such that $\mathcal{C} = L \cup L'$ forms a simple, closed, smooth contour with the positive direction running from $t$ to $t'$ on $L$ and from $t'$ to $t$ on $L'$. The domain bounded by $\mathcal{C}$, denoted by $\mathcal{D}^+$, is assumed to lie to the left of $\mathcal{C}$ with respect to the positive direction. The unbounded region outside the contour is denoted by $\mathcal{D}^-$. As long as these requirements are fulfilled, the choice of $L'$ is arbitrary and has no influence on the result. The Hilbert problem (A.15) can be extended to the contour $\mathcal{C}$ by putting $\mathcal{S}(\tau) = 1$, the $N \times N$ unit matrix, on $L'$. With this choice $\mathcal{S}(\tau)$ has discontinuities at the points $t$ and $t'$.  

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The method presented below consists in a simplified version of Vekua’s technique to suppress the discontinuities of $S(\tau)$. Generally, this transforms the coefficient $S(\tau)$ into a smooth function only and does not give a solution to (A.15). However, in the present case of a constant, unitary coefficient it is already sufficient to solve the problem.

We define the matrices

$$
\gamma = \left[ S(t + 0) \right]^{-1} S(t - 0) = S^{-1},
\gamma' = \left[ S(t' + 0) \right]^{-1} S(t' - 0) = S.
$$

(A.16)

The unitarity of $S$ assures that we can find a unitary matrix $B_0$ that diagonalizes simultaneously $\gamma$ and $\gamma'$ such that

$$
\lambda = B_0^{-1} \gamma B_0,
\lambda' = B_0^{-1} \gamma' B_0,
$$

(A.17)

are diagonal and inverse to each other. Further we may choose the real numbers $\delta_\alpha$, with $-\pi < \delta_\alpha < +\pi, \alpha = 1, \ldots, N$, such that

$$
\lambda_\alpha = e^{-2i\delta_\alpha},
\lambda'_\alpha = e^{+2i\delta_\alpha}.
$$

(A.18)

The condition $-\pi < \delta_\alpha < +\pi$ is a mathematical requirement that ensures the convergence of the expressions, but it is shown in Appendix C that the same restrictions result from purely physical arguments. Even more, the physical constraints fix uniquely the angles $\delta_\alpha$ to be obtained from the phase shifts from the quotient of the scattering matrices immediately before and after a transition (see Eq. (A.16)).

We choose an arbitrary point $z_0$ in $D^+$ and define the diagonal matrix functions $\xi_0, \xi_1$ and $\xi$ as

$$
\left( \xi_0(z) \right)_\alpha = \left( z - z_0 \right)^{\frac{\delta_\alpha}{\pi}},
$$

(A.19)

$$
\left( \xi_1(z) \right)_\alpha = \left( z - t \right)^{\frac{\delta_\alpha}{\pi}},
$$

(A.20)

$$
\left( \xi(z) \right)_\alpha = \left( \frac{z - t}{z - z_0} \right)^{\frac{\delta_\alpha}{\pi}},
$$

(A.21)

for $\alpha = 1, \ldots, N$. Let $\ell$ be a not self-intersecting smooth line that starts at $z_0$, intersects $C$ once in $t$ and goes then to infinity. The whole line $\ell$ is chosen to be the branch line of $\xi_0(z)$, its part starting at $t$ the branch line of $\xi_1(z)$, and its segment $(z_0, t)$ the branch line of $\xi(z)$. Similarly we construct the functions $\xi'_0(z), \xi'_1(z)$ and $\xi'(z)$ which are given by Eqs. (A.19)–(A.21) with the substitutions $t'$ for $t$, and with a branch line $\ell'$ that starts at $z_0$, crosses $C$ at $t'$ and goes then to infinity.
In this way, the functions $\xi(z)$ and $\xi'(z)$ are holomorphic in $D^-$, whereas $\xi_1(z)$ and $\xi'_1(z)$ are holomorphic in $D^+$. All four functions can be continued analytically to the contour $C$ with the exception of their respective branch points $t$ or $t'$. 

Now introduce the matrices

$$A_0 = \mathcal{S}(t + 0) B_0 \left[ \xi_0(t + 0) \right]^{-1} = \mathcal{S}(t - 0) B_0 \left[ \xi_0(t - 0) \right]^{-1},$$

$$A'_0 = \mathcal{S}(t' + 0) B_0 \left[ \xi_0(t' + 0) \right]^{-1} = \mathcal{S}(t' - 0) B_0 \left[ \xi_0(t' - 0) \right]^{-1},$$

and define the functions

$$Q(z) = A_0 \xi_1(z),$$

$$Q'(z) = \left[ Q(t') \right]^{-1} A'_0 \xi'_1(z),$$

for $z \in D^+$, and

$$P(z) = B_0 \xi(z),$$

$$P'(z) = \left[ P(t') \right]^{-1} B_0 \xi'(z),$$

for $z \in D^-$. These functions allow us to substitute the sectionally holomorphic function $\Psi(z)$ in the homogeneous Hilbert problem (A.15) by the new functions

$$\tilde{\Psi}(z) = \begin{cases} 
\left[ Q'(z) \right]^{-1} \left[ Q(z) \right]^{-1} \Phi(z) & \text{for } z \in D^+, \\
\left[ P'(z) \right]^{-1} \left[ P(z) \right]^{-1} \Phi(z) & \text{for } z \in D^-, 
\end{cases}$$

which leads to the new Hilbert problem

$$\tilde{\Psi}^+(\tau) = \tilde{\mathcal{S}}(\tau) \tilde{\Psi}^-(\tau)$$

with the new coefficient

$$\tilde{\mathcal{S}}(\tau) = \left[ Q'(\tau) \right]^{-1} \left[ Q(\tau) \right]^{-1} \mathcal{S}(\tau) P(\tau) P'(\tau).$$

An investigation of the phases of the six functions $\xi_{...}(\tau)$ and $\xi'_{...}(\tau)$ shows that $\tilde{\mathcal{S}}(\tau)$ equals the unit matrix on the whole contour $C$, including the points $t$ and $t'$. The Hilbert problem (A.15) has therefore been reduced to the trivial problem $\tilde{\Psi}^+(\tau) \equiv \tilde{\Psi}^-(\tau)$, which consist in seeking a function which is holomorphic in the whole plane $\mathbb{C}$. This condition, together with the requirements of Sec. A.3.1, shows that the fundamental solution of (A.24) must be a constant matrix, which we choose to be the unit matrix, $\tilde{X}(z) \equiv 1$. Inverting the relations (A.23) leads to the fundamental solution $X(z)$ of the original
problem (A.15),

\[
X(z) = \begin{cases} 
Q(z) Q'(z) & \text{for } z \in D^+, \\
P(z) P'(z) & \text{for } z \in D^-,
\end{cases}
\]  
(A.26)

and it can readily be verified that this function also satisfies the requirements of Sec. A.3.1.

A.3.3 Extension to a coefficient fluctuating between two values

Let us now extend the above method to the case where \(S(\tau)\) is of the form

\[
S(\tau) = \begin{cases} 
\mathbb{G} & \text{for } \tau \in (\tau_j, \tau'_j), \ j = 1 \ldots n \\
\mathbb{1} & \text{otherwise}
\end{cases}
\]

where \(\tau_1, \tau'_1, \tau_2, \tau'_2, \ldots, \tau_n, \tau'_n\) are subsequent points (with respect to the positive direction) on \(L\), and where \(\mathbb{G}\) is a unitary matrix.

We now apply the same regularization method as above. Let us introduce the functions \(\xi_0(z), \xi_1(z)\) and \(\xi(z)\), as well as \(\xi'_0(z), \xi'_1(z)\) and \(\xi'(z)\), for \(k = 1, \ldots, n\), which are defined by Eqs. (A.19)–(A.21) with the substitutions \(\tau_k\) for \(t\) and \(\tau'_k\) for \(t'\), respectively, and the appropriate choice of their branch lines. Consider now the points \(\tau_1\) and \(\tau'_1\) and define

\[
\begin{align*}
\frac{1}{P}(z) &= B_0 \frac{1}{\xi}(z), & \frac{1}{Q}(z) &= A_0 \frac{1}{\xi_1}(z), \\
\frac{1}{P'}(z) &= \left[\frac{1}{\hat{P}(\tau'_1)}\right]^{-1} B_0 \frac{1}{\xi}(z), & \frac{1}{Q'}(z) &= \left[\frac{1}{\hat{Q}(\tau'_1)}\right]^{-1} A_0 \frac{1}{\xi_1}(z),
\end{align*}
\]

where

\[
\begin{align*}
A_0 &= \mathbb{G}(\tau_1 \pm 0) B_0 \left[\frac{1}{\xi_0}(\tau_1 \pm 0)\right]^{-1}, \\
A'_0 &= \mathbb{G}(\tau'_1 \pm 0) B_0 \left[\frac{1}{\xi'_0}(\tau'_1 \pm 0)\right]^{-1}.
\end{align*}
\]

The new coefficient of the Hilbert problem is given by

\[
\mathbb{G}^{(1)}(\tau) = \left[\frac{1}{Q'(\tau)}\right]^{-1} \frac{1}{\hat{Q}(\tau)} \frac{1}{\mathbb{G}(\tau)} \frac{1}{P(\tau)} \frac{1}{P'(\tau)}.
\]

As we have seen above, in the interval \((\tau_1, \tau'_1)\) this new coefficient is equal to \(\mathbb{1}\). But since \(\mathbb{G}(\tau)\) takes only the two values \(\mathbb{1}\) and \(\mathbb{G}\), which are both unitary matrices, and since \(B_0\) diagonalizes \(\mathbb{G}(\tau)\) on the whole line \(L\), the module of \(\mathbb{G}^{(1)}\) is equal to \(\mathbb{1}\) everywhere on \(L\). However, the phases vary between the
different segments on the line, such that
\[
\mathcal{S}^{(1)}(\tau) = \begin{cases} \mathcal{E}^{2i\tilde{\Delta}} & \text{for } \tau \not\in (\tau_1, \tau_1') \text{ and where } \mathcal{S}(\tau) = \mathcal{E} \\ \mathbb{I} & \text{otherwise} \end{cases}
\]
for the diagonal real matrix \(\tilde{\Delta} = \text{diag}(\delta_1, \ldots, \delta_N)\).

If the original Hilbert problem is written in the form
\[
\Psi^+(\tau) = \mathcal{S}(\tau) \Psi^-(\tau)
\]
we have now found an equivalent Hilbert problem expressed by
\[
\left(\left[\mathcal{C}^+(\tau)\right]^{-1} \Psi^+(\tau)\right) = \mathcal{S}^{(1)}(\tau) \left(\left[\mathcal{C}^-(\tau)\right]^{-1} \Psi^-(\tau)\right)
\]
where
\[
\mathcal{C}^+(\tau) = \frac{1}{Q(\tau)} \frac{1}{Q'(\tau)}, \quad \mathcal{C}^-(\tau) = \frac{1}{P(\tau)} \frac{1}{P'(\tau)}.
\]
This is a system of scalar (decoupled) Hilbert problems with discontinuities at the points \(\tau_2, \tau'_2, \ldots, \tau_n, \tau'_n\) which can readily be solved. We can use the functions \(\xi_{k,0,1}(\tau)\) to eliminate the jumps of \(\mathcal{S}^{(1)}\) between the segments. What remains is again a trivial Hilbert problem, \(\tilde{\Psi}^+ \equiv \tilde{\Psi}^-\), for which a fundamental solution is given by \(\tilde{X} = \mathbb{I}\). In fact, we introduce into \(\Psi(z)\) for each point of discontinuity \(\tau_k\) the factor
\[
\begin{align*}
\prod_{k=1}^n \xi(z) \xi'(z) \left[\xi_{k}(\tau'_{k}) \xi'_0(\tau'_{k} + 0)\right]^{-1} & \quad \text{for } z \in \mathcal{D}^+; \\
\prod_{k=1}^n \xi(z) \xi'(z) \left[\xi_{k}(\tau'_{k})\right]^{-1} & \quad \text{for } z \in \mathcal{D}^-.
\end{align*}
\]
Notice the factors with \(\tau'_{k}\) as argument. Their effect is to assure the validity of the solution to the Hilbert problem for any choice of the origin of the phases of complex numbers (i.e. the axis with respect to which they are measured). The final fundamental solution to the Hilbert problem, denoted by \(X(z)\), can then be written in the form
\[
X(z) = \begin{cases} 
B_0 \prod_{k=1}^n \xi_{k}(z) \xi'_{k}(z) B_0^{-1} & \text{for } z \in \mathcal{D}^+ \\
B_0 \prod_{k=1}^n \xi(z) \xi'(z) \xi_{0}(\tau'_{k}) \xi'_0(\tau'_{k} + 0) B_0^{-1} & \text{for } z \in \mathcal{D}^-
\end{cases}
\]
where we have chosen to take \(\xi'_0(\tau'_{k} + 0)\) into the definition of \(\Psi^-(z)\) and we have multiplied all expressions by \(B_0^{-1}\) from the right (which does not change
the Hilbert problem, but assures that \( X(z) \) tends to the unit matrix \( \mathbb{I} \) as \( z \) goes to infinity).

A.3.4 Limits of the method

We show briefly why the above method of regularization does not give the solution for the case where \( \mathcal{S}(\tau) \) is a more general piecewise constant function, taking the values \( \mathcal{S}_1, \mathcal{S}_2, \ldots \) on \( L \).

For instance, assume that the coefficient has the form

\[
\mathcal{S}(\tau) = \begin{cases} \\
\mathcal{S}_1 & \text{for } \tau \in I_1 \equiv (\tau_1, \tau_2) \\
\mathcal{S}_2 & \text{for } \tau \in I_2 \equiv (\tau_2, \tau_3) \\
\mathbb{I} & \text{otherwise}
\end{cases}
\]

for \( \tau_1, \tau_2, \tau_3 \) some subsequent points on \( L \).

For the Hilbert problem

\[
\Psi^+(\tau) = \mathcal{S}(\tau) \Psi^-(\tau)
\]  
(A.28)

the regularization above consists in an ansatz in form of a product, \( \Psi(z) = \psi_1(z) \psi_2(z) \) where \( \psi_k(z) \) is the solution of

\[
\psi_k^+(\tau) = \begin{cases} \\
\mathcal{S}_k \psi_k^-(\tau) & \text{if } \tau \in I_k \\
\psi_k^-(\tau) & \text{otherwise}
\end{cases}
\]

for \( k = 1, 2 \). If we put this expression into Eq. (A.28) we must have

\[
\psi_1^+(\tau) \psi_2^+(\tau) = \mathcal{S}(\tau) \psi_1^-(\tau) \psi_2^-(\tau).
\]

This equation is satisfied for \( \tau \in I_1 \). But if \( \tau \in I_2 \), the function \( \psi_2(z) \) must simultaneously satisfy the equations

\[
\psi_2^+(\tau) = \mathcal{S}_2 \psi_2^-(\tau),
\]

\[
\psi_2^+(\tau) = \left( [\psi_1^+(\tau)]^{-1} \mathcal{S}_2 \psi_1^-(\tau) \right) \psi_2^-(\tau).
\]

In other words, since \( \psi_1^+(\tau) = \psi_1^-(\tau) \equiv \psi_1(\tau) \) on \( I_2 \), it is required that

\[
\mathcal{S}_2 = [\psi_1(\tau)]^{-1} \mathcal{S}_2 \psi_1(\tau) \quad \forall \tau \in I_2.
\]

This means that \( \mathcal{S}_2 \) and \( \psi_1(\tau) \) must commute, which is equivalent to saying (by the construction of \( \psi_1 \)) that \( \mathcal{S}_2 \) and \( \mathcal{S}_1 \) must commute. Generally, there is no reason why they should, and the regularization method sketched above
cannot be used to solve the problem. In such cases, Vekua’s complete theory which uses Fredholm integral equations is required.

If, however, \( S_1 \) and \( S_2 \) (or all matrices \( S_k \) in an extension to more than two different matrices) commute, they can all be diagonalized simultaneously, and the procedure of the previous section applies. The only modification in the result (A.27) is that the matrices \( \hat{\Delta} \) in the definition of the functions \( \xi \) have additional indices \( k \) indicating their origin from \( [S_k]^{-1} S_{k-1} \).

A.4 Solution of the Dyson equations

We turn now to the solution of the Dyson equations (28) and (53). Consider first Eq. (28) which is almost of the form of the singular integral equation (A.1) considered in the previous section. The only difference in (28) is the dependence of the coefficients \( \tilde{A}(\tau) \) and \( \tilde{B}(\tau) \) on the phase factors \( e^{i\mu\tau} \). In the transformation to a Hilbert problem this difference is of no significance. Therefore, if we follow the lines indicated in Sec. A.1 we are lead to the equation

\[
\Psi^+(\tau) = \tilde{\mathcal{S}}(\tau) \Psi^-(\tau) + b(\tau)
\]  
(A.29)

with

\[
\tilde{\mathcal{S}}(\tau) = \left[ \tilde{A}(\tau) + \tilde{B}(\tau) \right] \left[ \tilde{A}(\tau) - \tilde{B}(\tau) \right]^{-1}
\]

\[
= e^{i\mu\tau} \left[ A(\tau) + B(\tau) \right] \left[ A(\tau) - B(\tau) \right]^{-1} e^{-i\mu\tau}
\]

\[
=e^{i\mu\tau} \mathcal{S}(\tau) e^{-i\mu\tau},
\]

and

\[
b(\tau) = \left( \tilde{\mathcal{S}}(\tau) - \mathbb{1} \right) \tilde{f}(\tau, \tau').
\]

The coefficient \( \mathcal{S}(\tau) \) fulfills the requirement of being a constant unitary matrix function on the line \( L = (\tau_1, \tau_2) \) with the value (from Eq. (34))

\[
\mathcal{S} = \left( \mathbb{1} - \pi(\tan \vartheta + i\mathbb{1})g \right) \left[ \mathbb{1} - \pi(\tan \vartheta - i\mathbb{1})g \right]^{-1}. \quad \text{(A.30)}
\]

By comparison with the result of Appendix B, Eq. (B.8), this function is the inverse scattering matrix for electrons at the Fermi surfaces, and we can define the hermitian matrix \( \Delta \) by

\[
\mathcal{S} = e^{2i\Delta}. \quad \text{(A.31)}
\]

The eigenvalues of \( \Delta \) are the phase shifts which we choose, as discussed in Appendix C, to lie between \(-\pi\) and \(+\pi\).
Hence, the homogeneous Hilbert problem

\[ \Phi^+(\tau) = \mathcal{G}(\tau) \Phi^-(\tau) \]

obtained from (A.29) by the substitution \( \Phi(z) = e^{-i\mu z} \Psi(z) \) and by putting \( b(\tau) \equiv 0 \), can be solved by the method described above. This leads to the fundamental matrix \( X(z) \), given by Eq. (A.27),

\[
X(z) = \begin{cases} 
B_0 \xi_1(z) \xi'_1(z) B^{-1}_0 & \text{for } z \in \mathcal{D}^+, \\
B_0 \xi(z) \xi'(z) \xi_0(\tau'_k) \xi'_0(\tau'_k + 0) B^{-1}_0 & \text{for } z \in \mathcal{D}^-. 
\end{cases}
\]

Since the line \( L \) coincides with the segment \([\tau_1, \tau_2]\) of the real axis, this formula can be simplified. If we choose for the logarithm the usual cut on the negative real axis, the function \( X(z) \) can be written in the form

\[
X(z) = \left( \frac{z - \tau_2}{z - \tau_1} \right)^\Delta \left( \frac{z - \tau_2}{z - \tau_1} \right)^\Delta B^{-1}_0 \quad \text{(A.32)}
\]

for any \( z \), not on \([\tau_1, \tau_2]\), with the definition \( t^\Delta = \exp(\Delta \log t) \).

To establish the fundamental solution, \( \tilde{X}(z) \), of the original homogeneous problem obtained from (A.29), it is not sufficient to substitute \( \tilde{X}(z) = e^{i\mu z} X(z) \), because this function is singular at infinity. For \( \tilde{X}(z) \) to be bounded at infinity, we use the fact that \( X(z) \to I \) as \( |z| \to \infty \), and that a solution to the homogeneous Hilbert problem remains a solution when it is multiplied by any matrix from the right. Therefore, the matrix function

\[
\tilde{X}(z) = e^{i\mu z} X(z) e^{-i\mu z} \quad \text{(A.33)}
\]

fulfills all requirements for a fundamental solution to the original homogeneous Hilbert problem.

The inhomogeneous term \( \tilde{f} \) is given by Eq. (31),

\[
\tilde{f}(\tau, \tau') = e^{i\mu \tau} G_0(\tau - \tau') = (-i\nu) \left[ \mathcal{P}\left( \frac{1}{\tau - \tau'} \right) + \pi \tan \delta(\tau - \tau') \right] e^{i\mu \tau'}
\]

and is thus of the form of Eq. (A.12). The solution of the integral equation (28) is then provided by Eq. (A.13), which reads explicitly, for \( \tau, \tau' \in \mathbb{R} \),

\[
G(\tau, \tau') = (-i) S^{-1}(\tau) e^{-i\Delta(\tau)} \left[ \frac{\tau - \tau_2}{\tau - \tau_1} \right]^\Delta e^{-i\mu(\tau - \tau')} e^{+i\Delta(\tau')} \left[ \frac{\tau' - \tau_1}{\tau' - \tau_2} \right]^\Delta \mathcal{P}\left( \frac{1}{\tau - \tau'} \right) + \pi \Theta(\tau') \delta(\tau - \tau') \right] M(\tau') \nu, \quad \text{(A.34)}
\]
where we have used the identities
\[
\begin{align*}
1 - i \tan \vartheta &= (S - 1)B^{-1}, \\
1 + i \tan \vartheta &= (1 - D)B^{-1}, \\
D^{-1} - S^{-1} &= 2S^{-1}BD^{-1},
\end{align*}
\]
and where we have defined
\[
\begin{align*}
\Theta(\tau') &= \begin{cases} 
  i(SD - A)B^{-1} & \text{if } \tau' \in (\tau_1, \tau_2), \\
  \tan \vartheta & \text{otherwise,}
\end{cases} \\
M(\tau') &= \begin{cases} 
  BD^{-1}B^{-1} & \text{if } \tau' \in (\tau_1, \tau_2), \\
  1 & \text{otherwise,}
\end{cases} \\
S(\tau) &= \begin{cases} 
  S & \text{if } \tau \in (\tau_1, \tau_2), \\
  1 & \text{otherwise,}
\end{cases} \\
\Delta(\tau) &= \begin{cases} 
  \Delta & \text{if } \tau \in (\tau_1, \tau_2), \\
  0 & \text{otherwise.}
\end{cases}
\end{align*}
\]

Now consider the Dyson equation (53) at higher orders in perturbation. The new feature is that the potential \( W \) is nonzero only within the time intervals \((\tau_{2j-1}, \tau_{2j}), j = 1, \ldots, n, \) on the real axis. Hence only on these intervals the matrix \( S \) takes the value \((A.30)\), everywhere else it is equal to the unit matrix. By Eq. (A.32) the fundamental matrix reads
\[
X(z) = \left( \prod_{j=1}^{n} \frac{z - \tau_{2j}}{z - \tau_{2j-1}} \right)^{\frac{\Delta}{\pi}} B_0 \left( \prod_{j=1}^{n} \frac{z - \tau_{2j}}{z - \tau_{2j-1}} \right)^{\frac{\Delta}{\pi}} B_0^{-1},
\]
and this expression must now replace the \( X^+ \) in the solution \((A.34)\),
\[
G(\tau, \tau') = (-i)S^{-1}(\tau) e^{-i\Delta(\tau)} \prod_{j=1}^{n} \frac{\tau - \tau_{2j}}{\tau - \tau_{2j-1}}^{\frac{\Delta}{\pi}} e^{-i\mu(\tau-\tau')} \prod_{j=1}^{n} \frac{\tau' - \tau_{2j-1}}{\tau' - \tau_{2j}}^{\frac{\Delta}{\pi}} \left[ \mathcal{P}\left(\frac{1}{\tau - \tau'}\right) + \pi \Theta(\tau') \delta(\tau - \tau') \right] M(\tau') \nu,
\]
with corresponding definitions of the matrices \( \Theta(\tau), M(\tau), S(\tau) \) and \( \Delta(\tau) \) as in Eqs. (A.35)–(A.38).

\section{The matrix \( \mathcal{G} \) is unitary}

We show that the matrix \( \mathcal{G} \) appearing in the Hilbert problem obtained from the Dyson equations is equal to the scattering matrix \( S \) associated to the
external potential $W$. This is a generalization of a result of Kohn [10] who determined the phase shift by similar scattering theory arguments for the scalar case. In this appendix $H_0$ denotes the free Hamiltonian and $H = H_0 + W$ the Hamiltonian with the static potential.

B.1 $T$ operator and $S$ matrix

Let $G(z)$ and $G_0(z)$ be the resolvents

\[
G = [z - H]^{-1}, \\
G_0 = [z - H_0]^{-1},
\]

for a point $z$ in the complex plane, not in the spectrum of $H$ or $H_0$.

The operator $T(z)$ is defined as follows

\[
T(z) = W + W G(z) W,
\]

and satisfies the two identities

\[
G_0(z) T(z) = G(z) W, \\
T(z) G_0(z) = W G(z).
\]

Combining the definition (B.1) with (B.2), the Lippmann-Schwinger equation for the $T$ operator follows

\[
T(z) = W + W G_0(z) T(z).
\]

In a plane wave basis of electrons with momentum $p$ and additional quantum number $\alpha$, the scattering matrix $S$ is connected to the $T$ operator by the relation (see [11])

\[
\langle p'\alpha'|S|p\alpha\rangle = \delta^{(3)}(p - p') \delta_{\alpha\alpha'} - 2\pi i \delta(E_{p'\alpha'} - E_{p\alpha}) \lim_{\epsilon \downarrow 0} \langle p'\alpha'|T(E_p + i\epsilon)|p\alpha\rangle.
\]

B.2 Case of a separable potential

Consider now the physical situation described in Sec. 2. The potential $W$ is assumed to be due to a localized scatterer and sufficiently short ranged. Its matrix elements between the plane wave states $|p\alpha\rangle$ can then be written in the form (see Eq. (5))

\[
W_{pp'}^{\alpha\alpha'} = u_p^\alpha W^{\alpha\alpha'} u_{p'}^{\alpha'}.
\]
with
\[ \int dp \left| u_p^\alpha \right|^2 = 1 \quad \text{and} \quad u_{p^\alpha}^\alpha = 1 \]
for any vector \( p_\alpha \) on the “Fermi surface” of the channel \( \alpha \). With this envelope function \( u_p^\alpha \) we can define the orthonormal localized conduction electron state
\[ |\zeta^\alpha\rangle = \int dp \, u_p^\alpha |p\alpha\rangle \]
in which the potential decomposes as
\[ W = \sum_{\alpha\alpha'} |\zeta^\alpha\rangle W^{\alpha\alpha'} \langle\zeta^{\alpha'}|. \quad \text{(B.5)} \]
Taking the matrix elements between \( |\zeta^\alpha\rangle \) and \( |\zeta^{\alpha'}\rangle \) of the Lippmann-Schwinger equation (B.3) yields
\[ T^{\alpha\alpha'}(z) = W^{\alpha\alpha'} + \sum_\beta W^{\alpha\beta} G_0^{\beta}(z) T^{\beta\alpha'}(z), \]
where \( T^{\alpha\alpha'} = \langle\zeta^\alpha|T|\zeta^{\alpha'}\rangle \), and
\[ G_0^{\beta}(z) = \langle\zeta^\beta|G_0(z)|\zeta^{\beta}\rangle = \int dp \frac{|u_p^{\beta}|^2}{z - E_{p\beta}}. \]
In matrix notation for the indices \((\alpha,\alpha')\) this becomes
\[ T(z) = W + W G_0(z) T(z) \]
which has the solution
\[ T(z) = [\mathbb{1} - W G_0(z)]^{-1} W = W [\mathbb{1} - G_0(z) W]^{-1}. \quad \text{(B.6)} \]
An expression for the \( S \) matrix (seen as a finite matrix with indices \((\alpha,\alpha')\)) can be found from (B.4) together with (B.6). This yields
\[ \langle p'\alpha'|S|p\alpha\rangle = \delta^{(3)}(p - p') \\delta_{\alpha\alpha'} - 2\pi i \delta(E_{p\alpha} - E_{p'\alpha'}) \lim_{\varepsilon \downarrow 0} \langle p'\alpha'|T(E_{p\alpha'} + i\varepsilon)|p\alpha\rangle \]
\[ = \delta^{(3)}(p - p') \\delta_{\alpha\alpha'} - 2\pi i \delta(E_{p\alpha} - E_{p'\alpha'}) \sum_{\beta\beta'} \langle p'\alpha'|\zeta^{\beta'}\rangle \left(W[\mathbb{1} - G_0(E_{p\alpha} + i0) W]^{-1}\right)^{\beta'\beta} \langle\zeta^\beta|p\alpha\rangle \]
\[ = \delta^{(3)}(p - p') \\delta_{\alpha\alpha'} - 2\pi i \delta(E_{p\alpha} - E_{p'\alpha'}) \]
\[ u_{p'}^{\alpha'} \left(W[\mathbb{1} - G_0(E_{p\alpha} + i0) W]^{-1}\right)^{\alpha'\alpha} u_p^{\alpha*}. \]
An integration over the momenta \( p \) and \( p' \) for the fixed energies \( E \) and \( E' \) then gives

\[
S^{\alpha'\alpha}(E, E') = \int dp \, dp' \, \delta(E' - E_{\alpha'\alpha'}) \delta(E - E_{p\alpha}) \langle p'\alpha' | S | p\alpha \rangle \\
= \left[ \bar{\nu}_\alpha \delta_{\alpha\alpha'} - 2\pi i \bar{\nu}_\alpha' u^{\alpha'}(E) \left( W[1 - G_0(E + i0)W]^{-1} \right)^{\alpha'\alpha} \right] u^{\alpha}(E) \tilde{\nu}_\alpha(E) \delta(E - E') \\
\equiv S^{\alpha'\alpha}(E) \delta(E - E'),
\]

where \( \tilde{\nu}_\alpha(E) \) is the density of states at the total energy \( E \) of the system.

We fix the energy of the incoming electrons at the value \( \mu_\alpha \) and consider a scattering onto an outgoing state with energy \( \mu_{\alpha'} \). Since generally \( \mu_\alpha \neq \mu_{\alpha'} \), the energy difference must be contributed by the localized scatterer, such that \( E = \mu_\alpha + E_{ls,\alpha} = \mu_{\alpha'} + E_{ls,\alpha'} \) remains constant, for \( E_{ls,\alpha} \) the initial and \( E_{ls,\alpha'} \) the final energy of the scatterer. This allows us to calculate

\[
G_0^\alpha(E + i0) = \int dp \frac{|u_p^\alpha|^2}{E - E_{p\alpha} + i0} = \int dp \frac{|u_p^\alpha|^2}{\mu_\alpha - \epsilon_{p\alpha} + i0}
\]

for \( \epsilon_{p\alpha} = E_{p\alpha} - E_{ls,\alpha} \). If \( \nu_\alpha(\epsilon) = \tilde{\nu}(\epsilon + E_{ls,\alpha}) \), and if \( \mathcal{P} \) denotes the principal value of the integral,

\[
G_0^\alpha(E + i0) = \int d\epsilon \frac{|u_{\epsilon}^\alpha|^2 \nu_\alpha(\epsilon)}{\mu_\alpha - \epsilon + i0} \\
= -\pi i \nu_\alpha |u_{\mu_\alpha}^\alpha|^2 + \oint d\epsilon \frac{|u_{\epsilon}^\alpha|^2 \nu_\alpha(\epsilon)}{\mu_\alpha - \epsilon} \\
= -\pi i \nu_\alpha - \pi \nu_\alpha \tan \theta_\alpha
\]

where \( \nu_\alpha = \nu_\alpha(\mu_\alpha) \). The angle \( \theta_\alpha \) is given by the relation (see also \( \mathbb{I} \), Eq. (39))

\[
\tan \theta_\alpha = \frac{1}{\pi \nu_\alpha} \oint d\epsilon \frac{|u_{\epsilon}^\alpha|^2 \nu_\alpha(\epsilon)}{\epsilon - \mu_\alpha},
\]

and is identical to the angle appearing in Eq. (27). Hence,

\[
S^{\alpha'\alpha}(E) = \nu_\alpha \delta_{\alpha\alpha'} - 2\pi i \nu_\alpha' \left( W[\mathbb{I} + \pi (\tan \theta + i\mathbb{I})\nu W]^{-1} \right)^{\alpha'\alpha} \nu_\alpha,
\]

or, in matrix notation with \( \nu = \{ \nu_\alpha \delta_{\alpha\alpha'} \} \), \( \tan \theta = \{ \tan \theta_\alpha \delta_{\alpha\alpha'} \} \), and \( g = \{ \nu \nu W^{\alpha\alpha'} \} \),

\[
S(E) = \left( \mathbb{I} - 2\pi i g [\mathbb{I} + \pi (\tan \theta + i\mathbb{I})g]^{-1} \nu \right) \\
= \left( \mathbb{I} + \pi (\tan \theta - i\mathbb{I})g \right) [\mathbb{I} + \pi (\tan \theta + i\mathbb{I})g]^{-1} \nu \quad (B.7)
\]

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B.3 Unitarity of the matrix $S$

In order to check the unitarity of the matrix $S(E)$ given in (B.7), we investigate the product $S(E)S(E')$:

$$\sum_{\alpha''} S^{\alpha''\alpha''}(E) S^{\alpha'\alpha''}(E') = \sum_{\alpha''} \int dp\,dp' \, dp'' \, \delta(E_{p\alpha} - E) \, \delta(E_{p'\alpha'} - E') \, S^{\alpha''\alpha''}_{pp''} S^{\alpha'\alpha''}_{p'p''}. $$

The unitarity of $S(p,p')$ implies that

$$\sum_{\alpha''} \int dp'' \, S^{\alpha''\alpha''}_{pp''} S^{\alpha'\alpha''}_{p'p''} = \delta_{\alpha\alpha'} \delta^{(3)}(p - p').$$

and hence

$$\sum_{\alpha''} S^{\alpha''\alpha''}(E) S^{\alpha'\alpha''}(E') = \int dp\,dp' \, \delta(E_{p\alpha} - E) \, \delta(E_{p'\alpha'} - E') \, \delta^{(3)}(p - p') = \nu_{\alpha} \nu_{\alpha'} \delta(E - E').$$

In other words

$$S(E)S(E') = \nu^2 \delta(E - E').$$

Therefore, the matrix $S(E)\nu^{-1}$, expressing the scattering matrix at fixed energy $E$ per state at the Fermi surfaces, is unitary. By comparison with Eq. (A.30) we see that

$$\mathcal{S}^{-1} \equiv S(E)\nu^{-1} = \left(1 + \pi (\tan \vartheta - i \nu W) \nu W \right) \left(1 + \pi (\tan \vartheta + i \nu W) \nu W \right)^{-1} (B.8)$$

which is the same matrix that was obtained in the Hilbert problem of Sec. 4 and 5 and yields the physical interpretation of this matrix $\mathcal{S}$.

C Discussion of the choice of the phase shifts

In Sec. A.3.2 we have seen that the numbers $\delta_{\alpha}$ are not uniquely defined, and can be chosen to be positive or negative within the limits $\pm 1$. It will now be shown, that the physical constraints determine uniquely all these numbers.

For this purpose, let us first focus on the scalar case ($N = 1$). The matrix $\mathcal{S}(\tau) = e^{2i \delta(\tau)}$ is then a scalar, piecewise constant function, where $\delta(\tau)$ is a real number. As has been shown in Sec. B, $\mathcal{S}(\tau)$ is nothing else than the scattering matrix on the Fermi surface. This explains why $\mathcal{S}(\tau)$ is unitary, and that the values $\delta(\tau)$ are the phase shifts which the wave functions acquire during the scattering on the local potential $W(\tau)$. These phase shifts are
defined in $[-\pi, +\pi]$ modulo $2\pi$ only, and for two different values of $\mathcal{S}(\tau)$ on $L$ the offset from this central interval, $2\pi m$ for $m$ an integer, is generally not identical. A possible situation is sketched in Fig. C.1. The arrows in this figure indicate the increments or decrements of $\delta(\tau)$ at the points of discontinuity. Exactly these in-/decrements enter the exponents of the functions $\xi$ defined in (A.19)–(A.21). The condition $-\pi < \delta < +\pi$ tells us moreover that the different phase shifts $\delta(\tau)$ can only differ by less than $\pm 2\pi$. They must therefore all have the same offset $2\pi m$ from the interval $[-\pi, +\pi]$. As long as this condition is satisfied, the value of $m$ is of irrelevan. For instance we may take $m = 0$ (which is perhaps the most intuitive choice for the regions where $\mathcal{S} = 1$).

The main condition is therefore seen to be the requirement $-\pi < \delta_\alpha < +\pi$ but it must be emphasized, that it is so far a purely mathematical constraint which ensures the integrability of the equations. However, there is a physical argument for this choice which was given in ND’s paper: only the perturbative solution must be retained. Take Eq. (A.40) for $G(\tau, \tau')$ into consideration. We know that the function $X^+$ contains the factors

$$\left(\frac{\tau - \tau_k}{\tau - \tau'_k}\right)^{\delta_k \pi}$$

for the different $\delta_k = \delta(\tau_k + 0) - \delta(\tau_k - 0)$ at the points of discontinuity $\tau_k$. If we let the scattering potentials tend to zero, $W(\tau) \to 0$, we must obtain the free propagator $G^{(0)}(\tau - \tau')$ given in (27). If in this limit $\delta(\tau_k + 0) \to 2\pi m_+$ and $\delta(\tau_k - 0) \to 2\pi m_-$ (for $m_+, m_-$ some integers), there would still remain the factor

$$\left(\frac{\tau - \tau_k}{\tau - \tau'_k}\right)^{2(n_+ - n_-)}$$

in $G(\tau, \tau')$ which does not appear in $G^{(0)}(\tau - \tau')$. Hence the requirement $m_+ = m_- \equiv m$ at all $\tau_k$.

In the matrix case where all matrices $\mathcal{S}(\tau)$ commute (for any other case, we do not possess a closed solution, as has been shown in Sec. A.3.4) all matrices
can be diagonalized simultaneously. The system transforms then into a set of
decoupled scalar problems to which the same arguments as above apply.

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