The density matrix for quantum impurities out of equilibrium

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1 Introduction

This set of somewhat informally written notes is a greatly extended version of the material I presented at two lectures during the Capri Spring School 2009. The goal of these lectures was to present some ideas and techniques used to describe and study quantum impurities in metallic environments out of equilibrium.

The phrase *quantum impurities* refer to the fact that we are studying objects that are very small (essentially can be thought of as zero-dimensional) and very different from the environment in which they are. In practice, they can be actual impurities in a conducting environment, like the magnetic impurities that lead to the Kondo effect, an increase of resistivity with decreasing temperature at low temperatures. However, for our purpose, it will be more appropriate to think of quantum impurities as quantum dots, small islands of conducting material connected to metallic sheets by thin barriers through which electrons can tunnel[1]. Quantum dots are "mesoscopic" objects, between microscopic and macroscopic. This means that taken "on their own" (with infinite tunnelling barriers), one finds that the separations between the energy levels are much larger than the separation between energy levels in the metallic environments (that is, quantum dots are small enough objects); yet, a large quantity of electrons may be contained in a quantum dot so that there are very many energy levels (that is, quantum dots are large enough). Although we will keep the picture of the quantum dot in mind, we will stay open with the precise interpretation of our quantum impurity. We will simply consider it as a quantum system with discrete energy levels, connected to metallic sheets in a way that allow the sheets to gain or loose electrons.

On the other hand, the phrase *out of equilibrium* above refers to the fact that the situation we are considering is not described by the usual density matrix of equilibrium quantum statistical mechanics, for instance in the macro-canonical ensemble $\rho = e^{-(H+\mu N)/T}$ (where H is the quantum Hamiltonian, N the number operator, μ the chemical potential and T the temperature). This definition of being out of equilibrium is not very restrictive, and does not provide very much insight into what is fundamentally different from situations at equilibrium. A more precise and physical definition is that a situation is out of equilibrium if there is production of entropy. This points to the fact that what we have in mind is a system and an environment, the latter absorbing the entropy produced, and that there are processes describing the action of the environment on the system, and *vice versa*. Out of equilibrium, as we will see, the consideration of these processes is crucial.

One of the interesting aspects of quantum impurities out of equilibrium is that the effects of quantum mechanics occur at a similar scale as those having to do with being out of equilibrium: we need to describe

[1]The system is made by plating, on a non-conducting substrate, conducting material in a configuration that reproduces the dot, the metallic sheets, and the small conducting connections between them. These small connections are made into barriers by applying *gate voltages*, that can be adjusted in order to adjust the tunnelling strengths.

the out-of-equilibrium situation using quantum mechanical states and observables. In other words, we expect that the processes describing the interaction between the system and the environment are quantum in nature. There is a way of theoretically describing an environment connected to a quantum system, developed by Caldeira and Leggett [1]. The basic idea is simply to connect the quantum system to a family of quantum oscillators of all possible frequencies; this should be able to absorb and provide energy as necessary in order to keep the temperature fixed, for instance. This family of quantum oscillators can be understood to represent a conformal field theory model [2].

In the cases in which we are interested, there are two separate semi-infinite (that is, very large compared to the size of the quantum dot) metallic sheets connected to the quantum dot, and these two sheets are kept at a fixed difference of potential. In this way, a constant electric current flows from one sheet to another through the quantum dot, thanks to tunnelling. This setup has the property of being out of equilibrium, because there is a constant electric current flowing (so that, for instance, the power generated is IV where I is the current and V is the potential difference, and the entropy generated is IV/T, by purely thermodynamic thinking). Yet, this is a simple enough situation, because the current is *constant*. The system is then said to be in a *steady state*, which we may define generally as a situation where the change, with time, of extensive quantities is constant, while intensive quantities are themselves constant in time. This, of course, includes situations at equilibrium, where everything is constant, but it also includes the situation we are looking at, a steady state out of equilibrium. For instance, in our case, the number of particles in any given metallic sheet changes in a constant way, with a rate of change proportional to the current.

2 Impurity models: the dynamics

We will now be more precise about the quantum systems of interest. In general, in order to describe a quantum system, we need to provide a set of observables, including the Hamiltonian, and their algebra (in the usual canonical quantisation, this algebra is induced from the Poisson brackets of classical mechanics). Then, the Hilbert space is a representation space where the Hamiltonian is bounded from below. Although this sounds like a somewhat formal approach, it will be useful to remember as we go along, because subtleties will arise in the discussion of the Hilbert space. Here, we will be describing the dynamics in a very general way, stating what the observables are, including the Hamiltonian, and some properties of the algebra they satisfy. We will not keep this level of generality throughout, as we will eventually specialise mainly to the interacting resonant level model.

First, recall that we consider the impurity to be essentially a zero-dimensional object; at low energies, or large distances, this is a good approximation. On the other hand, the metallic sheets are represented, through Landau's Fermi liquid theory, by two sets of free Fermions with dispersion relations characteristic of the conducting bands. In order to be precise, suppose these metallic sheets have the shape of large half-disks, with the impurity at the center of the corresponding full disk. Then, the wave functions associated to a free Fermionic mode in any half-disk can be obtained from the wave functions on the full disk by collapsing on a sector of fixed parity with respect to inversion about the axis defining the half-disks. This means that these wave functions may be separated into radial and angular parts (the angular part contains the boundary conditions on the flat piece of the bounary of the half-disk). In the usual way in quantum mechanics, the corresponding radial part of the Hamiltonian can be brought to the form of a Hamiltonian for a one-dimensional free Fermion on a line segment, whose length is the

radius of the half-disk. One end-point of the line segment, say the one that is to the right, is where the impurity lies. The other end-point, the left one, is the part of the boundary of the half-disk far from the impurity. If the "average" energy we are looking at is in the conducting band, and if we are only looking at low-energy processes, then we may linearise the one-dimensional dispersion relation about that average energy. Hence, we obtain free *massless* relativistic Fermions on a line segment, with a "velocity of light" equal to the Fermi velocity (we will just set it to 1, by appropriate choice of units). Naturally, these Fermions can be decomposed into a chiral and an anti-chiral parts: the former travelling "to the right" (towards the impurity), the latter "to the left" (away from the impurity). The boundary conditions at the end-points (for now, without considering the effect of the interaction with the impurity) correspond to pure reflections. This means that we can in fact "open up" the line segment into a line segment twice the length, with Fermions everywhere travelling to the right and the impurity in the middle, say at $x = 0$. We have two of these opened-up line segments of right-moving Fermions, for the two metallic sheets.

Keeping everything general, the Fermions may have spin and other internal degrees of freedom, and we will denote them by vectors of Fermionic fields $\Psi_1(x)$, $\Psi_2(x)$, with non-zero anti-commutation relations

$$\{\Psi_j(x), \Psi^\dagger_{j'}(x')\} = \mathbf{1}\delta_{j,j'}\delta(x - x') \tag{2.1}$$

(here, $\mathbf{1}$ is in the space of internal degrees of freedom). These are the observables corresponding to the electrons in the metallic sheets. The Hamiltonian representing their dynamics is

$$H_e = -\mathrm{i}\int_{-L}^{L} dx \sum_{j=1,2} \Psi^\dagger_j(x)\frac{d}{dx}\Psi_j(x) \tag{2.2}$$

where L is the radius of the half-disks. In particular, we find

$$[H_e, \Psi_j(x)] = \mathrm{i}\frac{d}{dx}\Psi_j(x). \tag{2.3}$$

It may seem as though the precise shape of the metallic sheets matter in order to obtain the exact form of this Hamiltonian. However, we will be interested at the end in taking the limit $L \to \infty$ (in an appropriate way), and their precise shape far from the impurity does not affect this limit. In order to assess the effect of the impurity, we only need the structure of the wave functions around the impurity, and this is correctly described by this Hamiltonian. But, it is convenient to have a finite radius initially, in order to clarify the limit process. Another viewpoint is that, independently from the derivation above, we would like to have a description of thermal and particle baths, from which we will correctly describe the situation out of equilibrium. The conformal Hamiltonian H_e has the potential of providing such a description in accordance with the Caldeira-Leggett model; this will depend on the particular interaction with the impurity. It will be good to keep this in mind: the metallic sheets not only constitute part of our quantum system, but can also play the rôle of baths (which are essential to the establishment of a steady state out of equilibrium).

On the other hand, the impurity has its own set of observables. We will consider a set of independent Fermionic observables d_α and their Hermitian conjugate $d^\dagger_\alpha$ (where the index α parametrises the elements of this set), and a set of independent bosonic observables D_β (where the index β parametrises the elements of this different set), which we take Hermitian for simplicity: $D^\dagger_\beta = D_\beta$. The impurity Hamiltonian is in the linear space of bosonic observables, and will be denoted H_i. Of course, one can be more precise, and represent d_α and D_β by matrices on a finite-dimensional vector space, for instance. We will give examples below.

The interaction between the impurity and the Fermionic fields that we will be looking at has in general two distinct components. One is that of tunnelling: electrons can be absorbed or given back by the impurity. These have to do with the observables d_α. For each α, we may form a coupling vector T_α representing the tunnelling strength (with possible phase shifts), so that the corresponding interaction terms are $\sum_{\alpha,j}\left(\Psi_j^\dagger(0)T_\alpha d_\alpha + d_\alpha^\dagger T_\alpha^\dagger \Psi_j(0)\right)$. For simplicity, we will assume the dot to be completely symmetric with respect to inversion of the metallic sheets, so that there is no j dependence on the tunnelling strength. Note that the interaction involves the Fermionic fields at $x = 0$, where the impurity lies.

Another component of interaction is that of *co-tunnelling*: electrons may change type (internal degree of freedom) and metallic sheet, but are neither absorbed nor given back by the impurity. This represents processes where the electrons are energetically forbidden to jump on or off the impurity, so that two tunnelling events have to occur. Such processes have to do with the bosonic obversables D_β. The processes can involve both sheets at the same time, or just one sheet. Hence, for each β, we form three square coupling matrices of co-tunnelling strengths, $U_\beta^{(0)}$ and $U_\beta^{(\pm)}$, corresponding to same-sheet co-tunnelling and cross-sheet co-tunnelling. The corresponding interaction terms are of the form $\sum_{\beta,j,k}\Psi_j^\dagger(0)U_\beta^{(j-k)}\Psi_k(0)D_\beta$ with $(U_\beta^{(\ell)})^\dagger = U_\beta^{(-\ell)}$. Note part of the terms of this interaction where $j = k$ can as well be understood as a repulsion (or attraction) term of the Hamiltonian as an energy observable.

Hence, the interaction Hamiltonian is

$$I = \sum_j \left(\Psi_j^\dagger(0)T_\alpha d_\alpha + d_\alpha^\dagger T_\alpha^\dagger \Psi_j(0)\right) + \sum_{j,k}\Psi_j^\dagger(0)U_\beta^{(j-k)}\Psi_k(0)D_\beta \tag{2.4}$$

where here and below summations over repeated impurity indices (α and β) are implied.

Hence, the total Hamiltonian is

$$H = H_e + H_i + I \tag{2.5}$$

and we will denote the part without impurity interaction by

$$H_0 = H_e + H_i. \tag{2.6}$$

Two models of high current interest in this subject are just particular cases of this general model. We will be mainly interested in the interacting resonant-level model (IRLM). It is obtained by taking single-component vectors (that is, spin-less Fermions) which we will denote $\Psi_j = \psi_j$. We have also a single fermionic observable $d_1 = d$ (and its Hermitian conjugate) with

$$\{d, d^\dagger\} = 1, \quad \{d, d\} = \{d^\dagger, d^\dagger\} = 0 \tag{2.7}$$

representing creation and annihilation of an electron on the impurity, and one bosonic observable $D_1 = d^\dagger d$, representing the number of electrons on the impurity (which can only be 0 or 1). Note that these fermionic and bosonic observables indeed form a closed algebra. The impurity Hamiltonian is simply $H_i = \epsilon d^\dagger d$, the one-component single tunnelling vector is $T_1 = t$ (not to be confused with the time!) and the co-tunnelling 1x1 matrices are $U_1^{(0)} = U$ and $U_1^{(\pm)} = 0$. Hence, the Hamiltonian is

$$H_{IRLM} = \sum_{j=1,2}\left[-\mathrm{i}\int_{-L}^{L} dx\, \psi_j^\dagger(x)\frac{d}{dx}\psi_j(x) + t\psi_j^\dagger(0)d + t^* d^\dagger\psi_j(0) + U\psi_j^\dagger(0)\psi_j(0)d^\dagger d\right] + \epsilon d^\dagger d. \tag{2.8}$$

Another model of interest included in this general setup is the Kondo model. In this model, the Fermions have spin 1/2 but no other internal degrees of freedom (hence the Fermion vectors have two

components). There is no direct tunnelling, but there are co-tunnelling terms. The three bosonic observables form the angular-momentum algebra, $[S_\alpha, S_\beta] = \mathrm{i}\epsilon_{\alpha\beta\gamma}S_\gamma$, meaning that we have a magnetic impurity. The associated co-tunnelling matrices are proportional to the Pauli matrices σ_α, for the spin-1/2 representation in which the Fermions are, $U_\alpha^{(0)} = g_0\sigma_\alpha$ and $U_\alpha^{(\pm)} = g_1\sigma_\alpha$. The impurity Hamiltonian represents a local magnetic field at the impurity site, $H_i = h_\alpha S_\alpha$. Hence, the Hamiltonian is

$$H_{Kondo} = -\mathrm{i}\sum_{j=1,2}\int_{-L}^{L} dx\, \Psi_j^\dagger(x)\frac{d}{dx}\Psi_j(x) + \sum_{j,k=1,2} g_{|j-k|}\Psi_j^\dagger(0)\sigma_\alpha\Psi_k(0)S_\alpha + h_\alpha S_\alpha. \tag{2.9}$$

These two models illustrate well the dual nature of the Hamiltonian: as the observable of energy, and as the generator of the dynamics. For instance, in the IRLM, the U-term (as it is often called) has the meaning of a Coulomb repulsion, being proportional to the product of the number operator of electrons on the metallic sheets at the impurity site, and the number operator of electrons on the impurity. This is certainly an energy term, and does not come *a priori* from the intuition of a co-tunnelling dynamical process. On the other hand, the same-sheet co-tunnelling term of the Kondo model can be seen as an energy term, a magnetic interaction as we would have in the case of a magnetic impurity in a conducting material, but the cross-sheet is more naturally a dynamical term, a co-tunnelling process whereby the spin of a metallic electron is flipped. The latter interpretation is in fact the reason why this term appears in the context of quantum dots.

Finally, it is worth mentioning that in fact, although the algebras of metallic observables (Fermion fields, their derivatives, and H_e) and of impurity observables that we talked about above are indeed closed, the adjunction of the full, interacting Hamiltonian as an observable in general will impose the adjunction of more observables, and may modify part of the algebra through the renormalisation process.

3 Quantum quench: constructing the steady state in real time

3.1 The large-time limit

Now that we have described the dynamics of the system we are looking at, we need to understand how to setup a steady state out of equilibrium in this dynamics. The basic idea that we first develop is that of a real-time construction, where we represent at the theoretical level, in an idealised way, the operations one would do in the laboratory in order to generate a steady state where a constant current flows. This idea goes back to Schwinger and Keldysh (and many others), and we will refer to it as the Schwinger-Keldysh formulation. In fact, often one understands by this the Keldysh method, which is a particular way of doing perturbation theory via diagrams, generalising Feynman's diagrams. But, as was emphasized in [3], it is not necessary to, and sometimes fruitful not to, talk about diagrams or perturbation theory with respect to some free model. We are rather interested here in the general aspects of the method, and in particular its physical meaning; its actual implementation may then be done via Keldysh diagrams or via other devices.

The Schwinger-Keldysh formulation starts with a system where there is no interaction between the impurity and the metallic sheets. Here, then, the set of observables we introduced above forms a closed algebra, and we may choose an appropriate representation. This system is then put in contact with a common thermal and particle bath and we wait for thermalisation. But in order to have the possibility

of a steady state, the two metallic sheets are set at different chemical potentials (we keep the same temperature everywhere). This is like connecting two glasses of water through a straw full of water, but putting these two glasses at different heights (different gravitational potential). The water levels will eventually equalise, so that one glass will be more full than the other. In terms of our quantum system, this means that the sheets will be described, after thermalisation, by the density matrix

$$\rho_e = e^{-(H_e - \mu_1 N_1 - \mu_2 N_2)/T} \tag{3.1}$$

where

$$N_j = \int_{-L}^{L} dx\, \Psi_j^\dagger(x)\Psi_j(x) \tag{3.2}$$

are the number operators on both sheets, and where μ_j are the chemical potentials. Note that we have

$$[N_j, \Psi_k(x)] = -\delta_{j,k}\, \Psi_k(x), \quad [N_j, \Psi_k^\dagger(x)] = \delta_{j,k}\, \Psi_k^\dagger(x). \tag{3.3}$$

As for the impurity, if there are fermionic creation and annihilation operators $d_\alpha^\dagger$, d_α, we can always adjoin (if it is not there already) a number operator N_i amongst the bosonic observables, with

$$[N_i, d_\alpha] = -d_\alpha, \quad [N_i, d_\alpha^\dagger] = d_\alpha^\dagger, \quad [N_i, D_\beta] = 0. \tag{3.4}$$

In particular, this number operator commutes with the impurity Hamiltonian, which just means that on its own, the impurity does not gain or loose electrons,

$$[H_i, N_i] = 0. \tag{3.5}$$

We will assume the impurity to be set at the average chemical potential, so that it is described by the density matrix

$$\rho_i = e^{-\left(H_i - \frac{\mu_1+\mu_2}{2} N_i\right)/T}. \tag{3.6}$$

The full initial density matrix is then

$$\rho_0 = \rho_e \rho_i = e^{-(H_0 - VQ - \mu N)/T} \tag{3.7}$$

where

$$Q = \frac{N_1 - N_2}{2}, \quad N = N_1 + N_2 + N_i, \quad V = \mu_1 - \mu_2, \quad \mu = \frac{\mu_1 + \mu_2}{2}. \tag{3.8}$$

In particular, the quantity V is the difference of chemical potentials, essentially the voltage applied, and will be responsible for the generation of a current; we will take $V > 0$ (so that the current should flow from sheet 1 to sheet 2). The average of an observable $\mathcal{O}$ is evaluated using

$$\langle \mathcal{O} \rangle_0 = \frac{\mathrm{Tr}\,(\rho_0 \mathcal{O})}{\mathrm{Tr}\,(\rho_0)} \tag{3.9}$$

The next step in the physical picture of the Schwinger-Keldysh formulation is to simply disconnect the common thermal and particle bath. This does not change anything in the density matrix, since we already have a statistical distribution of quantum states, but it allows us to consider this as a statistical distribution of initial states, that we may then evolve with some unitary evolution operator as is usual in quantum mechanics.

This is just what we do in the third step: we turn on the interaction between the impurity and the metallic sheets, and let the system evolve unitarily. The evolution is described by the full Hamiltonian H,

including the interaction term I. This is an operation that is nowadays called a *quantum quench* (here, a local quantum quench). Performing a quantum quench means that we start with a ground state or a natural, equilibrium density matrix associated to a certain Hamiltonian, and evolve this state or density matrix with a different Hamiltonian, obtained from the initial one by varying one or many parameters. In particular, it should be that the initial density matrix is not an equilibrium one with respect to the evolution Hamiltonian. In the present case, we only modify the Hamiltonian around the point $x = 0$, so it is a local quench. Since both Q and N are local conserved charges with respect to the dynamics H_0, the density matrix ρ_0 is indeed an equilibrium density matrix with respect to this dynamics. On the other hand, H does not commute with $H_0 - VQ$ (but note that it commutes with μN). The evolved density matrix is

$$\rho(t) = e^{-\mathrm{i}Ht}\rho_0 e^{\mathrm{i}Ht} \tag{3.10}$$

(with $\hbar = 1$). Note that since N commutes with $H_0 - VQ$ as well as with H, it will only produce a factor $e^{\mu N/T}$ independently of time. This will not affect any of the physical quantities we will be looking at, so for simplicity, we will set (slighlty formally) $N = 0$ throughout.

The hope is then that the limit where t is very large should give rise to a steady state. Physically, this means that we wait for a long time, until the system settles to something that looks steady – where, for instance, the average of the current flowing from sheet 1 to sheet 2 is constant. The current operator is easy to obtain:

$$\mathcal{J} = -\frac{dQ}{dt} = -\mathrm{i}[H, Q] = -\mathrm{i}[I, Q] = \mathrm{Im}\left(d_\alpha^\dagger T_\alpha^\dagger \Psi_1(0) - d_\alpha^\dagger T_\alpha^\dagger \Psi_2(0) + 2\Psi_2^\dagger(0) U_\alpha^{(+)} \Psi_1(0) D_\alpha\right). \tag{3.11}$$

Hence, we hope that, in a certain sense,

$$\text{“}\lim_{t\to\infty} \frac{\mathrm{Tr}\left(\rho(t)\mathcal{J}\right)}{\mathrm{Tr}\left(\rho(t)\right)} \quad \text{exists.”} \tag{3.12}$$

Let us now address three questions associated to this hope.

3.2 Does the limit exist? (relaxation processes)

Standard arguments of quantum mechanics tell us that in general, the unitary evolution of a quantum system should display the phenomenon of quantum recurrence: the system will eventually come back very close to its initial condition, at some later time. Hence, it is impossible that the large-time limit give rise to something steady, unless it was constant in the first place! The solution to this problem lies in the way in which we take the large-time limit. Indeed, in order to avoid recurrence, we need in fact to take the limit where the system length L is very large before that where the time t is very large. More precisely, we should be looking into the region $L \gg t \gg T^{-1}$ [3]. In this limit, the baths of electrons that the metallic sheets are may provide the relaxation necessary in order to obtain something that looks steady. This is in fact not immediate, because it depends on the type of interaction between the metallic sheets and the impurity, I. In general, we would expect that if the interaction is such that all states of the impurity may be reached by emitting or absorbing electrons, through hopping (or tunnelling) terms, then indeed the Caldeira-Leggett theory should work (as it is rather like the linear coupling used in the initial Caldeira-Leggett model, modelling absorption and emission of phonons or photons). This is the case, for instance, of the interacting resonant-level model; we will see later clear signs of the presence of relaxation in this model. However, if only co-tunnelling terms are present, then relaxation may in general not occur.

In the case of the Kondo model, which only contains co-tunnelling terms, it was shown in [3] that relaxation does occur when the impurity magnetic field h_α is zero. That is, it was shown that to all orders of perturbation theory in the co-tunnelling strengths, the integrals have finite limit $L \gg t \gg T^{-1}$. The idea of the proof is as follows. Consider the average of the current operator $\mathcal{J}$, for instance. Using interaction picture, it can be written

$$\langle \mathcal{J} \rangle(t) = \left\langle \mathcal{P} \exp\left[-\mathrm{i}\int_t^0 dt'\, I(t')\right]\ \mathcal{J}\ \mathcal{P} \exp\left[-\mathrm{i}\int_0^t dt'\, I(t')\right]\right\rangle_0 \tag{3.13}$$

where $\langle\cdot\rangle(t)$ is evaluated using $\rho(t)$ and $\langle\cdot\rangle_0$ using ρ_0. Here $\mathcal{P}\exp$ is the path-ordered exponential, where the ordering is from the lower limit on the left to the upper limit on the right. The interaction-picture interaction Hamiltonian $I(t)$ is simply

$$I(t) = e^{-\mathrm{i}H_0 t} I e^{\mathrm{i}H_0 t} = \sum_{j,k=1,2} g_{|j-k|} \Psi_j^\dagger(t) \sigma_\alpha \Psi_k(t) S_\alpha \tag{3.14}$$

where the Fermion fields are now at the position $x = t$ (we used the fact that they are right-moving).

Now, we may as well write the denominator on the right-hand side of (3.13) as

$$\left\langle \mathcal{P} \exp\left[-\mathrm{i}\int_t^0 dt'\, I(t')\right] \mathcal{P} \exp\left[-\mathrm{i}\int_0^t dt'\, I(t')\right]\right\rangle_0 = 1.$$

But in general, expressions like

$$\frac{\mathrm{Tr}\left(\mathcal{P}\exp\left[\int_{x_1}^{x_1'} dx\, A_1(x)\right]\ \mathcal{O}\ \mathcal{P}\exp\left[\int_{x_2}^{x_2'} dx\, A_2(x)\right]\right)}{\mathrm{Tr}\left(\mathcal{P}\exp\left[\int_{x_1}^{x_1'} dx\, A_1(x)\right] \mathcal{P}\exp\left[\int_{x_2}^{x_2'} dx\, A_2(x)\right]\right)}, \tag{3.15}$$

when expanded in powers of A_1 and A_2, lead to path-ordered integrals of *connected* correlation functions. The connection is between $\mathcal{O}$ and all operators $A_1(x)$ and $A_2(x)$. We will not recall here the technical definition of connected correlation functions (see, for instance, [3]), but only their fundamental property. If the unconnected correlation functions (i.e. simply the averages of products of the fields involved) *factorise* when any group of $A_1(x)$'s or $A_2(x)$'s are positionned far from where $\mathcal{O}$ lies, then the connected correlation functions *vanish* in that limit – connected correlation functions are just linear combinations where the factorised forms are substracted. Hence, the proof that the large-time limit of $\langle\mathcal{J}\rangle(t)$ exists lies on the proof that correlation functions of the type $\langle A_1(x_1)A_2(x_2)\cdots A_n(x_n)\rangle_0$ factorise when some group $x_1, x_2, \ldots, x_{m_L}, x_{m_R}, x_{m_R+1}, \ldots, x_n$ of positions are very far from the rest, where $A_m(x)$ is of the type $J_{m,\alpha}(x)S_\alpha \equiv \Psi_j^\dagger(x)\sigma_\alpha\Psi_k(x)S_\alpha$ for some j,k that may depend on m (this includes the operators in $I(t)$ which are at $x = t$, as well as those in $\mathcal{J}$, which are at $x = 0$). We only need to take the positions of consecutive left-most (up to m_L) and consecutive right-most (from m_R) operators, because we have left- and right- time orderings in $\langle\mathcal{J}\rangle(t)$.

Such a correlation function may be written as a sum of products of two factors, one being the CFT correlation function of Fermion fields, the other the trace over the impurity space of the product of S_α's:

$$\langle J_{1,\alpha_1}(x_1) J_{2,\alpha_2}(x_2) \cdots J_{n,\alpha_n}(x_n)\rangle_{CFT} \mathrm{Tr}\left(S_{\alpha_1} S_{\alpha_2} \cdots S_{\alpha_n}\right).$$

The CFT correlation function factorises in the limit by local QFT principles. It is here that we use $L \gg t$, so that we may use infinite-volume correlation functions, and $t \gg T^{-1}$, so that we may use the finite-temperature form of these, which reach their asymptotic values exponentially fast. The non-trivial part is the impurity average. But since the CFT correlation functions factorise, and the CFT is

$SU(2)$ invariant (simultaneous spin $SU(2)$ transformation on both metallic sheets), this means that in the limit, we may make independent $SU(2)$ transformations on the two factorised groups of fields. This translates into independent $O(3)$ transformations of the indices $\alpha_1, \ldots$. Since this is dotted into the trace of impurity spin matrices, this means that in the limit, we can make independent $SU(2)$ transformations of two corresponding groups of spin matrices. Using cyclicity of the trace, we then obtain, for the trace over spin matrices,

$$\mathrm{Tr}\left(U\, S_{\alpha_{m_R}} \cdots S_{\alpha_n} S_{\alpha_1} \cdots S_{\alpha_{m_L}}\, U^{-1}\, U'\, S_{\alpha_{m_L+1}} \cdots S_{\alpha_{m_R-1}}\, (U')^{-1}\right),$$

where U and U' are independent $SU(2)$ transformations. But for the spin-1/2 representation, we can always write $S_{\alpha_{m_R}} \cdots S_{\alpha_{m_L}} = a\mathbf{1} + bS_x + cS_y + dS_z$ for some numbers a, b, c, d; that is, the identity matrix and the matrices corresponding to all the algebra elements span the whole space of 2 by 2 matrices. We can do similarly for $S_{\alpha_{m_L+1}} \cdots S_{\alpha_{m_R-1}}$ for numbers a', b', c', d'. Since

$$\mathrm{Tr}\left[(a\mathbf{1} + bS_x + cS_y + dS_z)(a'\mathbf{1} + b'S_x + c'S_y + d'S_z)\right] = 2(aa' + bb' + cc' + dd')$$

and since U and U' correspond to independent $O(3)$ transformations of the vectors b, c, d and b', c', d', we can make these vectors orthogonal, so that we are left with aa', which is indeed the product of the traces of the individual groups of impurity spin matrices. This completes the proof of factorisation, hence of existence of the large-time limit in the Kondo model.

It is worth noting that it is physically natural to associate the large-time factorisation of correlation functions to the presence of appropriate relaxation processes. Indeed, relaxation corresponds essentially to information loss at large times, and indicates that quantum observations made at large time intervals should not affect each other.

If the impurity magnetic field is non-zero, then the impurity part of the Hamiltonian does not possesses the $SU(2)$ invariance that we need to provide the proof of factorisation. In his case, in fact, the large-time limit of the perturbative integrals does not exist. However, it is still possible to provide an expression for the current, for instance, from the Schwinger-Keldysh formulation [4], using a clever trick. We will not go into the details of this, but we just mention that the result has somewhat strange features, as it does not have a well-defined small-coupling limit (it has the form of a ratio between two perturbative series starting at non-zero order). It is not clear, to our opinion, if this result is physically correct, as it is not clear if there is, in a certain non-perturbative sense, relaxation in this model. In general, as we will see below and as was emphasized in [3], it seems likely that the presence of relaxation is necessary not only to reach the steady state out of equilibrium, but also to maintain it. A non-trivial check would be to verify, using the methods of [4], that the current-current correlation function factorises at large time.

Recapitulating, we argued that if the impurity interaction exchanges particles with the metallic sheets in such a way that all states of the impurity can be reached, like in the IRLM, then relaxation should occur; and we saw that with only co-tunnelling terms, if there is a symmetry that allows us to reach all states of the impurity, like in the Kondo model without magnetic field, then relaxation also occurs. Interestingly, we will see below that these facts allow us, in these two models respectively, to complete the definition of the density matrix out of equilibrium in the space of scattering states.

3.3 What is the result of the limit? (reaching the equilibrium density matrix)

Now that we have understood in which sense the limit may exist, and that we have seen quite explicitly that the limit does exist in the case of the Kondo model without impurity magnetic field, we should ask what the result of the limiting process exactly is. Let us look again at the average of the current, and write it in the form

$$\langle\mathcal{J}\rangle(t) = \frac{\left\langle \mathcal{P}\exp\left[-\mathrm{i}\int_{\mathrm{i}/T}^{t+\mathrm{i}/T} dt'\, I_V(t')\right]\ \mathcal{P}\exp\left[-\mathrm{i}\int_t^0 dt'\, I(t')\right]\ \mathcal{J}\right\rangle_0}{\left\langle \mathcal{P}\exp\left[-\mathrm{i}\int_{\mathrm{i}/T}^{t+\mathrm{i}/T} dt'\, I_V(t')\right]\ \mathcal{P}\exp\left[-\mathrm{i}\int_t^0 dt'\, I(t')\right]\right\rangle_0} \tag{3.16}$$

where we have used cyclicity of the trace and moved $\rho_0 = e^{-(H_0-VQ)/T}$ through one of the path-ordered integrals (and we have done the same in the denominator for later convenience). This has produced an imaginary shift of time, up to factors introduced by the potential term:

$$I_V(x) = \sum_j \left(e^{-\mu_j/T}\Psi_j^\dagger(x)T_\alpha d_\alpha(x) + e^{\mu_j/T}d_\alpha^\dagger(x)T_\alpha^\dagger\Psi_j(x)\right) + \sum_{j,k} e^{V(j-k)/T}\Psi_j^\dagger(x)U_\beta^{(j-k)}\Psi_k(x)D_\beta(x) \tag{3.17}$$

where $\mu_1 = V/2$ and $\mu_2 = -V/2$. Here, we use the notation

$$d_\alpha(x) = e^{-\mathrm{i}H_i x}d_\alpha e^{\mathrm{i}H_i x},\quad d_\alpha^\dagger(x) = e^{-\mathrm{i}H_i x}d_\alpha^\dagger e^{\mathrm{i}H_i x},\quad D_\beta(x) = e^{-\mathrm{i}H_i x}D_\beta e^{\mathrm{i}H_i x}. \tag{3.18}$$

Note that in the particular case of the Kondo model without impurity magnetic field that we discussed above, we had $H_i = 0$, so that there was no need for this extra notation.

For $V = 0$, we clearly have $I_V(x) = I(x)$. Then, if the limit $L \gg t \gg T^{-1}$ exists, we may change the upper limit of the first path-ordered integral $t + \mathrm{i}/T$ to t, which just cancels the lower limit of the second path-ordered integral, giving

$$\lim_{L\gg t\gg T^{-1}}\langle\mathcal{J}\rangle(t) \overset{V=0}{=} \frac{\left\langle \mathcal{P}\exp\left[-\mathrm{i}\int_{\mathrm{i}/T}^0 dt'\, I(t')\right]\ \mathcal{J}\right\rangle_0}{\left\langle \mathcal{P}\exp\left[-\mathrm{i}\int_{\mathrm{i}/T}^0 dt'\, I(t')\right]\right\rangle_0} = \frac{\mathrm{Tr}\left(e^{-H/T}\mathcal{J}\right)}{\mathrm{Tr}\left(e^{-H/T}\right)}. \tag{3.19}$$

This is the usual thermal density matrix: we have just shown that if the metallic sheets play the rôle of thermal baths, à la Caldeira-Leggett, then the large-time limit of the Schwinger-Keldysh formulation in the equilibrium situation correctly reproduces the expected thermal density matrix. That is, if there is relaxation in the model, then the state of the system relaxes to the correct thermal density matrix. Note that it was necessary to shift $t + \mathrm{i}/T$ to t in the denominator as well, in order to keep the correlation functions connected (so that the large-time limit exists). Note also that the density matrix we reach depends strongly on the initial density matrix we used. This is essentially because it is this initial density matrix that determines the state of the bath giving rise to relaxation, and the bath itself is represented by just a set of non-interacting oscillators; in order to indeed have a physical thermal bath, we need a thermal distribution from the start (there are no processes that would allow the bath itself to relax to a thermal distribution). Finally, note that this local quantum quench situation is very different from that of global quantum quenches: the quench does not change the system in a macroscopic way, just locally, so that the energy of the initial configuration is not "macroscopically" far from that of the final configuration (hence, indeed the initial thermal distribution may give rise to a final thermal distribution with the same temparature).

In the case where $V \neq 0$, then because $I_V(x) \neq I(x)$, there is no cancellation possible, and no immediate simple form of the density matrix (we will come back in subsection 4.2 to the expression of

the density matrix we obtain in this way; this leads to interesting expressions for physical quantities like the current response functions and noise). But, if the large-time limit exists, then there is relaxation; why, then, would the system not relax to the ground state, for instance, when the temperature is zero? What is happening is that here, we in fact have a *global* quantum quench, with both a local change at the impurity site introducing the impurity interaction with the metallic sheets, and a global change on the sheets themselves, putting the difference of potential to zero. Then, the averages of the operator Q, for instance, with the initial density matrix, and with $e^{-H/T}$, differ by an amount that scales like L when L is large, whereas the average of the derivative of the operator Q, the current, is a quantity that is finite at all times in the large-L limit because it is localised at the impurity site. Hence, we certainly cannot expect to reach $e^{-H/T}$ in the limit $L \gg t \gg T^{-1}$. That is, in a zero-temperature language, the initial state is far from the ground state of H, and the approach towards the ground state of H, which indeed occurs thanks to relaxation, is too slow (see [3] for some more details). At finite temperature, we do not expect to have a thermal distribution. But, if the limit exists, the result in the equilibrium case $V = 0$ suggests that the metallic sheets are correct thermal baths, so that for $V \neq 0$ the system should reproduce the correct physics of a driven impurity in a steady state out of equilibrium, in contact with an external thermal bath at a fixed, well-defined temperature.

There are a number of subtle differences between the cases at and out of equilibrum (besides the obvious difference that V is zero or not!). First, in the equilibrium case, if the model didn't have appropriate relaxation processes *a priori*, we may well have started with a more complicated model including more physical interactions so that relaxation mechanisms are present, and the large-time limit exists. This large-time limit is then described by the density matrix $e^{-H/T}$, in which we may, then, neglect these additional interactions if the physics we are interested in does not involve them. On the other hand, out of equilibrium, this cannot be done: if the model does not contain the proper relaxation mechanisms, then the large-time limit simply does not exist, and the Schwinger-Keldysh formulation does not provide an answer for the steady-state average. The interpretation is simply that in order to actually maintain the steady state out of equilibrium in a real-time formulation, we need relaxation mechanisms at all times, because energy and entropy need to be absorbed steadily. This is in contrast to the equilibrium case, where once the equilibrium density matrix is obtained, we may forget about how it was obtained.

The second point is that the result in the equilibrium case also holds at zero temperature, whereas that out of equilibrium may well not hold. Indeed, at equilibrium, we only need the connected correlation functions to vanish at large times, so that we may shift the contours and get the equilibrium density matrix; the zero-temperature, power-law vanishing of CFT correlation functions is enough. Out of equilibrium, we need the integrals themselves to exist, forward and backward contours do not cancel, so that the exponential vanishing provided by the temperature may be necessary. Again, this points to the fundamental rôle played by the thermal baths in the case out of equilibrium.

Finally, the usual approach to the real-time formulation is not that of a quantum quench, but rather of adiabatically turning on the interaction. This can be implemented, for instance, by a factor of the type $e^{\nu(t-t_0)}$ in front of the impurity interaction, where t_0 is the final time, so that we have an explicitly time-dependent Hamiltonian. With the shift $t \to t + t_0$ so that the starting time is $-t_0$ instead of 0, and the final time is 0, it is clear then that all large-time integrals exist in the interaction picture for any $\nu > 0$. That is, here we do not have to worry about having proper relaxation mechanisms; they are in a sense implemened by the presence of ν. But the adiabatic process is actually obtained when we take the limit $\nu \to 0^+$, so that the interaction is turned on very slowly. Hence, we have to worry again about the

existence of a limit. We expect that in fact, out of equilibrium, if there are no relaxation processes, then the limit $\nu \to 0^+$ at $t_0 = \infty$ is not convergent (this is what seems to happen in the Kondo model with an impurity magnetic field). Hence, the adiabatic process is in fact of no help. In order to understand what is happening, consider the following arguments, in the equilibrium case. In quantum mechanics, we know that adiabatically turning on the interaction guarantees that, for instance, the ground states are mapped to one another. However, there is a "ghost" of the phenomenon of quantum recurrence that plays a fundamental rôle for this to happen. In the cases where no relaxation mechanisms are present, we would need to keep L finite before taking the limit $\nu \to 0^+$. Technically, with L infinite, the part that we wish to cancel in making the shift $t + \mathrm{i}/T \mapsto t$ would instead give integrals of the type $\sin(\nu/T) \int_{-\infty}^{0} e^{\nu t}\, dt$, which do not vanish as $\nu \to 0^+$ (but give some spurious finite values). With L finite, oscillatory terms will appear in these integrals, $\sin(\nu/T) \int_{-\infty}^{0} e^{(\nu+i\omega)t}\, dt$, and guarantee that they vanish as $\nu \to 0^+$. Then indeed, at equilibrium, we would get the density matrix $e^{-H/T}$ for finite L, in which we may then take the limit $L \gg T^{-1}$. That is, we do not need to explicitly have relaxation mechanisms in the model, an adiabatic change of the Hamiltonian implements the correct physics, but this works by doing the adiabatic process at finite L. But, out of equilibrium, we certainly need to take L large in the first place, otherwise the steady state cannot be reached. Then, the adiabatic process is of no help, relaxation mechanisms are essential. Physically, this is again the same principle: relaxation mechanisms not only allow us to reach the steady state, but also to maintain it.

3.4 The limit of what objects are we looking at? (irreversibility)

Although we have talked about the meaning and existence of the large-time limit, and what result it may give, we have not been very precise about the objects of which we take the large-time limit. This is quite important, and point to one more deep physical property of the construction. Basically, in order for the large-time limit to exist, we needed factorisation of correlation functions, but this can occur only if the operator of which we evaluate the average is *finitely supported* in space. For instance, the current operator $\mathcal{J}$ or the impurity number operator N_i are supported at the impurity site $x = 0$, which is just one point, so are finitely supported. Operators like $\Psi_j^\dagger(x)\Psi_j(x)$ for any fixed x are supported at x, again just one point. The operator $\int_{-\ell}^{\ell} dx\, \Psi_j^\dagger(x)\Psi_j(x)$ is supported on the interval $[-\ell, \ell]$, so is also finitely supported for any finite ℓ. If the factorisation property needs a symmetry, like the $SU(2)$ symmetry of the Kondo model, then the operator should also be invariant under that symmetry. In all these examples, we expect that the factorisation property will hold if relexation mechanisms are present. (A more formal definition of a finitely supported operator is one that commutes with the Hamilonian density $h(x)$ for any x large enough.)

Hence, only for finitely supported operators do we expect the steady-state average to exist. Their main property is of being non-extensive: loosely speaking, a change of L does not affect them. Extensive quantities in general do not have a well-defined steady state average out of equilibrium, because their averages may be subject to a constant flow. In our impurity models, the time variations of extensive quantities that are conserved by H_0, are finitely supported operators (supported at $x = 0$), so that these time variations have well-defined averages (so that we are indeed describing steady states).

The restriction on the set of operators of which we may take steady-state averages answers the question of irreversibility in the unitary, quantum quench formulation. Clearly, using the unitary evolution operator e^{iHt}, the state we reach after time t can be used to get back the initial state simply by the backward

unitary evolution. But a steady state is not affected by that unitary evolution, since it is steady; hence it has, in a sense, lost the information of the initial state. This loss of information is essentially the loss of the extensive observables in the set of observables of which we may take steady-state averages. The finitely supported operators constitute just enough observables to fully describe the steady state, but not to describe the full time evolution that led to it. Note that in the equilibrium case, if we use the adiabatic formulation, there is no need to restrict the set of operators, since we consider finite L. However, in this case, the time evolution reaching the equilibrium state is generated by a different operator, with an explicit time dependence, so that there is clearly no interpretation problem.

4 The density matrix out of equilibrium

The real-time formulation described above contains too much information if we are just interested in steady states: it tells us about the full time evolution, from the initial density matrix $e^{-(H_0-VQ)/T}$, to the steady state itself. Can we describe only the steady state, using something similar to the equilibrium density matrix $e^{-H/T}$? The first suggestion that this can be done is found in Hershfield's proposition of a density matrix out of equilibrium [5], through a so-called Y operator. Here, we will put the accent on the use of scattering states in order to describe this density matrix, as suggested by Hershfield [5]. We will first show how to derive the Y operator, and the density matrix out of equilibrium, from the real time formulation described above, based on the fundamental properties proposed in [6]. For this purpose, we will introduce and describe scattering states through the Lippman-Schwinger equation. We will also provide an expression for Y directly related to the real-time formulation, following [5] and [3]. We will show how it can be useful by deriving from it interesting expressions for the current response function and the current noise (reproducing results of Fujii [7] for the latter), that can be used more conveniently in the scattering-state formulation. Then, we will give more explanations about the Y operator by considering a "free" (from the viewpoint of operator algebra) model, the resonant level model (RLM). We will construct the Y operator explicitly, describe with more precision, for the first time, its property of non-locality that was predicted in [3] (this is, we believe, at the basis of the out-of-equilibrium aspect of the density matrix – the initial explanation of Hershfield [5] is not entirely enough), and give some explanations as to how to obtain efficiently a full operator construction in the interacting case (perturbation theory for the density matrix out of equilibrium was considered by Han [8], but we will present a different approach, based on constructing observables, which we believe is simpler). We will also provide some clarifications about the "resolution of the impurity" that is needed in the scattering-state formulation, a concept that was emphasized in [6], showing that there are strong consistency constraints. Finally, following [6], we will explain how to use equations of motion in order to obtain various results, including the all-order perturbative expansions, in the scattering-state formulation for a large family of steady-state averages, focusing on the interacting resonant-level model.

4.1 The scattering-state definition of the Y operator

We first wish to derive the scattering-state formulation of steady states out of equilibrium from the real-time formulation of the previous section. Although the resulting scattering-state formulation is quite simple, its careful derivation from the real-time formulation is quite non-trivial. We will be presenting mostly general arguments, but we will specialise to the interacting resonant-level model and to the Kondo

model for clarifying some more technical parts.

4.1.1 General conditions on the density matrix out of equilibrium

In quantum mechanics, a usual scattering state is obtained from the large-time evolution of the large-volume limit of a (unnormalised) state that represents a density of particles present only in a flat "asymptotic" region of the potential (the "incoming" region). That is, it is obtained by taking the limit $L \gg t \gg a$ where a is some length scale characterising the initial state. This limit has to be taken in an appropriate way, and the important notion is that we wish to probe only the resulting state in finite regions near to where the potential is not flat. The result is, in general, *not* the large-volume limit of a finite-volume eigenstate of the Hamiltonian, because, for instance, in the outgoing region of the potential, the state only contains outgoing particles (there is no wave corresponding to the other direction of probability current). In general, starting with any finite-volume state and taking the limit $L \gg t \gg a$, we expect to obtain a linear combination of such scattering states. This will involve scattering states obtained from incoming particles in all possible directions (so that the resulting state will not, in general, have a clear outgoing region with only one probability current direction). The space of scattering states is not exactly a Hilbert space, as its basis forms a continuum and is not normalisable on L^2. Yet, it is of much use, and from scattering states physical quantities can be evaluated (like the reflection and transmission coefficients).

In the present case of impurity models, we start with a statistical distribution of finite-volume states given by the density matrix $e^{-(H_0-VQ)/T}$, and, as we saw above, we need to take the limit $L \gg t \gg T^{-1}$ with the time evolution obtained from the interacting Hamiltonian H, and probe the result of the limit in finite regions around $x = 0$. Hence, it is natural to expect that the result of the limit can be described in the space spanned by scattering eigenstates of H. What we need to assess is the various resulting statistical weights of these scattering states, recalling that these states will be in general linear combinations of states both with incoming particles on metallic sheets 1 and 2 (hence without clear outgoing metallic sheet). One may worry about the possible presence of bound states when there is interaction with the impurity. However, the initial density matrix describes scattering states of the model without impurity interaction, and when the impurity interaction is added, all such scattering states are mapped to the scattering region of the interacting spectrum (by the Lippman-Schwinger equation) – if there are bound states, they do not contribute to the statistical distribution.

Hence there should exist a Hermitian operator ρ_{NE} acting on the space of scattering states such that all steady-state averages of finitely supported operators are reproduced by formal traces:

$$\lim_{L\gg t\gg T^{-1}} \langle \mathcal{O}\rangle(t) = \langle \mathcal{O}\rangle_{NE} \equiv \frac{\mathrm{Tr}\,(\rho_{NE}\,\mathcal{O})}{\mathrm{Tr}\,(\rho_{NE})}. \tag{4.1}$$

If we had an N-dimensional Hilbert space for finite N, there would be N^2 linearly independent operators $\mathcal{O}$, so that we would have N^2 conditions, which should be just enough to fully fix the N by N matrix ρ_{NE} – indeed ρ_{NE} should exist and be unique. Of course, the Hilbert space is infinite-dimensional, so this counting argument fails, and in principle we would still need to prove its existence and uniqueness. However, we will show in this subsection that assuming its existence, it can be uniquely fixed, in a way that allows us to evaluate steady-state averages. We will then discuss in the next subsection its existence when making more explicit the connection to the real-time formulation.

We start by describing two properties of the steady-state trace (i.e. of ρ_{NE}), based on the existence of the large-time limit. The first is the steady-state condition. In general, for any finitely supported

operator $\mathcal{O}$, the "time-differentiated" operator $[H, \mathcal{O}]$ is also finitely supported. This means that the large-time limit of the average of $[H, \mathcal{O}]$ exists, so should be described by ρ_{NE}. Since this is proportional to the time derivative of the average of $\mathcal{O}$, whose large-time limit also exists, the average $\langle [H, \mathcal{O}] \rangle_{NE}$ must be zero. Hence, if ρ_{NE} is fixed by knowing the averages of all finitely supported operators, it must be that

$$[H, \rho_{NE}] = 0. \tag{4.2}$$

This is the very natural steady-state condition. In fact, by similar arguments, it is also true that ρ_{NE} should commute with any local conserved charge, operators that commute with H and whose action on any finitely supported operator gives a finitely supported operator.

The second condition is slightly more subtle, and is based on chirality: that $\Psi_j(x)$ are right-movers. Let us consider an operator

$$\mathcal{O}(x_1, x_2, \ldots, x_n) = \Psi^\dagger_{j_1,a_1}(x_1)\Psi^\dagger_{j_2,a_2}(x_2)\cdots\Psi_{j_{n-1},a_{n-1}}(x_{n-1})\Psi_{j_n,a_n}(x_n) \tag{4.3}$$

that is a product of Fermion operators on the metallic sheets j_i, of particle numbers ± 1, of internal indices a_i, and at positions x_i. The important point is that we will consider all the positions to be "on the left", $x_i < 0$, that is, in a region that corresponds to right-moving particles that have not yet interacted with the impurity. Let us look at the time-evolved average of such an operator, which we write in the interaction picture as in (3.13), but now in the form

$$\langle \mathcal{O}(x_1, x_2, \ldots, x_n) \rangle(t) = \left\langle \mathcal{P} \exp\left[-\mathrm{i} \int_t^0 dt' \, [I(t'), \cdot] \right] \, \mathcal{O}(x_1, x_2, \ldots, x_n) \right\rangle_0 \tag{4.4}$$

where $[I(t'), \cdot]$ should be understood as acting on $\mathcal{O}(x_1, x_2, \ldots, x_n)$ by generating commutators (it is the adjoint representation of $I(t')$ on the space of operators). Since $I(t')$ is made up of impurity operators and Fermion operators at positions $x = t' > 0$, it commutes with $\mathcal{O}(x_1, x_2, \ldots, x_n)$ for any $x_1 < 0, x_2 < 0, \ldots, x_n < 0$, so that in general we obtain the strong statement that

$$\langle \mathcal{O}(x_1, x_2, \ldots, x_n) \rangle(t) \overset{x_1<0, x_2<0, \ldots, x_n<0}{=} \langle \mathcal{O}(x_1, x_2, \ldots, x_n) \rangle_0$$

for any $t > 0$. That is, we find the second condition,

$$\langle \mathcal{O}(x_1, x_2, \ldots, x_n) \rangle_{NE} \overset{x_1<0, x_2<0, \ldots, x_n<0}{=} \langle \mathcal{O}(x_1, x_2, \ldots, x_n) \rangle_0. \tag{4.5}$$

It turns out that in general, conditions (4.2) and (4.5) are essentially enough to fully fix the operator ρ_{NE}. The first condition tells us that ρ_{NE} can be diagonalised simultaneously with H, so that we only need to describe the eigenvalues of ρ_{NE} on a basis of scattering eigenstates of H. The second condition tells us what these eigenvalues are. We will present here arguments that rely on a scattering state construction. This will also allow us to fully define ρ_{NE} as an operator on the space of scattering states. These two conditions were first written and used in [6].

First, though, we start by recasting the problem into the language of the Y operator. Let us write ρ_{NE} in the form

$$\rho_{NE} = e^{-(H - VY)/T} \tag{4.6}$$

for some Hermitian operator Y. This can always be done, but in general the operator Y may depend on V and T. Condition (4.2) immediately implies that

$$[H, Y] = 0 \tag{4.7}$$

so that we may diagonalise simultaneously H and Y. In order to use condition (4.5), we may look at both sides as analytic functions of $x_1, x_2, \ldots, x_n$ in the region $\Re(x_1) < 0, \ldots$. On the right-hand side, with the density matrix ρ_0, there is a quasi-periodicity property under $x_i \mapsto x_i + \mathrm{i}/T$ that can be obtained by using cyclicity of the trace as well as the canonical commutation relations (2.1). This relies on evaluating $e^{(H_0-VQ)/T}\Psi_j(x)e^{-(H_0-VQ)/T}$. Condition (4.5) implies that there is the same quasi-periodicity property on the left-hand side. This occurs if and only if $H - VY$ has the same commutation relations, with Fermion operators, as $H_0 - VQ$. But we know that $[H, \Psi_j(x)] = [H_0, \Psi_j(x)]$ for any $x < 0$, so that we must impose

$$[Y, \Psi_j(x)] = [Q, \Psi_j(x)] = \frac{(-1)^j}{2}\Psi_j \quad (x < 0) \tag{4.8}$$

where we recall that $j = 1, 2$. Hence, we have recast conditions (4.2) and (4.5) into (4.7) and (4.8) respectively. These latter strongly suggest that Y is indeed independent of V and T. In fact, the quasi-periodicity property, along with analytic conditions coming mainly from the canonical commutation relations, and some asymptotic conditions, are enough to fully determine the averages. Hence, this also strongly suggests that Y defined through (4.7) and (4.8) is unique, possibly up to conserved impurity operators. In order to complete its description, we need to construct (at least formally) scattering eigenstates of H and deduce the eigenvalues of Y on these states, which we now proceed to do.

4.1.2 Scattering states and Lippman-Schwinger equation

The construction of scattering eigenstates of H in general is of course quite involved, but we will only need here some of the main principles. Our first step is the construction of scattering eigenstates for the uninteracting Hamiltonian H_0. We will consider here the "bare" construction, whereby the "bare ground state" is empty, and must be filled in in order to construct a Fermi sea corresponding to the true ground state. We will discuss Hilbert spaces at more length in the last two subsections, but for now this will be sufficient. The bare construction is simply that of a Fock space $\mathcal{F}$ over the algebra of real-space Fermion operators (2.1), tensored into a representation space $\mathcal{I}$ of the impurity degrees of freedom, $\mathcal{S} = \mathcal{F} \otimes \mathcal{I}$. The space $\mathcal{F}$ is constructed from a vacuum $|0\rangle$ defined by $\Psi_j(x)|0\rangle = 0$, and then by acting on it with $\Psi_j^\dagger(x)$, creating particles at positions x. Scattering eigenstates of H_0 are simply of the form

$$\int dx_1 dx_2 \cdots dx_n \, e^{\mathrm{i}p_1x_1 + \mathrm{i}p_2x_2 + \ldots + \mathrm{i}p_nx_n} \Psi^\dagger_{j_1,a_1}(x_1)\Psi^\dagger_{j_2,a_2}(x_2)\cdots\Psi^\dagger_{j_n,a_n}(x_n)|0\rangle \otimes |i\rangle \tag{4.9}$$

where $|i\rangle$ is an eigenstate of H_i. These states have energies $p_1 + p_2 + \ldots + p_n + e_i$ by the linear dispersion relation, where e_i is the energy of the state $|i\rangle$.

A basis of scattering eigenstates of H can then be constructed using the Lippman-Schwinger formulation. This tells us that if $|v\rangle_0$ is an eigenstate of H_0 with some energy E_v, then there is a unique state $|v\rangle$ that satisfies

$$|v\rangle = |v\rangle_0 + \frac{1}{E_v - H_0 + \mathrm{i}0^+} I|v\rangle, \tag{4.10}$$

and this state is an eigenstate of $H = H_0 + I$ also with energy E_v. The latter assertion is easy to check formally:

$$(H - E_v)|v\rangle = (H_0 - E_v)|v\rangle + I|v\rangle = (H_0 - E_v)\frac{1}{E_v - H_0 + \mathrm{i}0^+} I|v\rangle + I|v\rangle = 0.$$

The uniqueness is just by inverting the linear operator, assuming it can be inverted (equivalently, by a recursive construction if this converges). The subtlety is that we need $\pm\mathrm{i}0^+$ in the denominator in the

second term on the right-hand side of (4.10); we chose $+\mathrm{i}0^+$, which corresponds to so-called *in* states. The need for $\pm\mathrm{i}0^+$ is in order to have a well-defined inverse operator $(E_v - H_0)^{-1}$, and more explicitly our choice leads to

$$|v\rangle = |v\rangle_0 - \mathrm{i}\int_0^\infty dt\, e^{\mathrm{i}(E_v - H_0 + \mathrm{i}0^+)t} I|v\rangle. \tag{4.11}$$

Hence, we have a map giving us an eigenstate of H for any eigenstate of H_0.

With this space of scattering states, we may now analyse the states $|v\rangle$. An important characteristic is its associated bare wave function,

$$\langle i| \otimes \langle 0|\Psi_{j_1,a_1}(x_1)\Psi_{j_2,a_2}(x_2)\cdots\Psi_{j_n,a_n}(x_n)|v\rangle.$$

The knowledge of the full bare wave function obviously fixes $|v\rangle$ uniquely. Moreover, if $|i\rangle$ is chosen to be an eigenstate $|i\rangle_{min}$ of H_i that has the least number of particles, i.e. that is annihilated by all operators d_α present in the tunneling term of I (if there is such a term), then it is clear that $|i\rangle_{min} \otimes |0\rangle$ is also an eigenstate of H with energy e_i (we will refer to states generated from it by applications of $\Psi_j^\dagger(x)$ as *minimal-particle states*). Hence, using that $[H, \Psi_j(x)] = [H_0, \Psi_j(x)]$ for any $x < 0$, we find that the associated minimal bare wave function must satisfy, for negative positions, the eigenvalue equation of H_0 with energy $E_v - e_i$. Since the states $|v\rangle_0$ form a basis of solutions for this equation, we may write in general, for $x_1 < 0, x_2 < 0, \ldots, x_n < 0$,

$${}_{min}\langle i| \otimes \langle 0|\Psi_{j_1,a_1}(x_1)\Psi_{j_2,a_2}(x_2)\cdots\Psi_{j_n,a_n}(x_n)|v\rangle = {}_{min}\langle i| \otimes \langle 0|\Psi_{j_1,a_1}(x_1)\Psi_{j_2,a_2}(x_2)\cdots\Psi_{j_n,a_n}(x_n)|\tilde{v}\rangle_0 \tag{4.12}$$

for some state $|\tilde{v}\rangle_0$ eigenstate of H_0 with energy E_v. Two important statements from the scattering state theory are: 1) that the state $|\tilde{v}\rangle_0$ can be chosen to be the state $|v\rangle_0$ used to construct $|v\rangle$ from the Lippman-Schwinger equation, and 2) that the knowledge of the minimal bare wave function for negative positions is enough to fix the state $|v\rangle$ in the space of scattering eigenstate of H. Similar statements hold for positive positions, with a different $|\tilde{v}\rangle_0$ identified with an *out* state instead of an *in* state.

In order to explain the first statement, consider the left-hand side of (4.12) using (4.11) to replace $|v\rangle$. The first term on the right-hand side of (4.11) gives indeed the bare wave function of the associated states $|v\rangle_0$. On the other hand, the second term is zero for $x_1 < 0, x_2 < 0, \ldots, x_n < 0$. This is because the impurity interaction I preserves the number of particles, and in fact guarantees that $I|v\rangle$ will have a particle at $x = 0$ (on the metallic sheets or at the impurity). For the co-tunnelling term, this is the case because of the presence of two Fermion operators. The tunnelling term, on the other hand, may be destroying a particle on the sheets, but will then create a particle on the impurity, so that the resulting state cannot be of minimum particle number on the impurity. Likewise, if it destroys a particle on the impurity, it must create one on the metallic sheets at $x = 0$. Since the operator $e^{\mathrm{i}(E_v - H_0 + \mathrm{i}0^+)t}$ may only displace particles on the sheets towards the right for $t > 0$, the result has no overlap with ${}_{min}\langle i| \otimes \langle 0|\Psi_{j_1,a_1}(x_1)\Psi_{j_2,a_2}(x_2)\cdots\Psi_{j_n,a_n}(x_n)$. Hence, only the first term of (4.11) contributes, which shows that we may choose $|\tilde{v}\rangle_0 = |v\rangle_0$; more precisely, that all components of $|\tilde{v}\rangle_0$ that are minimal-particle eigenstates are equal to those of $|v\rangle_0$. Note that once we know the x_i-dependence of the wave function of $|v\rangle_0$ for negative positions, we also know it for positive positions, because it is just obtained by analytic continuation.

The second statement above is slighly more subtle in general. There are simple cases where all states $|i\rangle$ are minimal particle states; for instance, the Kondo model, where no particle on the impurity is ever created or destroyed, since the impurity is just a spin degree of freedom. In these cases, the derivation

above shows that we know $|v\rangle_0$ uniquely from the minimal bare wave function at negative positions, hence that we can indeed deduce $|v\rangle$ from this using the Lippman-Schwinger equation. In other cases, the situation is more complicated, because the minimal bare wave function does not tell us about the overlap of $|\tilde{v}\rangle_0$ with non-minimal-particle states. That is, we do not have enough information to fix $|v\rangle_0$ just from the minimal bare wave function, so it seems that we do not have enough information to fix $|v\rangle$. However, the map from eigenstates of H_0 to eigenstates of H given by the Lippman-Schwinger equation (4.10) in general is not expected to be invertible: different uninteracting eigenstates $|v\rangle_0$ may give rise to the same interacting eigenstate $|v\rangle$. More precisely, we expect that all states $|v\rangle_0$ with the same minimal-particle components lead to the same vector $|v\rangle$. Then, it is indeed sufficient to know the minimal-particle components of $|v\rangle_0$ in order to know $|v\rangle$; in other words, the minimal bare wave function of $|v\rangle$ fixes $|v\rangle$. What is happening is that there is *hybridisation*: the particles on the impurity get mixed up with those on the metallic sheets in one state, so that there is no good quantum number that would correspond to all states of the impurity with all particle numbers. The only good impurity quantum number is the one parametrising the minimal-particle states (the other quantum numbers for $|v\rangle$ are the momenta $p_1, p_2, \ldots, p_n$ and the particle types).

In order to see how this can happen, let us consider the IRLM for simplicity (see the Hamiltonian (2.8)). What we want to show is that if we consider a state $|v\rangle_0$ (eigenstate of H_0) that has no minimal-particle component at all, then the resulting state $|v\rangle$ is zero. By linearity of the Lippman-Schwinger equation, this will indeed guarantee that only the minimal-particle component of $|v\rangle_0$ determines $|v\rangle$.

In the case of the IRLM, there are only two impurity states, filled and empty. Let us denote the component of $|v\rangle$ that has a filled/empty impurity state by $|v\rangle^{f,e}$. The Lippman-Schwinger equation can be written, using the fact that $|v\rangle_0$ has no empty component,

$$\begin{aligned}
|v\rangle^e &= t\sum_j \frac{1}{E_v - H_0 + \mathrm{i}0^+}\psi_j^\dagger(0)d|v\rangle^f \\
|v\rangle^f &= |v\rangle_0 + \frac{1}{E_v - H_0 + \mathrm{i}0^+}I_U|v\rangle^f + t^*\sum_j \frac{1}{E_v - H_0 + \mathrm{i}0^+}d^\dagger\psi_j(0)|v\rangle^e
\end{aligned}$$

where $I_U = U\sum_j \psi_j^\dagger(0)\psi_j(0)$. We may easily simplify this into one equation for $|v\rangle^f$. We have to evaluate

$$\begin{aligned}
|t|^2\sum_{j,j'} d^\dagger\psi_j(0)\frac{1}{E_v - H_0 + \mathrm{i}0^+}\psi_{j'}^\dagger(0)d|v\rangle^f &= -\mathrm{i}|t|^2\sum_{j,j'}\int_0^\infty dx\,\psi_j(0)e^{\mathrm{i}(E_v+\epsilon-H_0+\mathrm{i}0^+)x}\psi_{j'}^\dagger(0)|v\rangle^f \\
&= -\mathrm{i}|t|^2\sum_{j,j'}\int_0^\infty dx\,\psi_j(0)\psi_{j'}^\dagger(x)e^{\mathrm{i}(E_v+\epsilon-H_0+\mathrm{i}0^+)x}|v\rangle^f \\
&= \mathrm{i}|t|^2\sum_{j,j'}\int_0^\infty dx\,\psi_{j'}^\dagger(x)\psi_j(0)e^{\mathrm{i}(E_v+\epsilon-H_0+\mathrm{i}0^+)x}|v\rangle^f + -\mathrm{i}|t|^2|v\rangle^f.
\end{aligned}$$

In the last line, we used the *resolution of the impurity*

$$\psi_j(0) = \frac{\psi_j(0^-) + \psi_j(0^+)}{2} \tag{4.13}$$

where $0^\pm$ are understood as limits from the right/left towards the point 0 (so that the integral over x of the delta-function arising from anti-commuting $\psi_j(0)$ and $\psi_{j'}^\dagger(x)$ only gets the 0^+ part). This is of course a natural choice, and we will show later that this is the only valid choice (we will discuss more about the resolution of the impurity later). Essentially, it says that in fact, we should think of $\psi_j(0)$ as being

$\int dx\, \rho(x)\psi_j(x)$ with a density $\rho(x)$ strongly peaked at $x = 0$, with total weight 1 equally distributed on both sides of $x = 0$. Using the notation

$$A = \mathrm{i}|t|^2 \sum_{j,j'} \int_0^\infty dx\, \psi_{j'}^\dagger(x)\psi_j(0) e^{\mathrm{i}(E_v+\epsilon-H_0+\mathrm{i}0^+)x},$$

what we found is that

$$|v\rangle^f = |v\rangle_0 + \frac{1}{E_v - H_0 + \mathrm{i}0^+} \left(I_U + A - \mathrm{i}|t|^2\right) |v\rangle^f. \tag{4.14}$$

The term $\frac{-\mathrm{i}t^2}{E_v-H_0+\mathrm{i}0^+}|v\rangle^f$ makes the matrix element ${}_0\langle v| \frac{1}{E_v-H_0+\mathrm{i}0^+} \left(I_U + A - \mathrm{i}|t|^2\right) |v\rangle_0$ be of order $1/0^+$ (more precisely, we would need to take two different states ${}_0\langle v'|$ and $|v\rangle_0$, and integrate on a small region over the momenta of ${}_0\langle v'|$); indeed, we have $H_0|v\rangle_0 = E_v|v\rangle_0$, whereas the terms with I_U and with A just have finite matrix elements. But, if a matrix has one element that is infinite, the inverse matrix has both the row and the column corresponding to this element equal to 0 (because the determinant is infinite, whereas the minors of elements on the row and on the column corresponding to the infinite element are finite). Since we must evaluate

$$\left[1 - \frac{1}{E_v - H_0 + \mathrm{i}0^+} \left(I_U + A - \mathrm{i}|t|^2\right)\right]^{-1} |v\rangle_0,$$

the result is a zero vector. Hence, the solution is $|v\rangle^f = 0$. But since $|v\rangle^e$ is a finite linear operator applied on $|v\rangle^f$, it must also be zero, so that we have $|v\rangle = 0$. Although our last considerations were expressed in the language of matrices, they hold here as well, where we should be thinking about solving linear integral equations.

Hence, we have shown that hybridisation occurs in the IRLM. The derivation makes it clear that it occurs thanks to the tunnelling terms, that allow particles to be absorbed and emitted from the impurity. We will see in the subsection 4.3 what consequence this has on the representation of the algebra of observables in the RLM, and in subsection 4.4 that this is associated to a construction of the set of scattering states as an embedding in $\mathcal{F} \otimes \mathcal{I}$. But the important point for us now is that this indeed guarantees that the minimal bare wave function fixes the state $|v\rangle$.

4.1.3 The general definition of Y on scattering states

Finally, we may now use (4.12) (with $|\tilde{v}\rangle_0 = |v\rangle_0$), along with (4.8), in order to provide a definition of Y. If $|v\rangle_0$ has Q-eigenvalue q_v, we may evaluate the bare wave function of the following commutator:

$$\begin{aligned} &{}_{min}\langle i| \otimes \langle 0|[Y, \Psi_{j_1,a_1}(x_1)\Psi_{j_2,a_2}(x_2)\cdots\Psi_{j_n,a_n}(x_n)]|v\rangle \\ &\overset{x_1<0,x_2<0,\ldots,x_n<0}{=} -q_v\ {}_{min}\langle i| \otimes \langle 0|\Psi_{j_1,a_1}(x_1)\Psi_{j_2,a_2}(x_2)\cdots\Psi_{j_n,a_n}(x_n)|v\rangle_0. \end{aligned} \tag{4.15}$$

The states $|0\rangle \otimes |i\rangle_{min}$ are eigenstates of H and of the number of particle operator N (the latter with eigenvalue 0). Since such states are the only ones with $N = 0$ and since Y commutes with both H and N we may assume that these states are also eigenstates of Y. Let us denote their Y eigenvalue by a_i. Then, we find

$$\begin{aligned} &{}_{min}\langle i| \otimes \langle 0|\Psi_{j_1,a_1}(x_1)\Psi_{j_2,a_2}(x_2)\cdots\Psi_{j_n,a_n}(x_n)\ Y|v\rangle \\ &\overset{x_1<0,x_2<0,\ldots,x_n<0}{=} (q_v + a_i)\ {}_{min}\langle i| \otimes \langle 0|\Psi_{j_1,a_1}(x_1)\Psi_{j_2,a_2}(x_2)\cdots\Psi_{j_n,a_n}(x_n)|v\rangle_0. \end{aligned} \tag{4.16}$$

In the IRLM, there is only one minimal-particle impurity eigenstate, so we may well shift Y in order to set $a_i = 0$. In the Kondo model without impurity magnetic field, there is an $SU(2)$ symmetry, which also preserves Y. Since this symmetry mixes the spin of the impurity with those of the metallic Fermions, we must also have both a_i (spin up and spin down) equal to each other, so that we can again shift Y to make them zero. Hence, using the fact that the minimal bare wave function fixes the state, in these two cases we have

$$Y|v\rangle = q_v|v\rangle \quad \text{if} \quad Q|v\rangle_0 = q_v|v\rangle_0. \tag{4.17}$$

This is expected to hold in general as well. This completely fixes the Y operator on the space of asymptotic eigenstates of H: given $|v\rangle_0$ that is eigenstate of both H_0 and Q, with eigenvalues E_v and q_v respectively, we may construct the unique $|v\rangle$ that is eigenstate of H through the Lippman-Schwinger equation, and we know that Y acts on it diagonally with eigenvalue q_v. This, then, also completely fixes ρ_{NE} through (4.6). Note that the Y operator is independent of V and T.

Recapitulating, we have found that there is a unique density matrix operator out of equilibrium (if it indeed exists), that can be defined by conditions (4.2) and (4.5). It can equivalently be defined through the Y operator by (4.6), where the Y operator is in general partially defined by the conditions (4.7) and (4.8) (to complete the definition, we need to say that it commutes with other internal symmetries), or completely defined by (4.17).

We note that we made use of hybridisation for the IRLM, and $SU(2)$ symmmetry for the Kondo model without magnetic field, in order to complete the definition of Y from its basic properties. It is interesting that it is these two concepts that lead, in the Schwinger-Keldysh formulation, to the fact that there is relaxation, so that a steady state can be established at large times. Indeed, the $SU(2)$ symmetry of the Kondo modal was used in order to prove the existence of the large-time limit; and hybridisation in the IRLM is simply related to the fact that the impurity can change its state by exchanging particles with the metallic sheets, a Caldeira-Leggett-like intraction. It would be interesting to understand further the relation between the real-time construction and the definition of the Y operator in this light.

An immediate question that arises, looking at (4.6), is: since the density matrix has the exponential form familiar to the equilibrium situation, why isn't it describing a system at equilibtium? Recall that in a system that has a conserved charge Q representing a certain quantity (number of particle, etc.), if this quantity is exchanged with an environement, the equilibrium will be described by putting a term $\mu Q/T$ in the exponential in the density matrix, for some associated "chemical potential" μ. However, an important aspect in this situation is that the conserved charge should be *strictly extensive*: the quantity represented should have a local density, and Q should be the sum over all space of that density (Q is then said to be a local conserved charge). This is what happens for the total energy, the number of particles, the volume, etc. In the case of (4.6), the Y operator is indeed a conserved quantity, but it is not strictly extensive. As we will see below in the case of a free impurity model, it does not have a local density; it is in fact a non-local conserved charge. It is this non-locality that is at the root of the fact that ρ_{NE} indeed describes a situation that is out of equilibrium.

Another question that may occur concerning the scattering state formulation is that of evaluating physical quantities. We have seen that the current $\mathcal{J}$ is a local operator (supported at $x = 0$), but there are other physical quantities that may be of interest, in particular quantities that involve explicitly a time evolution. In the scattering-state formulation, all meaningful physical questions must be translated into averages of finitely supported operators (or a slight extension of this, as we will see below), and in principle it is always possible to do so. The steady-state average of the integral $\int_0^t dt\, \mathcal{J}(t)$ of the current

evolved over a finite period of time can be obtained, for instance, by using the interaction picture and the fact that the time evolution with H_0 of Fermion operators corresponds to displacements in space. If the period of time t is finite, then these displacement will also be finite, so that we will indeed have a finitely supported operator. The interaction picture, however, does provide a nice expression for $\int_0^t dt\, \mathcal{J}(t)$ as a finitely supported operator. A more tricky, and more interesting, question is that of the current noise or of the zero-frequency response function, which in principle involves an integral over an infinite period of time. This is discussed in the next subsection.

Finally, although we defined the Y operator properly on the space of asymptotic eigenstates of H, in practice we do not need to use this definition. We will show below that the conditions (4.2) and (4.5) are in fact enough to evaluate averages out of equilibrium perturbatively, and that the conditions (4.7) and (4.8) are enough to construct the Y operator in the resonant level model and to develop an operator perturbation theory.

4.2 Connection to the real-time formulation, current noise and current response functions

In the previous subsection, we have shown how to define a density matrix out of equilibrium in the space of scattering states of H. It has a form very similar to an equilibrium density matrix, but the Y operator associated to voltage V is quite special, and had to be defined in a somewhat involved way. Here we will see how to obtain an expression for Y directly from the real-time formulation. This was in fact written in the initial paper by Hershfield [5], but a more careful analysis for the Kondo model was performed for the first time in [3], including the proof of the existence of the large-time limit (the presence of appropriate relaxation mechanisms), as we mentionned above, and the sligthly different proof of the existence of the Y operator itself and of its rôle in the density matrix.

Let us consider a finitely-supported operator $\mathcal{O}$, and its time-evolved average from the density matrix $\rho_0 = e^{-(H_0 - VQ)/T}$ via the dynamics given by H. We may write $\rho_0 = e^{-H_0/T} e^{VQ/T}$, and similarly to what we obtained in (3.16), we may write

$$\langle \mathcal{O} \rangle(t) = \frac{\left\langle \mathcal{P} \exp\left[-\mathrm{i} \int_{\mathrm{i}/T}^{t+\mathrm{i}/T} dt'\, I(t')\right]\ \mathcal{P} \exp\left[-\mathrm{i} \int_t^0 dt'\, I(t')\right]\ e^{VY(t)/T}\ \mathcal{O} \right\rangle_0}{\left\langle \mathcal{P} \exp\left[-\mathrm{i} \int_{\mathrm{i}/T}^{t+\mathrm{i}/T} dt'\, I(t')\right]\ \mathcal{P} \exp\left[-\mathrm{i} \int_t^0 dt'\, I(t')\right] e^{VY(t)/T}\ \right\rangle_0} \tag{4.18}$$

where we defined

$$Y(t) = \ \mathcal{P} \exp\left[-\mathrm{i} \int_0^t dt'\, I(t')\right]\ Q\ \mathcal{P} \exp\left[-\mathrm{i} \int_t^0 dt'\, I(t')\right] = e^{-iHt} Q e^{iHt} \tag{4.19}$$

(in the last equality, we used the fact that $[H_0, Q] = 0$). That is, instead of using $H_0 - VQ$ for the interaction picture, we only used H_0, so that we generated $I(t')$ everywhere instead of having some factors with $I_V(t')$.

Let us consider instead the quantity

$$\frac{\left\langle \mathcal{P} \exp\left[-\mathrm{i} \int_{\mathrm{i}/T}^{t_1+\mathrm{i}/T} dt'\, I(t')\right]\ \mathcal{P} \exp\left[-\mathrm{i} \int_{t_1}^0 dt'\, I(t')\right]\ e^{VY(t_2)/T}\ \mathcal{O} \right\rangle_0}{\left\langle \mathcal{P} \exp\left[-\mathrm{i} \int_{\mathrm{i}/T}^{t_1+\mathrm{i}/T} dt'\, I(t')\right]\ \mathcal{P} \exp\left[-\mathrm{i} \int_{t_1}^0 dt'\, I(t')\right]\ e^{VY(t_2)/T}\ \right\rangle_0}. \tag{4.20}$$

For $t_1 = t_2 = t$, this is the same as $\langle \mathcal{O} \rangle(t)$, but otherwise it is just a different quantity. However, as it was argued in [3], for the Kondo model without impurity magnetic field where we know how to prove

that the limit $\lim_{t\to\infty}\langle\mathcal{O}\rangle(t)$ exists (see subsection 3.2), we may take the limit $t_1 \to \infty$ of the quantity (4.20) first, which exists by the same arguments, and then $t_2 \to \infty$. The result is the same as that of $\lim_{t\to\infty}\langle\mathcal{O}\rangle(t)$. This is an important fact, because with $t_1 \to \infty$ first, we can shift the corresponding t' contour and we obtain

$$\lim_{L\gg t\gg T^{-1}}\langle\mathcal{O}\rangle(t) = \lim_{t_2\gg T^{-1}} \frac{\left\langle e^{-H/T}\, e^{VY(t_2)/T}\, \mathcal{O}\right\rangle_0}{\left\langle e^{-H/T}\, e^{VY(t_2)/T}\right\rangle_0}. \tag{4.21}$$

Hence, we see, from (4.1) and (4.6), that we may define

$$Y = \lim_{t\to\infty} Y(t) = \lim_{t\to\infty} e^{-iHt} Q e^{iHt} \tag{4.22}$$

where the limit is really to be understood in the sense of (4.21). That is, Y is nothing else than the evolution backward in time of Q for an infinite time.

This makes good sense with respect to the result (4.17) concerning the action of Y on asymptotic states. Indeed, naïvely, the backward evolution of a state $|v\rangle$ gives $\lim_{t\to\infty} e^{iHt}|v\rangle = |v\rangle_0$ (as it should be for an *in* state), the action of Q on this gives the eivenvalue q_v, and the forward evolution gives back $\lim_{t\to\infty} e^{-iHt}|v\rangle_0 = |v\rangle$. However, these are naïve arguments as they are presented; a better analysis of the limits taken would be required, but the derivation of the previous subsection circumvented this.

Another form of Y, directly derived from (4.22), is obtained as follows. Consider the operator $Y(t)$ from (4.19). We have that $Y(0) = Q$, and that $dY(t)/dt = \mathcal{J}(-t)$, hence we can write, using (4.22),

$$Y = Q + \int_{-\infty}^{0} dt\, \mathcal{J}(t) \tag{4.23}$$

(which was first written in [3]). As was pointed out by Fujii [7], this provides a connection between the Schwinger-Keldysh formalism and the formalism of MacLennan-Zubarev [9, 10].

Although not of practical use by itself as a definition for the density matrix out of equilibrium, the expression (4.23) gives rise to interesting results. Let us consider first the (zero-frequency) current response function associated to any other (finitely supported) observable $\mathcal{O}$:

$$R_{\mathcal{O}} = \mathrm{i}\int_{-\infty}^{0} dt\, \langle[\mathcal{J}(t), \mathcal{O}]\rangle_{NE}, \quad \mathcal{J}(t) = e^{\mathrm{i}Ht}\mathcal{J}e^{-\mathrm{i}Ht}. \tag{4.24}$$

That is, this measures the total average quantum mechanical response of the observable $\mathcal{O}$ upon past current measurements. It is possible to obtain a simple expression for this. Indeed, expression (4.23) leads to the following expression:

$$\mathrm{i}\int_{-\infty}^{0} dt\, [\mathcal{J}(t), \mathcal{O}] = \mathrm{i}[Y - Q, \mathcal{O}]. \tag{4.25}$$

From the fact that Y commutes with the density matrix ρ_{NE}, we immediately find the expression

$$R_{\mathcal{O}} = \mathrm{i}\langle[\mathcal{O}, Q]\rangle_{NE}. \tag{4.26}$$

The operator $[\mathcal{O}, Q]$ is now a local operator. For instance, with $\mathcal{O} = \mathcal{J}$, so that we are looking at the current-current response function, we have

$$\mathrm{i}[\mathcal{J}, Q] = \mathrm{Re}\left(\frac{1}{2}d_\alpha^\dagger T_\alpha^\dagger \Psi_1(0) + \frac{1}{2}d_\alpha^\dagger T_\alpha^\dagger \Psi_2(0) + 2\Psi_2^\dagger(0) U_\alpha^{(+)} \Psi_1(0) D_\alpha\right). \tag{4.27}$$

As usual, there are subtleties in this derivation concerning the large-time limits. In particular, the validity of (4.23) as an operator relation, that can be inserted inside averages, must be established.

However, we know that we may put powers of the Y operator inside averages of finitely supported operators; we only need to take derivatives with respect to V (we expect averages to be differentiable in V for all $V \geq 0$). More precisely,

$$T\frac{d}{dV}\langle \mathcal{O}\rangle_{NE} = \langle Y\mathcal{O}\rangle_{NE} - \langle Y\rangle_{NE}\langle \mathcal{O}\rangle_{NE} = \langle \mathcal{O}Y\rangle_{NE} - \langle Y\rangle_{NE}\langle \mathcal{O}\rangle_{NE}. \tag{4.28}$$

Hence, if we are evaluating an average where both terms in Q and in $\int_{-\infty}^{0} dt\, \mathcal{J}(t)$ exist, then we may write Y as (4.23). Then, the proper way of deriving (4.26) is as follows. Let us define the zero-average observable

$$\delta\mathcal{O} = \mathcal{O} - \langle \mathcal{O}\rangle_{NE} \tag{4.29}$$

and let us consider $\langle Y\delta\mathcal{O}\rangle_{NE}$ which exists because it is equal to $d\langle \mathcal{O}\rangle_{NE}/dV$. Since

$$Q = \frac{1}{2}\int_{-\infty}^{\infty} dx\, (\Psi_1^\dagger(x)\Psi_1(x) - \Psi_2^\dagger(x)\Psi_2(x)) \tag{4.30}$$

is an integral of a local observable (the difference of local Fermion densities), we have that

$$\langle Q\delta\mathcal{O}\rangle_{NE} \quad \text{exists} \tag{4.31}$$

by factorisation of correlation functions of local (or finitely supported) observables at large distances. Also, if there is relaxation (the condition for the Y operator to exist in the first place), then we also have that

$$\int_{-\infty}^{0} dt\, \langle \mathcal{J}(t)\delta\mathcal{O}\rangle_{NE} \quad \text{exists} \tag{4.32}$$

by large-time factorisation due to relaxation. Hence we can indeed write

$$\langle Y\delta\mathcal{O}\rangle_{NE} = \langle Q\delta\mathcal{O}\rangle_{NE} \; + \int_{-\infty}^{0} dt\, \langle \mathcal{J}(t)\delta\mathcal{O}\rangle_{NE}. \tag{4.33}$$

We can do similarly for Y on the other side of $\delta\mathcal{O}$, $\langle \delta\mathcal{O}\, Y\rangle_{NE}$. Taking the difference between these two quantities, and using the fact that Y commutes with the density matrix, we indeed find (4.26), since in the commutators we may replace $\mathcal{O} \leftrightarrow \delta\mathcal{O}$.

In impurity systems, another quantity that is of experimental interest is the current noise. It is defined essentially by the quantum average of the anti-commutator of current operators at different times, integrated over time (substracted by the large-time limit for convergence),

$$B = 2\int_{-\infty}^{0} dt\, \left(\langle\{\mathcal{J}(t),\mathcal{J}\}\rangle_{NE} - 2\langle\mathcal{J}\rangle_{NE}^2\right). \tag{4.34}$$

More generally, as we did above, we may consider the correlator of the past current with a finitely supported observable $\mathcal{O}$:

$$B_{\mathcal{O}} = 2\int_{-\infty}^{0} dt\, \langle\{\mathcal{J}(t),\delta\mathcal{O}\}\rangle_{NE}. \tag{4.35}$$

We wish to transform this into an average of operators at time 0, so that the expression may be more useful in the scattering-state formulation. Equation (4.23) along with the considerations above immediately lead to

$$B_{\mathcal{O}} = 2\langle\{Y-Q,\delta\mathcal{O}\}\rangle_{NE} = 4T\frac{d}{dV}\langle\mathcal{O}\rangle_{NE} - 2\int_{-\infty}^{\infty} dx\, \langle\{\Delta n(x),\delta\mathcal{O}\}\rangle_{NE} \tag{4.36}$$

where

$$\Delta n(x) = \frac{1}{2}(\Psi_1^\dagger(x)\Psi_1(x) - \Psi_2^\dagger(x)\Psi_2(x)). \tag{4.37}$$

In particular, this gives, for the current noise,

$$B = 4T\frac{d}{dV}\langle\mathcal{J}\rangle_{NE} - 2\int_{-\infty}^{\infty} dx\,\langle\{\Delta n(x), \delta\mathcal{J}\}\rangle_{NE} \tag{4.38}$$

which expresses the noise in terms of the differential conductance, and of the integral over x of the correlation between charge densities at x and the current. This formula was first obtained by Fujii [7] (by a slightly different derivation, in the real-time formulation). Putting the current noise and current-current response function in parallel, we obtained:

$$\begin{aligned} B &= 4T\frac{d}{dV}\langle\mathcal{J}\rangle_{NE} - 2\langle\{\delta\mathcal{J}, Q\}\rangle_{NE} \\ R &= \mathrm{i}\langle[\delta\mathcal{J}, Q]\rangle_{NE}. \end{aligned}$$

Note that although Q does not have a well-defined steady-state average (since it flows steadily), its *quantum correlations* with finitely supported observables reach a steady value in the steady state; this is why the quantities above are well defined. Also, note that for the noise, we do not have strictly speaking an average of a finitely-supported operator. However, we have a limit where the support becomes infinite (the limit is on the extent of the integral over x defininning Q), and this limit exists; that is, this is element of a certain *completion* of the space of finitely-supported operators.

4.3 Operator construction in the (I)RLM

We now provide a full operator construction of the Y operator in the case of the resonant-level model, where the dynamics is obtained from the Hamiltonian (2.8) with $U = 0$; we will then discuss briefly how to take into account the U-term. In quantum mechanics, we may define the Hilbert space of a quantum system as a vector space that forms a module for a closed algebra of observables that includes the Hamiltonian, in such a way that the Hamiltonian has a spectrum that is bounded from below – this gives rise to a bounded representation of the algebra of observables. In the case of the RLM, a closed algebra of observables can be obtained from $\psi_j(x)$ and $\psi_j^\dagger(x)$ for $j = 1, 2$ and $x \in \mathbb{R}$, d, $d^\dagger$ and H (of course, strictly speaking observables should be Hermitian operators, but we may consider the vector space of observables over $\mathbb{C}$). Once we have a bounded representation, since we are interested in steady-state averages out of equilibrium, we will have to construct the Y-operators on this. An operator construction of the Y operator was studied by Han [], and some of the concepts that we discuss here are similar. However, the main point of this subsection is to show that we do not need to construct the Y operator in terms of the impurity-less scattering-state creation and annihilation operators, which is a complicated matter. Indeed, we need only to concentrate on the algebra of observables, and we may use the full scattering creation and annihilation operators, where both the Hamiltonian and the Y operators are very simple (such an expression for the Y operator was already written by Hershfield in the initial paper [5]). Another goal of this subsection is to discuss further the resolution of the impurity in the RLM, and in particular show that we do not have as much freedom as one would initially think about this.

4.3.1 Operator construction and bounded representation in the RLM

Let us now consider the RLM. The (anti-)commutation relations that we need to represent are the canonical ones, (2.1) and (2.7), along with those related to the equations of motion. In fact, it is convenient, in

this model, to consider the *even* and *odd* combinations of the Fermion operators (a transformation which preserves the canonical anti-commutation relations),

$$\psi_{e,o}(x) = \frac{\psi_1(x) \pm \psi_2(x)}{\sqrt{2}} \tag{4.39}$$

along with the rescaling of the tunneling strength,

$$t = \frac{\tau}{\sqrt{2}}. \tag{4.40}$$

Then, the equations of motion are

$$\begin{aligned} [H, \psi_e(x)] &= \mathrm{i}\frac{d}{dx}\psi_e(x) - \tau\delta(x)d \\ [H, \psi_o(x)] &= \mathrm{i}\frac{d}{dx}\psi_o(x) \\ [H, d] &= -\epsilon d - \tau^*\psi_e(0). \end{aligned} \tag{4.41}$$

The set of (anti-)commutation relations formed by the canonical observables and the equations of motion is characteristic of a *free* model: the canonical observables and the Hamiltonian form a closed operator algebra. Moreover, clearly the even and odd sectors decouple, so we can consider them separately.

We know from the general analysis of the scattering states in paragraph 4.1.2 that the only quantum numbers of the scattering eigenstates are the momenta (which is the same as the energy by the linear dispersion relation) of the incoming particles (along with the particle types). Hence, we can expect to be able to write the Hamiltonian using canonical mode operators a_p and b_p (for the even and odd sectors, respectively),

$$\{a_p^\dagger, a_{p'}\} = \{b_p^\dagger, b_{p'}\} = \delta(p - p'), \tag{4.42}$$

other anti-commutation relations giving 0. The Hamiltonian will have the form

$$H = \int dp\, p\, :(a_p^\dagger a_p + b_p^\dagger b_p): \,. \tag{4.43}$$

In order to have a Hamiltonian that is bounded from below, the Fock space must be constructed out of the vacuum $|\mathrm{vac}\rangle$ defined by

$$a_p|\mathrm{vac}\rangle = b_p|\mathrm{vac}\rangle = a_{-p}^\dagger|\mathrm{vac}\rangle = b_{-p}^\dagger|\mathrm{vac}\rangle = 0 \quad (p > 0). \tag{4.44}$$

This represents a filled Fermi sea, where we can create a particle of energy $p > 0$ above it using $a_p^\dagger$, or a hole at an energy $-p < 0$ inside it (which propagates with an energy p) using a_{-p}. The normal-ordering above, $:\cdot:$, tells us to exchange the order of the factors (with an extra minus sign) for $p < 0$.

Thanks to the free-model property of the operator algebra, we can then expect the canonical observables to be linear combinations of the mode operators. For the odd sector, the solution is straighforward:

$$\psi_o(x) = \int \frac{dp}{\sqrt{2\pi}}\, b_p e^{\mathrm{i}px}. \tag{4.45}$$

For the even sector, we must simply try the form $\int \frac{dp}{\sqrt{2\pi}}\, a_p f_p(x)$ for both operators that are mixed by the Hamiltonian, $\psi_e(x)$ and d (with different functions $f_p(x)$). But we know that $f_p(x)$, for $\psi_e(x)$, should be proportional to $e^{\mathrm{i}px}$ for any $x \neq 0$, and that the x-derivative must give a delta-function that cancels the delta-function term in the equation of motion. So we must have a jump at $x = 0$:

$$\psi_e(x) = \int \frac{dp}{\sqrt{2\pi}}\, a_p e^{\mathrm{i}px} \begin{cases} 1 & (x < 0) \\ v_p & (x > 0) \end{cases} \tag{4.46}$$

for some v_p with $|v_p|^2 = 1$. The equation of motion for $\psi_e(x)$ then tells us that

$$-\mathrm{i}\tau d = \int \frac{dp}{\sqrt{2\pi}}\, a_p(v_p - 1). \tag{4.47}$$

That is, this tells us how the operator d is expressed in terms of the mode operators, once we know how to express the canonical observable $\psi_e(x)$. The equation of motion for d then gives us a constraint on v_p, which will finally fix the mode representation of both canonical observables ψ_e and d:

$$\int \frac{dp}{\sqrt{2\pi}}\, a_p(\epsilon - p)(v_p - 1) = \mathrm{i}|\tau|^2 \int \frac{dp}{\sqrt{2\pi}}\, a_p \frac{v_p + 1}{2}. \tag{4.48}$$

Here, we used, as in paragraph 4.1.2, the resolution of the impurity given by (4.13) in order to define $\psi_e(0)$. Since the mode operators a_p are independent for different values of p, we obtain

$$2(\epsilon - p)(v_p - 1) = \mathrm{i}|\tau|^2(v_p + 1) \Rightarrow v_p = \frac{\epsilon - p + \mathrm{i}|\tau|^2/2}{\epsilon - p - \mathrm{i}|\tau|^2/2} = \frac{\epsilon - p + \mathrm{i}|t|^2}{\epsilon - p - \mathrm{i}|t|^2}. \tag{4.49}$$

This should provide the solution to the problem of representing the algebra of observables. We still need to check that the canonical anti-commutation relations are indeed satisfied. The anti-commutation relation $\{\psi_e^\dagger(x), \psi_e(x')\} = \delta(x - x')$ along with (4.46) gives us, for both $x > 0$ and $x' > 0$, the condition that we already stated,

$$|v_p|^2 = 1 \tag{4.50}$$

which is easily checked to hold using (4.49). For $x < 0$ and $x' > 0$, we find instead the integral

$$\int \frac{dp}{2\pi} e^{\mathrm{i}p(x'-x)} v_p,$$

which is seen to give 0 by deforming the contour towards infinity in the positive imaginary direction, using the fact that v_p does not have pole in the region swept. A similar argument holds for $x > 0$ and $x' < 0$. For the impurity operators, we find, from the mode representation,

$$\begin{aligned} \{d^\dagger, d\} &= \frac{1}{|\tau|^2} \int \frac{dp}{2\pi} |v_p - 1|^2 \\ &= \frac{1}{|\tau|^2} \int \frac{dp}{\pi} \left(1 - \frac{(\epsilon - p)^2 - |\tau|^4/4}{(\epsilon - p)^2 + |\tau|^4/4}\right). \end{aligned}$$

The last integral can be evaluated by, for instance, getting the residues upon contour deformation towards $\mathrm{Im}(p) = \pm\infty$, at which line the integral is zero because the integrand goes proportionally to $1/p^2$ at large $|p|$. This indeed gives the correct anti-commutation relation $\{d^\dagger, d\} = 1$. A final anti-commutation relation that needs to be verified is $\{\psi_e^\dagger(x), d'\} = 0$, which is non-trivial because both observables are expressed in terms of the same set of mode operators. We find

$$-\mathrm{i}\tau\{\psi_e^\dagger(x), d\} = \int \frac{dp}{2\pi} (v_p - 1) e^{-\mathrm{i}px} \begin{cases} 1 & (x < 0) \\ v_p^* & (x > 0). \end{cases} \tag{4.51}$$

For $x < 0$, we may deform the p contour towards infinity in the positive imaginary direction, and v_p does not have any pole in the region swept, so this indeed gives 0. For $x > 0$, we must deform towards the negative imaginary direction instead, but we have the factor $(v_p - 1)v_p^* = 1 - v_p^*$ which again does not have pole in that direction, so we again find zero. There may still be delta-function contributions at $x = 0$ in principle, but evaluating $\int_{-L}^{L} dx\, x^n \{\psi_e^\dagger(x), d\}$, we find that for any integer $n \geq 0$ the result is

zero, by similar contour-deformation arguments and from the fact that $v_p - 1$ is proportional to $1/p$ for large $|p|$.

Hence we indeed have a solution to the problem of representing the algebra of canonical observables and the Hamiltonian. One very important subtlety, however, is as follows. From (4.47) and (4.46), we find that

$$\psi_e(0^+) - \psi_e(0^-) = -\mathrm{i}\tau d. \tag{4.52}$$

This is the discontinuity equation of $\psi_e(x)$ in operator terms. But this equation implies that, for instance, $\{\psi_e(0^\pm), d^\dagger\} \neq 0$. This may seem like a contradiction, but it is important to understand that $\psi_e(0^\pm)$ correspond to two "versions" of the field ψ_e at the impurity site 0. In the calculation of (4.51) above, we considered x *away* from the impurity site, $x \neq 0$, when looking at both sides $x > 0$ and $x < 0$. Hence, this excluded the operators $\psi_e(0^\pm)$. Taking $x = 0^\pm$ instead, we indeed find a non-zero result, given by half of the residue of the pole at $p = \infty$ (just half, because we must integrate on the upper half-plane or the lower half-plane, so we only get half of the contour around the pole at $p = \infty$):

$$\{\psi_e(0^\pm), d^\dagger\} = \mp\mathrm{i}\tau/2. \tag{4.53}$$

Hence, we indeed recover consistency with $\{d, d^\dagger\} = 1$. This result points to the fact that the operators $\psi_e(0^\pm)$ are reproduced by the limits $\lim_{x\to 0^\pm} \psi_e(x)$ only in matrix elements where no other operators are present at the impurity site.

The reason why the result (4.53) is not in contradiction with having a correct representation of the algebra of observables is that $\psi_e(0^\pm)$ cannot be interpreted as the limits $x \to 0^\pm$ of the *algebra element* $\psi_e(x)$; the algebra element $\psi_e(x)$ at the impurity site is simply $\psi_e(0)$ (there is no well-defined notion of a limit in x of algebra elements like $\psi_e(x)$). The impurity led us to define two "new" operators $\psi_e(0^\pm)$, which have the meaning of the limits $\lim_{x\to 0^\pm} \psi_e(x)$ of the operator representation of $\psi_e(x)$ in appropriate matrix elements, and satisfy non-trivial anti-commutation relations with the impurity operators. But the operator representing the algebra element $\psi_e(0)$, which is simply $(\psi_e(0^+) + \psi_e(0^-))/2$ by the resolution (4.13), still commutes with $d^\dagger$. Of course, the two operators $\psi_e(0^\pm)$ are not really new, since they are related to $\psi_e(0)$ and d; they are just, from the viewpoint of the algebra, linear combinations of certain algebra elements.

It is important to note that we only needed one set of modes, a_p, in order to represent the algebra involving both canonical observables $\psi_e(x)$ and d. This may seem strange at first, since without impurity interaction, we initially considered two separate representations, where d can be seen as a matrix and $\psi_e(x)$ as a conformal field. This is a consequence of the phenomenon of hybridisation: the impurity states do not have an associated quantum number parametrising the set of scattering states, only the momenta and particle types are quantum numbers. Hence, once we introduce mode operators for constructing the states, all operators have to be represented in terms of these mode operators.

4.3.2 Resolution of the impurity

In fact, one of the steps that was not completely deductive in the operator construction above was that of the resolution of the impurity, where we used (4.13). It is very interesting to see if there can be another resolution. What we want is an operator

$$\psi_e(0) \equiv \int \frac{dp}{\sqrt{2\pi}} a_p f_p$$

with the property that

$$[\psi_e^\dagger(x), \psi_e(0)] = \delta(x) \tag{4.54}$$

(a property which we used to derive the equations of motion – this is the main defining property of $\psi_e(0)$ in the Hamiltonian). First, we may simply wish to define

$$\psi_e(0) = a\psi_e(0^-) + b\psi_e(0^+), \quad a + b = 1, \tag{4.55}$$

which indeed satisfies the condition (4.54). However, solving the equation of motion for d we find, instead of (4.49),

$$v_p = \frac{\epsilon - p + \mathrm{i}a|\tau|^2}{\epsilon - p - \mathrm{i}b|\tau|^2},$$

which does *not* fulfill the requirement (4.50) for the canonical anti-commutation relation of the observable $\psi_e(x)$ except for $a = b$. Looking for a possibly more general f_p, the requirement (4.54) tells us that f_p does not have poles in the upper-half plane $\mathrm{Im}(p) > 0$, that $v_p^* f_p$ does not have poles in the lower-half plane $\mathrm{Im}(p) < 0$, and that $f_p = O(p^0)$ as $|p| \to \infty$. The possibilities are 1, v_p or any linear combinations of these, so that (4.55) is indeed the most general possibility, and we saw that it is consistent only for $a = b$. Hence, (4.13) is indeed the only consistent resolution of the impurity.

In fact, we can well *modify* the initial algebra of observables in order to account for a resolution like (4.55). We know from our operator construction that with this resolution, thanks to (4.53), we have $\{\psi_e(0), d^\dagger\} = (a - b)\mathrm{i}\tau/2$. Since we have an operator construction for this, it should lead to a consistent algebra. Taking that as part of the initial algebra of observables used in the Hamiltonian, the equation of motion for d is modified by a shift $\epsilon \mapsto \epsilon - (a - b)\mathrm{i}|\tau|^2/2$, which modifies the solution v_p in such a way that $|v_p|^2 = 1$; indeed, the construction is consistent. However, this simply comes from a different algebra of observables, which can in fact be obtained from the initial one by a simple shift $\psi_e(0) \mapsto \psi_e(0) - (a - b)d\mathrm{i}\tau/2$. We emphasize, though, that this is a modification of the original algebra, whereby the physical meaning of $\psi_e(0)$, as representing electrons on the metallic sheets at the impurity site, is lost.

How is it possible that the symmetric resolution be the only physical possibility? The idea is that *a priori*, with a spreaded impurity interaction $\tau \int dx\, \rho(x)\psi_e^\dagger(x)d + h.c.$, the point 0 does not have any particular status: there is no information about *where* the operator d is placed, besides the distribution $\rho(x)$ itself. What is happening is that, whatever the shape of the density $\rho(x)$ is, be it symmetric or not, in the limit where the density becomes supported at one point x_0, the interaction can be seen as involving the two parts $\psi_e(x_0^\pm)$ around the center of mass of the density, both parts with equal weight.

4.3.3 Bare scattering eigenstates

It is worth noting that from the operator construction above, it is possible as well to reproduce the bare scattering state construction referred to in paragraph 4.1.2. This does not form *a priori* a bounded representation, because the Hamiltonian is not bounded from below. However, we may make this a bounded representation simply by restricting the values of momenta to $p \in [-\Lambda, \Lambda]$ and by restricting the maximal number of particles. With these restrictions, both the bounded representation in the previous paragraph and the bare scattering state construction are equivalent. However, in order to properly obtain the states in the scaling limit (where $\Lambda \to \infty$ and where the maximal number of particles is infinite), we need to look at the states in the bounded representation of the previous paragraph.

In order to construct the bare scattering states, recall that we first construct a bare vacuum $|0\rangle$ through $\psi_e(x)|0\rangle = \psi_o(x)|0\rangle = 0$. We will also take it as a vacuum for the impurity space, $d|0\rangle = 0$. Then, the bare vacuum satisfies $a_p|0\rangle = b_p|0\rangle = 0$ for all $p \in \mathbb{R}$ (note how this differs from (4.44)), and bare scattering states are constructed by applications of $a_p^\dagger$ and $b_p^\dagger$. This can in turn be written in terms of the operators $\psi_e^\dagger(x)$, $d^\dagger$ and $\psi_o^\dagger(x)$ by inverse Fourier transform. The inverse Fourier transform is most easily found from the anti-commutation relations $\sqrt{2\pi}\{\psi_e(x), a_p^\dagger\} = e^{\mathrm{i}px}(1\ (x<0),\ v_p\ (x>0))$ and $-\mathrm{i}\tau\sqrt{2\pi}\{d, a_p^\dagger\} = v_p - 1$, giving

$$\sqrt{2\pi}a_p^\dagger = \int_{-\infty}^0 dx\, e^{\mathrm{i}px}\psi_e^\dagger(x) + \int_0^\infty dx\, v_p e^{\mathrm{i}px}\psi_e^\dagger(x) - \frac{v_p - 1}{\mathrm{i}\tau}d^\dagger \tag{4.56}$$

whereas we immediately have

$$\sqrt{2\pi}b_p^\dagger = \int_{-\infty}^\infty dx\, e^{\mathrm{i}px}\psi_o^\dagger(x). \tag{4.57}$$

Then, many-particle states are simply constructed as $a_p^\dagger|0\rangle$, $a_{p_1}^\dagger a_{p_2}^\dagger|0\rangle$, $a_{p_1}^\dagger b_{p_2}^\dagger|0\rangle$, etc.

This gives the scattering eigenstates as states in the space $\mathcal{F}\otimes\mathcal{I}$ formed by tensoring the Fock space $\mathcal{F}$ over the canonical algebra of $\psi_e(x)$, $\psi_e^\dagger(x)$, $\psi_o(x)$ and $\psi_o^\dagger(x)$, and the representation space $\mathcal{I}$ of d and $d^\dagger$. However, the resulting space of bare scattering states certainly cannot be simply related to $\mathcal{F}\otimes\mathcal{I}$. This is because, in $\mathcal{F}\otimes\mathcal{I}$, the discontinuity equation (4.52) certainly does not hold. What is happening is that the space of scattering states of the RLM is *embedded* into $\mathcal{F}\otimes\mathcal{I}$, and we need to define $\psi_e(0^\pm)$, the physical operator, as $P\psi_e^{(bare)}(0^\pm)P$ where $\psi_e^{(bare)}(0^\pm)$ is the unphysical operator acting in the "bare" way on $\mathcal{F}\otimes\mathcal{I}$ and P is the projection operator on the space of scattering states. Here we see how the operator construction based on the algebra of observable is more transparent. Subtleties of this type will turn out to be useful in the next subsection.

4.3.4 The Y-operator and its non-locality

Now that we have a bounded representation of the algebra of observables, we wish to represent the Y operator. We say above that, in the case of the IRLM, the conditions (4.7) and (4.8) are enough to fully determine the Y operator. In terms of modes, the solution is simple:

$$Y = \frac{1}{2}\int dp\ \left(a_p^\dagger b_p + b_p^\dagger a_p\right). \tag{4.58}$$

Using this and the representation of the algebra of observables constructed above, we may evaluate all traces involving the density matrix out of equilibrium. The trick is simply to use the cyclic properties of the trace, and the adjoint action of Y and H on the individual modes (i.e. the action by commutation), in the more natural combination $a_p \pm b_p$ where the adjoint actions of both Y and H are diagonal:

$$\begin{aligned}
&\frac{\mathrm{Tr}\left(e^{-(H-VY)/T}(a_p \pm b_p)(a_{p'}^\dagger \pm' b_{p'}^\dagger)\right)}{\mathrm{Tr}\left(e^{-(H-VY)/T}\right)} \\
&= e^{(p'\pm' V/2)/T}\frac{\mathrm{Tr}\left(e^{-(H-VY)/T}(a_{p'}^\dagger \pm' b_{p'}^\dagger)(a_p \pm b_p)\right)}{\mathrm{Tr}\left(e^{-(H-VY)/T}\right)} \\
&= e^{(p'\pm' V/2)/T}\left((1 + (\pm)(\pm')1)\,\delta(p-p') - \frac{\mathrm{Tr}\left(e^{-(H-VY)/T}(a_p \pm b_p)(a_{p'}^\dagger \pm' b_{p'}^\dagger)\right)}{\mathrm{Tr}\left(e^{-(H-VY)/T}\right)}\right)
\end{aligned}$$

where in the last equation we can solve for the initial ratio of traces. Traces with more factors of the mode operators are obtained using Wick's theorem. One can then easily calculate, using these results, the average current

$$\langle \mathcal{J} \rangle_{NE} = \left\langle \mathrm{Im}\left(\tau^* d^\dagger \psi_o(0)\right)\right\rangle_{NE} = -\mathrm{Re}\left(\int \frac{dpdp'}{2\pi}\,(v_p^*-1)\langle\, a_p^\dagger b_{p'}\rangle_{NE}\right). \tag{4.59}$$

We will not go into explicit calculations of physical averages using the modes, as this is somewhat tedious but completely straightforward. However, it is instructive to derive the form of the Y operator in terms of the localised observables $\psi_e(x), \psi_o(x)$ and d, and their hermitian conjugates. Using

$$v_p = 1 - |\tau|^2 \int_0^\infty dx\, e^{\mathrm{i}\left(p-\epsilon+\mathrm{i}\frac{|\tau|^2}{2}\right)x} \tag{4.60}$$

we find

$$Y = \frac{1}{2}\int_{-\infty}^{\infty} dx\, \psi_e^\dagger(x)\psi_o(x) - \frac{1}{2}\int_0^\infty dx\, e^{-\left(|\tau|^2/2+i\epsilon\right)x}\left(\mathrm{i}\tau^* d^\dagger\psi_o(x) + |\tau|^2\int_0^\infty dx' \psi_e^\dagger(x')\psi_o(x+x')\right) + h.c. \tag{4.61}$$

where $h.c.$ means the hermitian conjugates of all terms. That is, the Y operator contains a first term equal to Q, which is (up to a factor) the integral over all $x \in \mathbb{R}$ of the local density $\psi_e^\dagger(x)\psi_o(x) + h.c.$. But the other terms in the Y operator are not of this form: they are not integral of local densities. Indeed, one term contains the integral over x of $d^\dagger\psi_o(x)$, a product of local operators at 0 and x, and the other term contains the integral over both x and x' of $\psi_e^\dagger(x')\psi_o(x+x')$, a product of local operators at x and $x+x'$. The non-local terms are supported on the right, since the form of the state in the left region, corresponding to right-moving waves before they scatter with the impurity, is just that of the initial state – describes by the local charge Q. In the non-local part, the weight of the integrand decreases exponentially with the distance between the local factors (this distance is x in the integral in (4.61)). This means that although the Y operator is non-local, it can still be considered *quasi-local*: it is an integral over the position x' of a quantity with a support around x', whose "strength" is exponentially decreasing away from x'. This quasi-locality is directly related to the presence of a good relaxation mechanism that allows the steady state to exist. In order to see that, note that from (4.23), the non-local part of the Y operator is just $\int_{-\infty}^0 dt\, \mathcal{J}(t)$. Then, thanks to relaxation mechanisms providing large-time factorisation, the steady-state average of the non-local part of Y times $\delta\mathcal{O} = \mathcal{O} - \langle\mathcal{O}\rangle_{NE}$ should exist for any finitely supported $\mathcal{O}$. This is only possible thanks to quasi-locality. Here, we see explicitly that the tunnneling term, with strength τ, is at the source of the relaxation mechanisms. At a more technical level, the steady-state average of a finitely supported operator $\mathcal{O}$ should be differentiable with respect to V. Since the derivative is $T^{-1}\langle Y\delta\mathcal{O}\rangle_{NE}$, this quantity should be finite – which is possible thanks to quasi-locality.

We expect the non-locality to be at the basis of the fact that the density matrix formed out of Y describes a situation that is out of equilibrium. Take for instance the equilibrium density matrix $\rho_0 = e^{-(H_0-VQ)/T}$. Interpreted in terms of the result of equilibration where the system exchanges a quantity with an external environment, the coupling of the charge Q to the chemical potential V represents processes where an electron at x is given by the system to the environment and coherently put back at the same position. In evaluating traces, we are considering quantum states that are steady under these processes. What these processes tell us is that electrons given and received at *different* positions are incoherent. If we wished to interpret the non-local part of Y as coming from an "equilibration" with an environment, we would have to consider that the system may give an electron at x to the environment, while coherently receiving an electron at $x' \neq x$; we are looking for quantum states that are steady under

such non-local processes. The main point is that there must be quantum coherence non-locally in the hypothetical environment; this allows a flow of particles out of equilibrium to occur.

Finally, it is worth verifying the formula (4.23) in the operator formalism, which provides a non-trivial connection between the scattering-state formulation and the real-time formulation. We first would like to calculate

$$\int_{-\infty}^{0} dt\, \mathcal{J}(t) = -\frac{\mathrm{i}\tau^*}{2}\int_{-\infty}^{0} dt\, e^{\mathrm{i}Ht} d^\dagger \psi_o(0) e^{-\mathrm{i}Ht} + h.c. = -\frac{\mathrm{i}\tau^*}{2}\int_0^\infty dx\, e^{-\mathrm{i}Hx} d^\dagger e^{\mathrm{i}Hx}\psi_o(x) + h.c. \quad (4.62)$$

where we used $[H, \psi_o(x)] = \mathrm{i}d\psi_o(x)/dx$. Of course this can be evaluated using our solution in terms of mode operators. However, an instructive way of evaluating this that directly leads to an expression like (4.61) is to try to find $e^{-\mathrm{i}Hx} d^\dagger e^{\mathrm{i}Hx}$ (for $x > 0$) by writing its general form in terms of local operators, knowing that it can only be a linear combination of $d^\dagger$ and $\psi_e^\dagger(y)$ for $0 < y < x$:

$$e^{-\mathrm{i}Hx} d^\dagger e^{\mathrm{i}Hx} = f(x) d^\dagger + \int_{0^+}^{x} dy\, \psi_e^\dagger(y) g(y,x). \quad (4.63)$$

We then only have to calculate the following commutator in two different ways:

$$\begin{aligned}
[H, e^{-\mathrm{i}Hx} d^\dagger e^{\mathrm{i}Hx}] &= e^{-\mathrm{i}Hx}[H, d^\dagger] e^{\mathrm{i}Hx} \\
&= e^{-\mathrm{i}Hx}(\epsilon d^\dagger + \tau \psi_e^\dagger(0)) e^{\mathrm{i}Hx} \\
&= e^{-\mathrm{i}Hx}\left(\left(\epsilon - \frac{\mathrm{i}|\tau|^2}{2}\right) d^\dagger + \tau \psi_e^\dagger(0^+)\right) e^{\mathrm{i}Hx} \\
&= \left(\epsilon - \frac{\mathrm{i}|\tau|^2}{2}\right) e^{-\mathrm{i}Hx} d^\dagger e^{\mathrm{i}Hx} + \tau \psi_e^\dagger(x) \\
&= \left(\epsilon - \frac{\mathrm{i}|\tau|^2}{2}\right)\left(f(x) d^\dagger + \int_{0^+}^{x} dy\, \psi_e^\dagger(y) g(y,x)\right) + \tau \psi_e^\dagger(x) \qquad (4.64)
\end{aligned}$$

where we used (4.13) and (4.52), as well as the fact that $[H, \psi_e(x)] = \mathrm{i}d\psi_e(x)/dx$ for any $x > 0$; and

$$\begin{aligned}
[H, e^{-\mathrm{i}Hx} d^\dagger e^{\mathrm{i}Hx}] &= [H, f(x) d^\dagger + \int_{0^+}^{x} dy\, \psi_e^\dagger(y) g(y,x)] \\
&= f(x)\left(\left(\epsilon - \frac{\mathrm{i}|\tau|^2}{2}\right) d^\dagger + \tau \psi_e^\dagger(0^+)\right) + \int_{0^+}^{x} dy\, \left(\mathrm{i}\frac{d}{dy}\psi_e^\dagger(y) + \tau^* \delta(y) d^\dagger\right) g(y,x) \\
&= f(x)\left(\left(\epsilon - \frac{\mathrm{i}|\tau|^2}{2}\right) d^\dagger + \tau \psi_e^\dagger(0^+)\right) \\
&\quad - \int_{0^+}^{x} dy\, \psi_e^\dagger(y) \mathrm{i}\frac{d}{dy} g(y,x) + \mathrm{i}\left(\psi_e^\dagger(x) g(x,x) - \psi_e^\dagger(0^+) g(0,x)\right). \qquad (4.65)
\end{aligned}$$

Comparing (4.64) with (4.65), we find

$$-\mathrm{i}\tau f(x) = g(0,x), \quad -\mathrm{i}\tau = g(x,x), \quad \left(\epsilon - \frac{\mathrm{i}|\tau|^2}{2}\right) g(y,x) = -\mathrm{i}\frac{d}{dy} g(y,x) \quad (4.66)$$

with the solution

$$g(y,x) = -\mathrm{i}\tau e^{(|\tau|^2/2 + \mathrm{i}\epsilon)(y-x)}, \quad f(x) = e^{-(|\tau|^2/2 + \mathrm{i}\epsilon)x}. \quad (4.67)$$

Putting this in (4.63), then in (4.62), we find exact agrement with the non-local terms of (4.61).

This calculation provides a quite non-trivial check of the consistency between the real-time formulation and the scattering-state formulation, in this special "free" impurity model. This then implies that we can indeed correctly calculate, for instance, the current-current response function by evaluating the average of the local operator

$$\mathrm{i}[\mathcal{J}, Q] = \frac{\tau^*}{2} d^\dagger \psi_e(0) + h.c. \quad (4.68)$$

and the noise by using the formula (4.38).

4.3.5 Perturbation in U

The model we solved until now was the RLM, without the Coulomb-like U-term in the impurity interaction. In order to assess the model (2.8) with $U \neq 0$, we may wish to study the perturbation theory in U. This may seem complicated at first, because we need not only to perturb the Hamiltonian, which is simple to do (or at least, which has been considered before), but also the Y operator: it should be modified by the U-term, since it is defined via the Hamiltonian. This modification, at first, may seem hard to obtain.

However, there is a very simple way of doing perturbation theory, based on the algebra of observables, instead of a direct construction of the modified Hamiltonian and Y operator. We know that the space of scattering states has the same form for any U: the states are characterised by momenta of scattering particles (and particle types), and there are no other quantum numbers. We know as well that the energy of a scattering eigenstate is just the sum of the energies of the individual scattering particles. Hence, (4.43) with (4.42) and (4.44) still hold: we have an exact expression for the Hamilonian. This is not so surprising: remember that in massive quantum field theory, for instance, the space of states is exactly the same as that of a free theory with a given set of particle masses and internal quantum numbers (if any). In fact, there are many bases that take exactly that form, for instance the *in* and the *out* bases. What makes the model non-trivial, and what chooses the basis, is the exact form of the energy density on that space: this encodes the interactions (or, equivalently, the scattering matrix encodes the interactions). In other words, instead of considering that the Hamiltonian is modified, we consider that the *representation of the local observables* is modified. In our present case, this means that we cannot any longer assume that the observables $\psi_e(x)$, $\psi_o(x)$ and d (and their Hermitian conjugates) are linear in the modes a_p and b_p (and their Hermitian conjugates). What we can do is simply to start with the solution we obtained above for the local observables, and add terms proportional to U, U^2, etc, that contain more and more factors of the mode operators (3 factors, 5 factors, etc., keeping the total number of particles created or annihilated the same). Then, we only need to impose constraints coming from the equations of motion (the commutation relations with the Hamiltonian H), and self-consistently solve these constraints. That is, we perturbatively solve the equations of motion in the Heisenberg picture, starting with a solution that we know at $U = 0$. This uniquely fixes, perturbatively in U, all the observables.

An important point is that for $x \neq 0$, no matter what value U (or even t) takes, the observables $\psi_e(x)$ and $\psi_o(x)$ satisfy the same algebra, and the same equations of motion. As a consequence, for $x > 0$ or for $x < 0$, these observables can in fact be taken to be in the *free form* in terms of the modes. Above, for $U = 0$ but $t \neq 0$ we chose to have them in the free form for $x < 0$ (see (4.46) for instance). Then, turning on U, we can well choose to keep the free form for $x < 0$: the only modification that the U-term provides, when solving self-consistently the equations of motion, is for $x \geq 0$ (including the operator d, for instance). We emphasize that this is just a choice; essentially what it says is that we chose the creation and annihilation operators to be corresponding to *in* scattering eigenstates. But this is a very convenient choice, because it means that we can keep exactly the *same expression* (4.58) for the Y operator: it still satisfies the conditions (4.7) and (4.8). It is important to understand that we do not need to "proove" that (4.58) holds for $U \neq 0$. The structure of the space of scattering states implies the form (4.43) of the Hamiltonian, and the algebra of local observables for $x < 0$ implies that we may choose the free form for $x < 0$. Then, the fact that conditions (4.7) and (4.8) uniquely fix the Y, as proven in subsection 4.1, immediately tells us that (4.58) holds. This form of the Y operator was written by Hershfield [5], but what was not emphasised was that, in order to produce a perturbation theory, we

then only have to construct the observables perturbatively, we do not have to write the "interacting" mode operators in terms of simpler "uninteracting" modes in which the obervables would have a linear expression (that would make the calculation of the Y operator complicated). Hence, the perturbation-theory part of the calculation does not know anything about the fact that we are interested in a steady state out of equilibrium; it is purely operatorial. This, then, provides a complete way of evaluating any steady-state average perturbatively. Note that the expressions for the current operator in (4.59), for the response operator (4.68), and for the noise (4.38), in terms of local obervables, are unaffected by the perturbation in U; their expressions in terms of modes will be affected, and this will provide the perturbation theory for their averages. Naturally, we will need to have a cut-off, and then to perform an appropriate renormalisation of the observables of interest (and of the couplings) in order to obtain well-defined observables that have finite averages.

4.4 Equations of motion and full perturbative expansion

Finally, we present here a way of obtaining the full perturbative expansion of steady-state averages out of equilibrium in terms of averages in the model without impurity interaction (at equilibrium); we use the IRLM as an example. This methods was developed in [6]. It is not based on the operator construction of the previous subsection, but rather on the equations of motion, the stationarity condition, and the fundamental conditions (4.2) and (4.5) for the Y operator. It makes fundamental use of the discontinuity equation through the impurity, the generalisation to non-zero U of (4.52). In fact, the method is also useful and novel in order to obtain averages at equilibrium, as well as any scattering-state matrix elements of observables.

4.4.1 Discontinuity relations

First, we explain how to obtain the discontinuity condition without an explicit construction of the operators. The idea is to consider some general properties of the bare scattering eigenstates of the IRLM. In the previous subsection, we constructed these eigenstates by using the expression of the creation and annihilation operators in terms of the local observables, simply changing the definition of the vacuum from $|\mathrm{vac}\rangle$ to $|0\rangle$. It may seem hard, then, to construct the eigenstates for any $U \neq 0$, because the relation between the creation and annihilation operators is not linear anymore. However, if we directly start with the bare Fock space constructed out of the bare vacuum $|0\rangle$, we may choose the Hamiltonian to annihilate $|0\rangle$, and since it preserves the number of particles, we may calculate its action on any sector with a fixed number of bare particles. That is, we think of forming eigenstates of the form

$$\begin{aligned}
&|p_1, p_2, \dots, p_n\rangle_{a_1,a_2,\dots,a_n} \\
&\quad = \int_{-\infty}^{\infty} g_{a_1,a_2,\dots,a_n}(p_1, p_2, \dots, p_n | x_1, x_2, \dots, x_n) \psi^\dagger_{a_1}(x_1)\psi^\dagger_{a_2}(x_2)\cdots\psi^\dagger_{a_n}(x_n)|0\rangle \\
&\qquad + \int_{-\infty}^{\infty} g_{a_1,a_2,\dots,a_{n-1},0}(p_1, p_2, \dots, p_n | x_1, x_2, \dots, x_{n-1}, 0) \psi^\dagger_{a_1}(x_1)\psi^\dagger_{a_2}(x_2)\cdots\psi^\dagger_{a_{n-1}}(x_{n-1})d^\dagger|0\rangle \\
&\qquad + \int_{-\infty}^{\infty} g_{a_1,a_2,\dots,0,a_n}(p_1, p_2, \dots, p_n | x_1, x_2, \dots, 0, x_n) \psi^\dagger_{a_1}(x_1)\psi^\dagger_{a_2}(x_2)\cdots d^\dagger\psi^\dagger_{a_n}(x_n)|0\rangle \\
&\qquad + \dots
\end{aligned} \tag{4.69}$$

where $a_j = e, o$ (or $a_j = 1, 2$), for fixed n, and we wish to diagonalise the action of H on it. This simply recasts the problem to its first-quantised form, where we only need to evaluate the bare wave functions g. For few number of particles, this can be done analytically, for any finite U, and it does not depend on the integrability of the model. Moreover, the action of Y is simple to evaluate, we just have to make sure that the bare wave functions diagonalise the operator Q for $x_j < 0$. This may seem like a much more powerful method than the operator method of the previous subsection; however, it has the disadvantage of providing eigenstates that are very far from the true vacuum. The true vacuum (which exists in the bare construction with a cutoff on the momenta and the number of particles), has a filled Fermi sea, so corresponds to a very large number of bare particles; this, in general, is not possible to construct systematically, unless there is integrability[2]. Hence, reaching the universal limit is beyond these low-particle calculations.

Yet, we will only be interested in general properties of the bare scattering eigenstates, valid for all states, so that we may apply them to the true vacuum and its low-lying excited states as well. Since the dispersion relation is linear, the first-quantised Hamiltonian eigenvalue equations are first-order equations, and since there is an impurity that couples only with the Fermion operators $\psi_{e,o}(0)$, not with their derivatives, they contain delta-functions $\delta(x)$ but no derivatives of delta-functions. Integrating the first derivatives, we observe that the resulting wave functions should, in general, have jumps at the position of the impurity, $x = 0$, but, importantly, no delta-functions. This observation has the following consequence. Suppose we look at the matrix element

$$\langle v|\mathcal{O}\psi_e(x)|v'\rangle \tag{4.70}$$

where $|v\rangle$ and $|v'\rangle$ are some scattering eigenstates, and $\mathcal{O}$ is any operator. Then, the evaluation of this matrix element, by pushing $\psi_e(x)$ through to the right until it annihilates $|0\rangle$, will generate wave functions at the argument x, so this matrix element has no delta-function as a (generalised) function x. Likewise, then,

$$(E_v - E_{v'})\langle v|\mathcal{O}\psi_e(x)|v'\rangle = \langle v|[H, \mathcal{O}\psi_e(x)]|v'\rangle \tag{4.71}$$

has no delta-function as function of x, so we may write

$$\int_{-L}^{L} dx\, \langle v|[H, \mathcal{O}\psi_e(x)]|v'\rangle = \left(\int_{-L}^{0^-} dx + \int_{0^+}^{L} dx\right) \langle v|[H, \mathcal{O}\psi_e(x)]|v'\rangle. \tag{4.72}$$

But since $[H, \psi_e(x)] = [H_0, \psi_e(x)] = \mathrm{i}d\psi_e(x)/dx$ for $x \neq 0$, and since

$$[I, \psi_e(x)] = -(\tau d + U\psi_e(0)D)\delta(x) \tag{4.73}$$

where we define

$$D = d^\dagger d, \tag{4.74}$$

we find

$$-\langle v|\mathcal{O}(\tau d + U\psi_e(0)D)|v'\rangle = \mathrm{i}\langle v|\mathcal{O}(\psi_e(0^-) - \psi_e(0^+))|v'\rangle. \tag{4.75}$$

That is, the absence of delta-function tells us about the jump of the operator $\psi_e(x)$ around the impurity site $x = 0$.

[2]Out of equilibrium, we want integrability to be in agreement with the Y operator – the natural particles in the integrable basis must have definite Q-value for positions $x < 0$, that is, must be charge carrier. An attempt at using integrability in this way for the IRLM is [11].

Since this jump does not depend on the states that we chose, we have the equality when any matrix element of the operators on both sides are evaluated:

$$\mathcal{O}(\psi_e(0^+) - \psi_e(0^-)) \overset{\mathcal{H}}{=} -\mathrm{i}\mathcal{O}(\tau d + U\psi_e(0)D) \tag{4.76}$$

where $\mathcal{H}$ is the space of scattering states. This makes it clear that this space is embedded into the initial Fock space, since this equality certainly does not hold in general on the Fock space $\mathcal{F}\otimes\mathcal{I}$; it is important, in order to obtain the equality, that we do evaluate the matrix elements of both sides in some scattering states. In fact, since the operator $\mathcal{O}$ can be any operator on the Fock space, the only requirement for the equality to hold is that we *apply* both operators on a scattering state. That is, we have equality for both sides not only as operators on $\mathcal{H}$, but also as linear maps $\mathcal{H} \to \mathcal{F}\otimes\mathcal{I}$. We will indicate this by the symbol $\overset{|\cdot\rangle}{=}$, so that we have

$$\psi_e(0^+) - \psi_e(0^-) \overset{|\cdot\rangle}{=} -\mathrm{i}(\tau d + U\psi_e(0)D). \tag{4.77}$$

The fact that the application on the right is singled out can be traced back to our choice of bare vacuum; we could have chosen it, instead, to be annihilated by $\psi_e^\dagger(x)$, and we would have obtained the opposite. Equation (4.77) generalises (4.52) to the case $U \neq 0$.

In equation (4.77), we again have the problem of the evaluation of $\psi_e(x)$ at $x = 0$ while it has a jump at that point. Hence, we need to resolve this impurity term, in a similar way that we needed to resolve the tunnelling impurity term in the case $U = 0$ above. We did not provide a complete operatorial analysis of the possible resolutions for the U-term, but it seems natural that we may simply replace $\psi_e(0) \mapsto (\psi_e(0^+) + \psi_e(0^-))/2$. Doing so, we find

$$\left(1 + \frac{\mathrm{i}U}{2}D\right)\psi_e(0^+) - \left(1 - \frac{\mathrm{i}U}{2}D\right)\psi_e(0^-) \overset{|\cdot\rangle}{=} -\mathrm{i}\tau d. \tag{4.78}$$

In order to be able to use these discontinuity conditions, it will be convenient to be able to express all operators that are on the right $x > 0$ in terms of impurity operators and operators on the left $x < 0$. That is, we would like to solve for $\psi_e(0^+)$ in the equation (4.78). This is possible to do thanks to the fact that the equation is valid as a linear map $\mathcal{H} \to \mathcal{F}\otimes\mathcal{I}$: we can pre-multiply by any operator. Here, we simply have to invert, using $D^2 = D$:

$$\left(1 + \frac{\mathrm{i}U}{2}D\right)^{-1} = 1 - \frac{\mathrm{i}U}{2 + \mathrm{i}U}D \tag{4.79}$$

so that we find, using $Dd = 0$,

$$\psi_e(0^+) \overset{|\cdot\rangle}{=} -\mathrm{i}\tau d + (1 - \mathrm{i}uD)\psi_e(0^-) \tag{4.80}$$

where

$$u = \frac{2\mathrm{i}U}{2\mathrm{i} - U}. \tag{4.81}$$

Likewise, a similar calculation yields, for the odd sector,

$$\psi_o(0^+) \overset{|\cdot\rangle}{=} (1 - \mathrm{i}uD)\psi_o(0^-). \tag{4.82}$$

Also, the Hermitian conjugate relations hold, but this time as operators acting on the left on $\mathcal{H}^*$:

$$\psi_e^\dagger(0^+) \overset{\langle\cdot|}{=} \mathrm{i}\tau^* d^\dagger + (1 + \mathrm{i}u^* D)\psi_e^\dagger(0^-) \tag{4.83}$$

and

$$\psi_o^\dagger(0^+) \overset{\langle\cdot|}{=} (1 + \mathrm{i}u^* D)\psi_o^\dagger(0^-). \tag{4.84}$$

Note that these discontinuity equations circumvent the problems occuring when trying to take (anti-)commutators with impurity operators on both sides. The operator that we are talking about, here, are the "bare" operators, without projection onto $\mathcal{H}$, to the difference of the operators constructed in the previous subsection. Hence, they satisfy the bare anti-commutation relations, and we need to make sure that there is no inconsistency. But, although the equations (4.80) and (4.82) can be pre-multiplied by impurity operators, their validity is *not* guaranteed when they are post-multiplied. The same holds but for the opposite side for (4.83) and (4.84). Hence, (anti-)commutators cannot be taken on these equations. However, there is no problem in pre- or post-multiplying by Fermion operators at positions $x \neq 0$, since these preserve the space $\mathcal{H}$.

4.4.2 Equations of motion and stationarity condition

We are now in a position to obtain a useful form of the equations of motion. First, note that any observable that we are interested in can be, in principle, brought to a linear combination of operators of the form $e^{\mathrm{i}yH} b_j \mathcal{O}(x) e^{-\mathrm{i}yH}$ for $x < 0$ and for some $y < 0$, where

$$b_0 = \mathbf{1}, \quad b_1 = d, \quad b_2 = d^\dagger, \quad b_3 = D, \tag{4.85}$$

and where $\mathcal{O}(x)$ is a finitely supported operator whose support has x as its rightmost point. For instance, the current operator $\mathcal{J} = \mathrm{Im}\left(\tau^* d^\dagger \psi_o(0)\right)$ in (4.59) can be written

$$\mathcal{J} \overset{\mathcal{H}}{=} \mathrm{Im}\left(\tau^* d^\dagger \psi_o(0^-)\right) \tag{4.86}$$

using $\psi_o(0) = (\psi_o(0^+) + \psi_o(0^-))/2$ (which comes from (4.13)) as well as (4.82), along with $d^\dagger D = 0$. Note that we needed to use both the discontinuity relations for ψ_o and for its Hermitian conjugate, so that the result holds only as an operator on $\mathcal{H}$. Likewise, the response operator (4.68) is

$$\mathrm{i}[\mathcal{J}, Q] \overset{\mathcal{H}}{=} \frac{\tau^*}{2} d^\dagger \psi_e(0^-) + h.c. \tag{4.87}$$

where we additionally used the fact that the term $-\mathrm{i}\frac{|\tau|^2}{4} D$ occuring from the first term on the right-hand side of (4.80) is purely anti-hermitian. In these two cases, we have $y = 0$. For observables with a local operator at $x > 0$, like those involved in the integral in the expression for the noise (4.38), we can in principle use $e^{\mathrm{i}Hx}$ in order to bring the operator to $x = 0^+$, then use the discontinuity conditions; there we will have $y = -x$. However, this may be harder in general, because, for instance, the action of $e^{\mathrm{i}Hx}$ will have to be evaluated perturbatively on the current operator $\mathcal{J}$ in (4.38). In the following, we will just consider cases with $y = 0$.

In order to illustrate how we can use this form of observables along with the equations of motion, let us consider the current in the case $U = 0$. The equations of motion tell us that

$$\begin{aligned} [H, d^\dagger \psi_o(x)] &\overset{x \leq 0}{=} (\epsilon d^\dagger + \tau \psi_e^\dagger(0)) \psi_o(x) + \mathrm{i}\frac{d}{dx}(d^\dagger \psi_o(x)) \\ &\overset{\langle\cdot|}{=} \tau \psi_e^\dagger(0^-) \psi_o(x) + \left(\epsilon + \frac{\mathrm{i}|\tau|^2}{2} + \mathrm{i}\frac{d}{dx}\right)(d^\dagger \psi_o(x)). \end{aligned} \tag{4.88}$$

Hence, the matrix elements of this operator satisfy the equations

$$\left(E_v - E_{v'} - \epsilon - \frac{\mathrm{i}|\tau|^2}{2} - \mathrm{i}\frac{d}{dx}\right) \langle v | d^\dagger \psi_o(x) | v' \rangle \overset{x \leq 0}{=} \tau \langle v | \psi_e^\dagger(0^-) \psi_o(x) | v' \rangle. \tag{4.89}$$

We can now consider the true vacuum and its excited states, instead of bare scattering eigenstates, because the equation holds for any eigenstates $|v\rangle$ and $|v'\rangle$. Then, we can evaluate the right-hand side if we choose *in*-scattering eigenstates, because it only contains Fermion operators at negative positions. For these, we know that the free form like (4.46) (at $x < 0$) in terms of mode operators hold, and we know that the scattering states can be obtained simply by application of the mode operators on the true vacuum $|\text{vac}\rangle$ (Fock space). Hence, this calculation is a free, conformal field theory calculation:

$$\langle v|\psi_e^\dagger(0^-)\psi_o(x)|v'\rangle \overset{x\leq 0}{=} {}_{CFT}\langle v|\psi_e^\dagger(0^-)\psi_o(x)|v'\rangle_{CFT}. \tag{4.90}$$

What has happened is that we used the discontinuity conditions in order to bring to the left any operator, appearing from the equations of motion, that is on the right. Solving (4.89), we find

$$\langle v|d^\dagger\psi_o(x)|v'\rangle \overset{x\leq 0}{=} \mathrm{i}\tau e^{(-|\tau|^2/2+\mathrm{i}(\epsilon-E_v+E_{v'}))x}\int_{-L}^{x} dy\, e^{(|\tau|^2/2-\mathrm{i}(\epsilon-E_v+E_{v'}))y}\ {}_{CFT}\langle v|\psi_e^\dagger(0^-)\psi_o(y)|v'\rangle_{CFT}. \tag{4.91}$$

We still need to determine the integration constant L. But clearly, for any L finite, when $x \to -\infty$ the result diverges, whereas we know that the correlation function may at most be oscillating. Hence, we need to take $L = \infty$. Then, in order to evaluate matrix elements of the current operator, we only need to take the limit $x \to 0^-$ and substract the complex conjugate with $v \leftrightarrow v'$.

Clearly, the derivation holds as well when we consider the trace with the density matrix out of equilibrium, and in this case we have $E_v - E_{v'} = 0$ (because $[Y, H] = 0$) – this is the stationarity condition. Hence we find

$$\langle d^\dagger\psi_o(0^-)\rangle_{NE} = \mathrm{i}\tau\int_{-\infty}^{0} dy\, e^{(|\tau|^2/2-\mathrm{i}\epsilon)y}\langle\psi_e^\dagger(0^-)\psi_o(y)\rangle_0 \tag{4.92}$$

where the CFT average, denoted $\langle\cdot\rangle_0$ to agree with our previous notations, is evaluated using the *initial* density matrix

$$\rho_0 = e^{-(H_0-VQ)/T}. \tag{4.93}$$

Here, the fact that we obtained this CFT average for operators on the left of the impurity can also be seen simply as the use of the condition (4.5) at the basis of the definition of the Y operator. The CFT correlation function is easily evaluated by standard methods, where, with

$$f_{ab}(x_1 - x_2) = \langle\psi_a^\dagger(x_1)\psi_b(x_2)\rangle_0, \tag{4.94}$$

we have

$$f_{11}(x) = \frac{\mathrm{i}Te^{-\mathrm{i}Vx/2}}{2\sinh(\pi Tx)}, \quad f_{22}(x) = \frac{\mathrm{i}Te^{\mathrm{i}Vx/2}}{2\sinh(\pi Tx)}, \quad f_{12}(x) = f_{21}(x) = 0, \tag{4.95}$$

giving

$$f_{ee}(x) = f_{oo}(x) = \frac{\mathrm{i}T\cos(Vx/2)}{2\sinh(\pi Tx)}, \quad f_{eo}(x) = f_{oe}(x) = \frac{T\sin(Vx/2)}{2\sinh(\pi Tx)}. \tag{4.96}$$

Hence, we find

$$\langle\mathcal{J}\rangle_{NE} = \frac{|\tau|^2}{2}\int_{-\infty}^{0} ds\, e^{\frac{|\tau|^2 s}{2T}}\frac{\sin\frac{Vs}{2T}\cos\frac{\epsilon s}{T}}{\sinh\pi s} \tag{4.97}$$

which specialises, at zero temperature $T \to 0$, to

$$\langle\mathcal{J}\rangle_{NE} \overset{T=0}{=} \frac{|\tau|^2}{4\pi}\left(\arctan\frac{V+2\epsilon}{|\tau|^2} + \arctan\frac{V-2\epsilon}{|\tau|^2}\right). \tag{4.98}$$

Finally, we can generalise this calculation to $U \neq 0$. For $\mathcal{O}(x)$ as above, we know that $[H, \mathcal{O}(x)] = \mathrm{i} d\mathcal{O}(x)/dx$, so that we find the equations of motion:

$$\begin{aligned}
[H, d\mathcal{O}(x)] &= \Big[-\epsilon d - \tau^* \psi_e(0) - U d(\psi_e^\dagger(0)\psi_e(0) + \psi_o^\dagger(0)\psi_o(0)) \Big] \mathcal{O}(x) + \mathrm{i}\frac{d}{dx}(d\mathcal{O}(x)) \\
[H, d^\dagger \mathcal{O}(x)] &= \Big[\epsilon d^\dagger + \tau \psi_e^\dagger(0) + U d^\dagger(\psi_e^\dagger(0)\psi_e(0) + \psi_o^\dagger(0)\psi_o(0)) \Big] \mathcal{O}(x) + \mathrm{i}\frac{d}{dx}(d^\dagger \mathcal{O}(x)) \\
[H, D\mathcal{O}(x)] &= \Big[-\tau d\psi_e^\dagger(0) - \tau^* d^\dagger \psi_e(0) \Big] \mathcal{O}(x) + \mathrm{i}\frac{d}{dx}(D\mathcal{O}(x)). \qquad (4.99)
\end{aligned}$$

We need to use an appropriate resolution of the U-term, and simply replacing $\psi_{e,o}(0) = (\psi_{e,o}(0^+) + \psi_{e,o}(0^-))/2$ everywhere will be in agreement with that which we used in order to derive the discontinuity relations. Then, we simply need to replace all operators at 0^+ using the discontinuity relations. There are many terms. We find:

$$\begin{aligned}
-d\psi_e^\dagger(0^+)\psi_e(0^+) &= \psi_e^\dagger(0^+) d\psi_e(0^+) \\
&\overset{\mathcal{H}}{=} (\mathrm{i}\tau^* d^\dagger + (1 + \mathrm{i}u^* D)\psi_e^\dagger(0^-))\, d\, (-\mathrm{i}\tau d + (1 - \mathrm{i}uD)\psi_e(0^-)) \\
&= (1 - \mathrm{i}u)(\mathrm{i}\tau^* D\psi_e(0^-) - d n_e(0^-)) \qquad (4.100) \\
-d\psi_e^\dagger(0^+)\psi_e(0^-) &= \psi_e^\dagger(0^+) d\psi_e(0^-) \\
&\overset{\langle\cdot|}{=} (\mathrm{i}\tau^* d^\dagger + (1 + \mathrm{i}u^* D)\psi_e^\dagger(0^-))\, d\, \psi_e(0^-) \\
&= \mathrm{i}\tau^* D\psi_e(0^-) - d n_e(0^-) \qquad (4.101) \\
-d\psi_e^\dagger(0^-)\psi_e(0^+) &= \psi_e^\dagger(0^-) d\psi_e(0^+) \\
&\overset{|\cdot\rangle}{=} \psi_e^\dagger(0^-)\, d\, (-\mathrm{i}\tau d + (1 - \mathrm{i}uD)\psi_e(0^-)) \\
&= -(1 - \mathrm{i}u) d n_e(0^-) \qquad (4.102)
\end{aligned}$$

and the same hold for $e \mapsto o$ with $\tau \mapsto 0$:

$$\begin{aligned}
-d\psi_o^\dagger(0^+)\psi_o(0^+) &\overset{\mathcal{H}}{=} -(1 - \mathrm{i}u) d n_o(0^-) \qquad (4.103) \\
-d\psi_o^\dagger(0^+)\psi_o(0^-) &\overset{\langle\cdot|}{=} -d n_o(0^-) \qquad (4.104) \\
-d\psi_o^\dagger(0^-)\psi_o(0^+) &\overset{|\cdot\rangle}{=} -(1 - \mathrm{i}u) d n_o(0^-) \qquad (4.105)
\end{aligned}$$

where we used

$$n_e(x) = \psi_e^\dagger(x)\psi_e(x), \quad n_o(x) = \psi_o^\dagger(x)\psi_o(x). \qquad (4.106)$$

Taking the Hermitian conjugates:

$$\begin{aligned}
d^\dagger \psi_e^\dagger(0^+)\psi_e(0^+) &\overset{\mathcal{H}}{=} (1 + \mathrm{i}u^*)(\mathrm{i}\tau D\psi_e^\dagger(0^-) + d^\dagger n_e(0^-)) \qquad (4.107) \\
d^\dagger \psi_e^\dagger(0^-)\psi_e(0^+) &\overset{|\cdot\rangle}{=} \mathrm{i}\tau D\psi_e^\dagger(0^-) + d^\dagger n_e(0^-) \qquad (4.108) \\
d^\dagger \psi_e^\dagger(0^+)\psi_e(0^-) &\overset{\langle\cdot|}{=} (1 + \mathrm{i}u^*) d^\dagger n_e(0^-) \qquad (4.109) \\
d^\dagger \psi_o^\dagger(0^+)\psi_o(0^+) &\overset{\mathcal{H}}{=} (1 + \mathrm{i}u^*) d^\dagger n_o(0^-) \qquad (4.110) \\
d^\dagger \psi_o^\dagger(0^-)\psi_o(0^+) &\overset{|\cdot\rangle}{=} d^\dagger n_o(0^-) \qquad (4.111) \\
d^\dagger \psi_o^\dagger(0^+)\psi_o(0^-) &\overset{\langle\cdot|}{=} (1 + \mathrm{i}u^*) d^\dagger n_o(0^-). \qquad (4.112)
\end{aligned}$$

We also have

$$\begin{aligned}
-d\psi_e^\dagger(0^+) &\overset{\langle\cdot|}{=} \mathrm{i}\tau^* D - d\psi_e^\dagger(0^-) \qquad (4.113) \\
-d^\dagger \psi_e(0^+) &\overset{|\cdot\rangle}{=} \mathrm{i}\tau D - d^\dagger \psi_e(0^-). \qquad (4.114)
\end{aligned}$$

Putting all these terms together, and using the relation $U(2\mathrm{i}-u)=2u$, the equations of motion become

$$[H,b_j\mathcal{O}(x)]=\mathrm{i}\left(\frac{d}{dx}+A_j\right)(b_j\mathcal{O}(x))+\left(c_j+\sum_{i=1}^{3}b_iE_{ij}(0^-)\right)\mathcal{O}(x) \tag{4.115}$$

where

$$\begin{aligned} A_j &= \left(\frac{|\tau|^2}{2}+\mathrm{i}\epsilon,\frac{|\tau|^2}{2}-\mathrm{i}\epsilon,|\tau|^2\right)_j && (4.116)\\ c_j &= \left(-\tau^*\psi_e(0^-),\tau\psi_e^\dagger(0^-),0\right)_j && (4.117)\\ E_{ij}(x) &= \begin{pmatrix} -un(x) & 0 & -\tau\psi_e^\dagger(x)\\ 0 & u^*n(x) & -\tau^*\psi_e(x)\\ \mathrm{i}u\tau^*\psi_e(x) & iu^*\tau\psi_e^\dagger(x) & 0\end{pmatrix}_{ij} && (4.118)\end{aligned}$$

with

$$n(x)=n_e(x)+n_o(x). \tag{4.119}$$

Using these equations of motion in the steady state, from the stationary condition we obtain a first order differential equation involving $b_j\mathcal{O}(x)$:

$$-\mathrm{i}\frac{d}{dx}\langle b_j\mathcal{O}(x)\rangle_{NE}=\mathrm{i}A_j(b_j\mathcal{O}(x))+\left(c_j+\sum_{i=1}^{3}b_iE_{ij}(0^-)\right)\mathcal{O}(x). \tag{4.120}$$

However, it is not possible to immediately solve it, because it contains terms of the type $b_i\tilde{\mathcal{O}}(x)$ for new operators $\tilde{\mathcal{O}}(x)$ supported on the left.

4.4.3 Full perturbative expansion

What we can do, from (4.120), is simply to solve recursively. First, we integrate, so that we find

$$\langle b_j\mathcal{O}(0^-)\rangle_{NE}=\mathrm{i}e^{-A_jx}\int_{-\infty}^{x}dy\,e^{A_jy}\langle\left(c_j+\sum_{i=1}^{3}b_iE_{ij}(0^-)\right)\mathcal{O}(y)\rangle_{NE}. \tag{4.121}$$

Here we already used the asymptotic finiteness condition in choosing the integration constant, and we have specialised to $x=0^-$ for simplicity (and because this is of most interest in many situations). Note that the part of the average involving the factor $\langle c_j\mathcal{O}(y)\rangle_{NE}$ can be evaluated explicitly, because c_j only contains operators on the left of the impurity site:

$$\langle c_j\mathcal{O}(y)\rangle_{NE}=\langle c_j\mathcal{O}(y)\rangle_0. \tag{4.122}$$

Then we only have to interpret $E_{ij}(0^-)\mathcal{O}(y)$ as a new operator $\tilde{\mathcal{O}}(0^-)$ supported on the left, with rightmost support point at $x=0^-$, and use again the same integral solution for the averages $\langle b_iE_{ij}(0^-)\mathcal{O}(y)\rangle_{NE}$. Recursively doing this, we find

$$\langle\sum_{j=1}^{3}b_j\mathcal{O}_j(0^-)\rangle_{NE}=\sum_{n=0}^{\infty}\mathrm{i}^{n+1}\int_{-\infty}^{0}dx_0\cdots dx_n\langle c^te^{Ax_n}E(x_n)\cdots e^{Ax_1}E(x_1+\ldots+x_n)e^{Ax_0}\mathcal{O}(x_0+\ldots+x_n)\rangle_0 \tag{4.123}$$

where

$$A=\begin{pmatrix}A_1&0&0\\0&A_2&0\\0&0&A_3\end{pmatrix},\quad c^t=\begin{pmatrix}c_1&c_2&c_3\end{pmatrix},\quad \mathcal{O}(x)=\begin{pmatrix}\mathcal{O}_1(x)\\\mathcal{O}_2(x)\\\mathcal{O}_3(x)\end{pmatrix} \tag{4.124}$$

and $E(x)$ is the matrix with entries $E_{ij}(x)$. This provides the full perturbative expansion in U for the average of any operator at the site $x = 0$. That it is an expansion in U is clear upon realising that the n^{th} power of the matrix $E(x)$ (at different positions x_j) has powers n and $n-1$ of U, a structure which is not affected by multiplying the n factors by diagonal matrices e^{Ax_j}. Interestingly, the matrix structure has taken care of the combinatorics of the perturbation theory: there was no need for any Keldysh diagrams, for instance. Certainly, we will need to have a cut-off and renormalisation scheme, but the cutoff can be totally implemented in the CFT correlation functions themselves. Interestingly, however, it is possible to take the cutoff scheme where we have infinite-cutoff CFT correlation functions, but an upper limit on the x_j integrations set to $-\Lambda^{-1}$ instead of 0. This was shown in [6] to reproduce, for instance, the correct singularity structure, hence the correct renormalisation group equations.

There are other suggestive forms in which this infinite series can be written:

$$\langle \sum_{j=1}^{3} b_j \mathcal{O}_j(0^-) \rangle_{NE} = \mathrm{i} \int_{-\infty}^{0} dx \, \langle c^t \mathcal{P} \exp \int_0^x dy (-\mathrm{i}E(y) + A) \, \mathcal{O}(x) \rangle_0 \tag{4.125}$$

and

$$\langle \sum_{j=1}^{3} b_j \mathcal{O}_j(0^-) \rangle_{NE} = \mathrm{i} \int_{-\infty}^{0} dx \, \langle c^t e^{-\mathrm{i}(H_e + E(0) + \mathrm{i}A)x} \, \mathcal{O}(0) e^{\mathrm{i}H_e x} \rangle_0 \tag{4.126}$$

where we recall that H_e is the metallic-sheet Hamiltonian.

In the latter form, there is a new evolution operator that appears, with Hamiltonian

$$\tilde{H} = H_e + E(0) + \mathrm{i}A. \tag{4.127}$$

This is a Hamiltonian with an impurity interaction, but the impurity space is twice as big: it is the space of original impurity operators. Equation (4.125) tells us to first evolve the CFT state for a "time" $-x$ with the impurity-less Hamiltonian, apply $\mathcal{O}(0)$, then evolve backward for the same time, but with the evolution operator associated to $\tilde{H}$, then act with the special operators c^t; finally tracing over the CFT states and integrating over the "time" $-x$. In a sense, the forward part of the time evolution has been made trivial, and all the impurity action is in the backward part. Essentially, the use of the discontinuity relations is equivalent to using the impurity (anti-)commutation relations to bring all impurity operators on one side of the observable that we are interested in; we are left only with a structure in the space of impurity operators.

In the former form, (4.125), we have a path-ordered exponential of an integral of the impurity part of the new Hamiltonian $\tilde{H}$. There, it is important to note that all operators are always ordered in decreasing positions. Hence, we do not need to know about the commutation relations of the various operators involved in the matrix $E(x)$. That is, it is at that point possible to represent all operators as random (anti-commuting) variables, with a proper kernel reproducing the correct correlation functions for ordered positions: we may consider

$$\langle \cdots \rangle_0 \mapsto \int [d\psi_1 d\psi_1^\dagger d\psi_2 d\psi_2^\dagger] e^{\int_{-\infty}^{0} dx dx' \left(\psi_1^\dagger(x) K_1(x,x') \psi_1(x) + \psi_2^\dagger(x) K_2(x,x') \psi_2(x) \right)} \cdots . \tag{4.128}$$

It would be interesting to study further such a representation.

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