Transient dynamics of the nonequilibrium Majorana resonant level model

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The Majorana resonant level model (MRLM) describes the universality class of the two-channel/terminal Kondo model at the Toulouse point as well as of a resonant level between two half-infinite Tomonaga–Luttinger liquids. We analyze the time evolution of the electric current and of the population function after an instantaneous switching on of the tunneling coupling. We find that the only timescale, which governs the relaxation of the initial dot preparation is the inverse contact transparency $\Gamma$, whatever the dot offset energy $\Delta$, applied bias voltage or temperature. The voltage alone determines the superimposed oscillatory behavior of the observables for weak detuning $|\Delta| < \Gamma/2$. In the opposite case of strong detuning $|\Delta| > \Gamma/2$ a beating pattern emerges. For the current the finite temperature plays the similar role as the hybridization. The dot population function dynamics approaches that of a resonant ($\Delta = 0$) setup upon increasing the voltage or/and temperature.

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During the last decades we witnessed a soaring interest in the nonequilibrium properties of quantum impurity models. It has been motivated by the advances in manufacturing of semiconductor based nanostructures, in which only a small number of electronic levels participate in the charge and spin transport. The experimentalists not only succeeded in observing the Kondo effect in such structures, but also were able to demonstrate phonon-assisted charge transport through single molecules, see e. g. [1]. From the theoretical point of view such zero-dimensional systems can be seen as realizations of quantum impurity models with or without internal degrees of freedom. Typical examples are the Anderson model, Tomonaga–Luttinger liquids (TLLs) and fractional quantum Hall edge states with impurities, resonant levels coupled to a Holstein phonon etc. Many of their equilibrium properties can be calculated with the help of by now quite substantial number of techniques. On the contrary, in the nonequilibrium one is especially missing the extremely powerful Bethe ansatz and integrability methods. Although their adaptation to setups far from equilibrium has already begun, a number of open issues are yet to be settled.

Fortunately, at least in the universality class of Kondo models there are some exactly solvable points which occur at nontrivial constellations of system parameters: the Toulouse limits. Those turn out to be the only fully featured testing grounds (apart from numerical approaches, of course), which we have at our disposal in the moment. In its canonical incarnation it is a special point in the parameter space where a mapping of the conventional Kondo model onto a resonant level model is possible. [2] For transport phenomena a two terminal topology is necessary. [3] The original Hamiltonian is then mapped onto that of a Majorana resonant level model (MRLM). It turns out to be isomorph to the interacting resonant level in the TLL. [4] Hence, a solution of MRLM provides us with predictions to a considerably broader class of situations, than the original Kondo quantum dot. Thus far this kind of exact solvability has been taken advantage of in a number of contributions. [7, 8, 9] However, only a fraction of them went beyond the steady state calculations. [10, 11] The quantities of special interest are the transport current evolution, several aspects of which has bee discussed in Ref. [10], and the magnetization of the impurity in the Kondo case, or the population of the resonant level in the TLL resonant level setup. To the best of our knowledge, the latter observables have not yet been addressed. We would like to close this gap and present the full solution in the case of instantaneous switching on of the tunneling hybridization.

We first summarize the MRLM Hamiltonian in its most general form. It features local Majorana fermions $a, b$ as well as four different Majorana fermionic fields. They are organized into pairs describing a principal channel $\eta(x), \xi(x)$ and a flavor channel $\eta_f(x), \xi_f(x)$:

$$ H = H_0[\xi, \eta, \eta_f] - i [\Delta ab + J_- b \xi_f(0) + J_+ a \eta_f(0) + \gamma_+ b \xi(0) + \gamma_- a \eta(0)] . $$

(1)

$H_0$ is responsible for the dynamics of the free (decoupled from the local Majoranas) fields,

$$ H_0 = i \int dx \left[ \eta_f(x) \partial_x \eta_f(x) + \xi_f(x) \partial_x \xi_f(x) + \eta(x) \partial_x \eta(x) + \xi(x) \partial_x \xi(x) + V(x) \eta(x) \right] . $$

(2)

$\Delta, J_{\pm}$ and $\gamma_{\pm}$ are different constant couplings whereas $V$ is in a strict sense not a coupling but a chemical potential and is related to the bias voltage applied in the systems parental to MRLM. This is the reason why we employ nonequilibrium diagrammatics in order to calculate the observables of interest. These are the current

$$ I = \langle i/2 \rangle [\gamma_- \langle a \xi(0) \rangle + \gamma_+ \langle b \eta(0) \rangle] , $$

(3)
and the dot occupation probability,

$$n_d = (1 + i \langle ab \rangle) / 2.$$  \tag{4}$$

The origin of the MRLM is twofold: it emerges in the (i) two terminal Kondo model at the Toulouse point, and (ii) interacting resonant level between two TLLs. In the situation (i) one starts with the conventional Kondo Hamiltonian (we set $\hbar = v_F = e = k_B = 1$), $H = H_0 + H_J + H_M + H_V$, where, with $\psi_{\alpha \sigma}$ being the electron field operators in the R.L (right/left) terminals,

$$H_0 = i \sum_{\alpha = R, L, \sigma = \uparrow, \downarrow} \int dx \, \psi^{\dagger}_{\alpha \sigma}(x) \partial_x \psi_{\alpha \sigma}(x),$$

$$H_J = -\sum_{\alpha = R, L, \nu = x, y, z} J^\nu_{\alpha \beta} \psi^{\dagger}_{\alpha \nu} \tau^\nu,$$

$$H_V = \frac{(V/2)}{\sigma} \int dx \left( \psi^{\dagger}_{L \sigma} \psi_{R \sigma} - \psi^{\dagger}_{R \sigma} \psi_{L \sigma} \right),$$

$$H_M = -\mu_B g_i \hat{H} \tau^z = -\Delta \tau^z. \tag{5}$$

Here $\tau^x, \tau^y, \tau^z$ are the Pauli matrices for the impurity spin and $(\alpha, \beta = R, L; \sigma = \uparrow, \downarrow; \gamma_{\sigma \gamma'})$ are the components of the $\nu$th Pauli matrix

$$\gamma^r_{\sigma \gamma'} = \sum_{\sigma, \gamma'} \psi^{\dagger}_{\sigma \gamma'}(0) \psi_{\sigma \gamma'}(0),$$

are the generalized electron spin densities in (or across) the leads biased by a finite $V$. The last term in Eq. (5) stands for the magnetic field, $\Delta = \mu_B g_i \hat{H}$. Following Ref. [7], we assume $J^\rho_{\alpha \beta} = J^\rho_{\beta \alpha}$. For $J^x, J^y, J^z$ and $J^L_R = J^{RL} = 0$. After bosonization, Emery-Kivelson rotation, and renormalization (see details in Ref. [2] or [12]) and setting $\tau = 2\pi$, one obtains the Toulouse point Hamiltonian [7], where $J^x = (J^{LL} + J^{RR}) / \sqrt{2} \nu a_0$, $\gamma_+ = J_+ = J^{LL} / \sqrt{2} \nu a_0$, $\gamma_- = 0$ ($a_0$ is the lattice constant of the underlying lattice model) and $a$ and $b$ being local Majorana operators originating from the impurity spin $\tau^x = (d^+ + d)$, $\tau^y = i(d^+ - d)$, and $\tau^z = 2d^+ d - 1$. In the chiral formulation the bias voltage amounts to a difference in the densities of the incoming particles in both channels far away from the constriction. [13] The current is then proportional to the difference between the densities of incoming and outgoing particles within each channel.

The setup (ii) is the spinless TLL resonant level model with the Hamiltonian $H = H_K + H_I + H_L$, where $H_K$ is the kinetic part, $H_K = \Delta d^d d + \sum_{i = R, L} H_0[\psi_i]$, describing the electrons in the leads $H_0[\psi_i]$, and the resonant level with energy $\Delta$, the corresponding electron operators being $d^d, d$. The dot can be populated from either of the two leads $(i = R, L)$ via electron tunneling with amplitudes $\gamma_i$, $H_I = \sum_i \gamma_i [d^\dagger \psi_i(0) + h.c.]$. $H_I$ describes the electrostatic Coulomb interaction between the strength $U$ between the leads and the dot, $H_I = U d^d d \sum_i \psi_i^\dagger(0) \psi_i(0)$. The contacting electrodes are one-dimensional half-infinite electron systems. We model them by chiral fermions living in an infinite system. [2] The bosonic representation $H_0[\psi_i]$ are diagonal even in presence of interactions (for a recent review see e.g. [4]: we set the renormalized Fermi velocity $v = v_F / g = 1$, the bare velocity being $v_F$):

$$H_0[\psi_i] = \frac{1}{4\pi} \int dx \left( \partial_x \phi_i(x) \right)^2. \tag{7}$$

Here the phase fields $\phi_i(x)$ describe the slow varying spatial component of the electron density (plasmons), $\psi_i^\dagger(0) \psi_i(0) = \partial_x \phi_i(x) / 2\pi \sqrt{\gamma}$. The electron field operator at the boundary is given by $\psi_i(0) = e^{i\phi_i(0)} / \sqrt{\gamma} \sqrt{\sqrt{\gamma} a_0}$. Here $g$ is the conventional TLL parameter related to the bare interaction strength $U_{\gamma LLL}$ via $g = \left(1 + U_{\gamma LLL} / \pi v_F \right)^{-1/2}$. [4] In the chiral formulation the bias voltage amounts to a difference in the densities of the incoming particles in both channels far away from the constriction. [14] The current is then proportional to the difference between the densities of incoming and outgoing particles within each channel.

At generic $g \neq 1$ the problem cannot be solved exactly though. However, at $g = 1 / 2$ after a transformation of $d^d$ and $d$ operators to the spin representation of the form $\tau^x = (d^+ + d)$, $\tau^y = i(d^+ - d)$, and $\tau^z = 2d^+ d - 1$ one immediately observes that the $U$-term is analogous to the $\tau^z$-spin density coupling in the Kondo problem. Indeed, a mapping onto the MRLM can be performed in the same way as in the Kondo case and one again obtains Hamiltonian [7] with $\gamma_\pm = \gamma_L \pm \gamma_R$ and $J_\pm = 0$. [6] As before we are interested in the transport current $I_L$ and dot population $I_d$. The time derivative of $n_d$ is the displacement current in the system $I_d^{\text{disp}}(t) = d n_d(\tau)/d\tau$. The currents through the individual contacts $I_{L/R}$ can then be conveniently evaluated using the relations [13]:

$$I_{L,R}(t) = I(t) \pm I_d^{\text{disp}}(t)/2.$$

The effect of the asymmetry $\gamma_- \neq 0$ is similar to that of a finite detuning $\Delta \neq 0$, that is why in order to make the calculations and results more lucid we concentrate on the latter case and set $\gamma_- = 0$. Then the current operators are identical in both (i) and (ii).

In general the calculation of the observables is simplified by their reduction to a related nonequilibrium Green’s function (GF). In the case of the transport current it is $G_{\gamma y}(t, t') = -i (T_C b(t) \eta(t'))$, where $T_C$ is the time ordering along the Keldysh contour $C$. [11] Then the time dependent current is given by $I(t) = -\langle \gamma \rangle / 2 G_{\gamma y}(t + 0^+, t)$, where by abuse of notation $G_{\gamma y}(t, t')$ denotes the time ordered GF and $\gamma = \gamma_+$. From now on we assume a steplike switching on of the tunneling when $\gamma(t) = \gamma \Theta(t)$, where $\Theta(t)$ is the Heaviside function. By an expansion in $\gamma$ and resummation of the series one can show, that
the resonant level TLL setup obtain:

\[ I(t) = i\gamma \int_0^\infty dt' [D_{bb}(t, t') g_{\xi}(t' - t) \]

\[ - D_{bb}^\xi(t, t') g_{\xi}(t' - t) ] . \tag{8} \]

\( D_{bb}(t, t') = -i(T_C b(t) b(t')) \) is the exact homogeneous b-Majorana GF. \( g_{\xi}(t, t') = -i(T_C \xi(t) \eta(t')) \) are the zero order in tunneling GFs. Remarkably, all its Keldysh components are equal and given by \( g_{\xi}(\omega) = (n_L - n_R)/2 \), where \( n_{R,L} \) are the Fermi distributions in the right(left) electrode.\] In the Kondo setup we model the electrodes by wide flat band with constant density of states \( \rho_0 \). In the resonant level TLL setup \( \rho_0 \) is equal to the energy-independent prefactor in the density of states in vicinity of the Fermi edge. Here the applied voltage must be doubled.\] Then for the current through the system we obtain:

\[ I(t) = i\frac{\Gamma T}{2} \int_0^\infty dt' D_{bb}^R(t - t') \frac{\sin[V(t' - t)]}{\sinh[\pi T(t' - t)]} , \tag{9} \]

where \( \Gamma = \rho_0 \gamma^2/2 \). Thus everything is determined by the retarded \( D_{bb}^R \) only. In the time domain we obtain:

\[ D_{bb}^R(t, t') = D_{bb}^{(0)R}(t - t') \]

\[ + \int_0^\infty dt_1 dt_2 D_{bb}^{(0)R}(t, t_1) \Sigma^R(t_1 - t_2) D_{bb}^R(t_2, t') , \tag{10} \]

where the self-energy is due to the tunneling only and is up to a prefactor identical to the homogeneous \( \eta \)-GF. It is most compact in the energy representation:

\[ \Sigma^R(\omega) = -i\Gamma \rho_0 , \Sigma^<(\omega) = -i\Gamma(n_L + n_R) , \]

\[ \Sigma^>(\omega) = -i\Gamma(n_L + n_R - 2) . \tag{11} \]

To make progress we use

\[ D_{bb}^{(0)R}(t, t') = -i\Theta(t - t') \cos[\Delta(t - t')] \tag{12} \]

for the GF in the absence of coupling, which is valid at \( J_+ = 0 \).\] It can be shown, that the solution of (10) is translationally invariant in time and has the structure

\[ D_{bb}^R(t, t') = D_{bb}^R(t - t') = -i\Theta(t - t') f(t - t') , \]

where

\[ f(t) = f^{(0)}(t) - \Gamma \int_0^t d\tau f^{(0)}(t - \tau) f(\tau) , \tag{13} \]

with \( f^{(0)}(t) = \cos(\Delta t) \). This is a Volterra integral equation of the second kind solvable by the Laplace transformation. We observe however, that the equation for the retarded dot GF in the static case without switching effects has exactly the same form.\] The explanation for that is the functional similarity of our switching method and of the natural steplike time dependence of the retarded GF. The solution in the energy domain is known to be given by

\[ D_{bb}^R(\omega) = \frac{\omega}{\omega^2 - \Delta^2 + i\omega\Gamma} . \tag{14} \]

FIG. 1: Full current through the constriction at zero temperature for different voltages \( V \) and dot offset energies \( \Delta \). The current is measured in units of \( G_0\Gamma/2 \), where \( G_0 = 2e^2/h \) is the conductance quantum.

Transformed back it yields

\[ f(t) = e^{-\Gamma t/2} \frac{2\Omega}{\Omega^2} [\cosh(\tau\omega) - \Gamma \sinh(\tau\omega)] , \tag{15} \]

with \( \Omega = |\sqrt{(\Gamma/2)^2 - \Delta^2} | \) for weak detuning \( |\Delta| < \Gamma/2 \). In case of strong detuning, when \( |\Delta| > \Gamma/2 \) the function is found by an analytic continuation. Knowing that the retarded GF is indeed translationally invariant in time allows for further simplification of (9):

\[ I(t) = \frac{\Gamma T}{2} \int_0^t d\tau f(\tau) \frac{\sin(\tau\omega)}{\sinh(\tau\pi T\omega)} . \tag{16} \]

In general the current shows up two constituents: the transient one and the time-independent static one, \( I(t) = I_{stat} + I_{trans}(t) \). For the weak detuning we obtain\,[6, 10]\]

\[ I_{stat} = \frac{\Gamma}{4\pi\Omega} \Im \sum_{p = \pm} (\Omega + p\Gamma/2) \]

\[ \times \Psi \left( \frac{1}{2} + \frac{iV + p\Omega + \Gamma/2}{2\pi T} \right) , \tag{17} \]

where \( \Psi \) denotes the digamma function. The transient part is given by

\[ I_{trans}(t) = \frac{\Gamma T}{2\Omega} \Im \sum_{p = \pm} (\Omega - p\Gamma/2) e^{(iV + p\Omega - \Gamma/2 - \pi T)t} \]

\[ \times 2F_1 \left( 1, \frac{1}{2}, \frac{iV + p\Omega - \Gamma/2}{2\pi T}, \frac{3}{2} - \frac{iV + p\Omega - \Gamma/2}{2\pi T}; e^{-2\pi Tt} \right) , \tag{18} \]

where \( 2F_1 \) denotes the hypergeometric function. For weak detuning the transient current oscillates with the frequency \( \propto V \)[10]. This situation changes in case of strong detuning when \( \Omega \) becomes imaginary and enters
the above equations in the same way as the voltage. Then there are two different frequencies \( \propto |V \pm \Omega| \) and a beating pattern emerges, s. Fig. 1. Of course these features can be observed only when the oscillation period is smaller than the competing time scale \( \propto \Gamma + \pi T \), which governs the overall current relaxation.

It turns out, that for the calculation of the dot population it is more convenient to work with the lesser Keldysh GF \( D_{\uparrow \downarrow}^{\leq}(t, t') = -i \langle a(t) b(t') \rangle \). The calculation of this GF is accomplished using the Dyson equation in the time domain (multiplication corresponds to time integrations):

\[
D_{\uparrow \downarrow} = D_{\uparrow \downarrow}^{(0)} + D_{\uparrow \downarrow}^{(0)} \Sigma D_{\uparrow \downarrow},
\]

where the self-energy is proportional to the unperturbed GF for the \( \xi \)-Majoranas \( \Sigma = \Gamma g_{\xi \xi} \). After the Keldysh disentanglement we obtain

\[
D_{\uparrow \downarrow} = D_{\uparrow \downarrow}^{(0)} + D_{\uparrow \downarrow}^{(0)} \Sigma R D_{\uparrow \downarrow} + D_{\uparrow \downarrow}^{(0)} \Sigma A D_{\uparrow \downarrow}^{(0)}.
\]

Thus the calculation of the inhomogeneous \( D_{\uparrow \downarrow} \)-GF is now reduced to the calculation of the homogeneous \( D_{\uparrow \downarrow} \).

The necessary zero order GFs are

\[
D_{\uparrow \downarrow}^{(0)}(t) = - (\kappa/2) e^{i \kappa \Delta t}, \quad D_{\uparrow \downarrow}^{(0)}(t) = -i \Theta(t) \sin(\Delta t),
\]

where \( \kappa = \pm 1 \) encodes the initially populated/empty dot level. For the retarded component of the homogeneous \( D_{\uparrow \downarrow} \) one obtains the equation

\[
D_{\uparrow \downarrow}^R = D_{\uparrow \downarrow}^{(0)R} + D_{\uparrow \downarrow}^{(0)R} \Sigma R D_{\uparrow \downarrow}^R.
\]

The resonant case \( \Delta = 0 \) is especially simple. Here the bare retarded inhomogeneous GF vanishes and one obtains

\[
n_d(t) = \frac{1 + \kappa e^{-\Gamma t}}{2}.
\]

This is a very remarkable result since the relaxation of the dot occupation/magnetization is independent on both temperature and applied voltage and is only governed by the timescale \( 1/\Gamma \).

In the off-resonant case the calculations are more complex since we need the full homogeneous \( D_{\uparrow \downarrow} \). It is given by

\[
D_{\uparrow \downarrow} = (1 + D_{\uparrow \downarrow}^R \Sigma R) D_{\uparrow \downarrow}^{(0)} + D_{\uparrow \downarrow}^R \Sigma D_{\uparrow \downarrow}^{(0)}.
\]

Putting the result into (19) we obtain for weak detuning

\[
n_d(t) = \frac{1}{2} \left( 1 + \kappa e^{-\Gamma t} \right) - \frac{\Gamma \Delta}{2\Omega^2} \int \frac{d\omega}{2\pi} \frac{4\Omega n_L}{(\Delta^2 - \omega^2)^2 + \omega^2 \Gamma^2} \times \left\{ \Omega \omega \left[ e^{\Gamma t} - e^{-\Gamma t/2} \right] \sin(\Omega t) \sin(\omega t) + 2\omega \Omega \cosh(\Omega t) \cos(\omega t) \right\}.
\]

The most striking feature of this result is that the relaxation behavior of the information about the initial preparation is exactly the same as in the resonant case and independent on either the temperature or the applied voltage. Thus the rate at which the system ‘forgets’ its initial preparation does not depend on these parameters. At zero temperature the effect of finite voltage is to fix the upper energy integration boundary. Since the integrand is an odd function of energy the whole correction due to finite \( \Delta \) vanishes towards larger \( V \), so that \( n_d \) approaches that of a system at resonance, see Fig. 2.

The effect of finite temperature is very similar: due to smearing off of the Fermi edge the contribution of the energy integration decreases so that the relative weight of the resonant contribution increases and becomes more and more dominant. For finite detuning \( n_d \) oscillates with the frequency \( \propto \Delta \). As soon as the applied voltage becomes nonzero a beating pattern emerges just as for the time dependence of the transport current.

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[19] The calculation without this restriction is exactly the same up to some minor adjustments. For the details see e. g. Appendix A of Ref. [17].
[20] This feature is shared by the corresponding equation for the conventional resonant level even beyond the wide flat band model [12].