Transient dynamics of the nonequilibrium Majorana resonant level model

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The Majorana resonant level model 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 time scale, which governs the relaxation of the initial dot preparation is the inverse contact transparency Γ , whatever the dot offset energy Δ , 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 (Δ =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., Ref. 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.²

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 at 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.^{3,4} For transport phenomena a two terminal topology is necessary.⁵ 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.⁶ Thus far this kind of exact solvability has been taken advantage of in a number of contributions.^{7–9} However only a fraction of them went beyond the steadystate calculations. 10,11 The quantities of special interest are the transport current evolution, several aspects of which has been 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 $\eta_f(x), \xi_f(x)$

$$H = H_0[\xi, \eta, \xi_f, \eta_f] - i[\Delta ab + J_-b\xi_f(0) + J_+a\eta_f(0) + \gamma_+b\xi(0) + \gamma_-a\eta(0)].$$
(1)

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

$$H_0 = i \int dx [\eta_f(x)\partial_x \eta_f(x) + \xi_f(x)\partial_x \xi_f(x) + \eta(x)\partial_x \eta(x)$$

+ $\xi(x)\partial_x \xi(x) + V\xi(x)\eta(x)$]. (2)

 Δ , J_{\pm} and γ_{\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

$$I = (i/2) [\gamma_{-} \langle a\xi(0) \rangle + \gamma_{+} \langle b\eta(0) \rangle]$$
 (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 $\hbar = v_F = e = k_B = 1$)

$$H = H_0 + H_I + H_M + H_V, (5)$$

where, with $\psi_{\alpha,\sigma}$ being the electron-field operators in the R (right) and L (left) terminals

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

$$H_{J} = \sum_{\alpha,\beta=R,L} \sum_{\nu=x,y,z} J_{\nu}^{\alpha\beta} s_{\alpha\beta}^{\nu} \tau^{\nu},$$

$$H_V = (V/2) \sum_{\sigma} \int dx (\psi_{L\sigma}^{\dagger} \psi_{L\sigma} - \psi_{R\sigma}^{\dagger} \psi_{R\sigma}),$$

$$H_M = -\mu_R g_i H \tau^z = -\Delta \tau^z. \tag{6}$$

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

$$s_{\alpha\beta}^{\nu} = \sum_{\sigma,\sigma'} \psi_{\alpha\sigma}^{\dagger}(0) \sigma_{\sigma\sigma'}^{\nu} \psi_{\beta\sigma'}(0)$$

are the generalized electron-spin densities in (or across) the leads biased by a finite V. The last term in Eq. (6) stands for the magnetic field $\Delta = \mu_B g_i H$. Following Ref. 7, we assume $J_x^{\alpha\beta} = J_y^{\alpha\beta} = J_\perp^{\alpha\beta}$, $J_z^{LL} = J_z^{RR} = J_z$, and $J_z^{LR} = J_z^{RL} = 0$. After bosonization, Emery-Kivelson rotation, refermionization (see details in Refs. 7 or 12), and setting $J_z = 2\pi$ one obtains the Toulouse-point Hamiltonian (1) where $J_\pm = (J_\perp^{LL} \pm J_\perp^{RR})/\sqrt{2\pi a_0}$,

 $\gamma_+ = J_\perp = J_\perp^{RL}/\sqrt{2\pi a_0}$, $\gamma_- = 0$ (a_0 is the lattice constant of the underlying lattice model), and a and b being local Majorana operators originating from the impurity spin $\tau = (\tau^x, \tau^y, \tau^z)$: $\tau^x = a$ and $\tau^y = b$. The fields η_f and ξ_f in the spin-flavor sector are equilibrium (real) Majorana fields whereas η and ξ in the charge-flavor sector are biased by the transport voltage V. The current through the system is then given by Eq. (3) and the impurity magnetization by

$$m = \langle \tau^z \rangle = -i \langle \tau^x \tau^y \rangle = i \langle ab \rangle = 2n_d - 1. \tag{7}$$

The setup (ii) is the spinless TLL resonant-level model with the Hamiltonian

$$H = H_K + H_t + H_I, \tag{8}$$

where H_K is the kinetic part, $H_K = \Delta d^{\dagger} d + \sum_{i=R,L} H_0[\psi_i]$, describing the electrons in the leads $H_0[\psi_i]$ and the resonant level with energy Δ , the corresponding electron operators being d^{\dagger} , d. The dot can be populated from either of the two leads (i=R,L) via electron tunneling with amplitudes γ_i

$$H_t = \sum_i \gamma_i [d^{\dagger} \psi_i(0) + \text{H.c.}]. \tag{9}$$

 H_I describes the electrostatic Coulomb interaction with the strength U between the leads and the dot

$$H_I = U d^{\dagger} d \sum_i \psi_i^{\dagger}(0) \psi_i(0).$$

The contacting electrodes are one-dimensional half-infinite electron systems. We model them by chiral fermions living in an infinite system.⁶ In the bosonic representation $H_0[\psi_i]$ are diagonal even in presence of interactions (for a recent review see, e.g., Ref. 4; we set the renormalized Fermi ve-

locity $v = v_F/g = 1$, the bare velocity being v_F)

$$H_0[\psi_i] = \frac{1}{4\pi} \int dx [\partial_x \phi_i(x)]^2. \tag{10}$$

Here the phase fields $\phi_i(x)$ describe the slow-varying spatial component of the electron density (plasmons)

$$\psi_i^{\dagger}(x)\psi_i(x) = \partial_x \phi_i(x)/2\pi\sqrt{g}$$
.

The electron-field operator at the boundary is given by $\psi_i(0) = e^{i\phi_i(0)/\sqrt{g}}/\sqrt{2\pi a_0}$. Here g is the conventional TLL parameter related to the bare interaction strength U_{TLL} via $g = (1 + U_{TLL}/\pi v_F)^{-1/2}$. 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^{\dagger} and d operators to the spin representation of the form $\tau^x = (d^{\dagger} + d)$, $\tau^y = -i(d^{\dagger} - d)$, and $\tau^z = 2d^{\dagger}d - 1$ one immediately observes that the U term is analogous to the τ^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 (1) with $\gamma_{\pm} = \gamma_L \pm \gamma_R$ and $J_{\pm} = 0.6$ As before we are interested in the transport current [Eq. (3)] and dot population [Eq. (4)]. The time derivative of n_d is the displacement current in the system

$$I_{\text{disp}}(t) = dn_d(t)/dt$$
.

The currents through the individual contacts $I_{L,R}$ can then be conveniently evaluated using the relations¹⁵

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

The effect of the asymmetry $\gamma_{-} \neq 0$ is similar to that of a finite detuning $\Delta \neq 0$, ¹² 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).

We would like to point out that although we remove a four-fermion coupling by choosing special parameter values, we do not expect distinct qualitative changes in the emerging physics in the case of generic couplings. One way to investigate these deviations is to perform perturbative expansion in these four-fermion operators. In fact this program was carried out in *nonequilibrium* in Ref. 16 with the result that in the low-energy sector the corrections are subleading and do not alter the generic Kondo picture. That is why we expect that also in the present situation the influence of the omitted four-fermion operators is far from being significant. Nonetheless, only a thorough study (which, even after restriction to perturbative expansion, would be quite involved from the mathematical point of view) can yield the ultimate answer to these questions.

During the last decade both setups have been experimentally realized by numerous research groups. Most of them were based on semiconductor heterostructures (for resonant

tunneling setup see, e.g., Ref. 17 and for Kondo Ref. 1), the others on nanotubes and single molecules (see, e.g., Ref. 18). While in the latter realizations it is quite difficult to generate time-dependent tunneling coupling v(t), one of the first reports of efficient real-time manipulation of this matrix element in the semiconductor heterostructures was published almost 20 years ago. 19 Nowadays the conductance of quantum point contacts can even be controlled by individual electrons populating side-coupled quantum dots.²⁰ That is why the investigation of such systems with explicitly timedependent coupling is not a purely academic question any more but rather can also be analyzed experimentally in the near future. The simplest time dependence is the sudden switching when the initially absent tunneling coupling (experimentally realized by a complete pinch off of the respective conducting channel) is switched on instantaneously to a constant value.

The quantities of interest are then the full transport current and the dot population in the setup (ii) and magnetization in the setup (i). We expect that the current can be measured by the standard techniques. The dot population measurement may require additional equipment such as, e.g., side-coupled quantum dot as demonstrated in Ref. 20. For the magnetization measurement one can, for instance, use the recently developed techniques discussed in Ref. 21.

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 $G_{b\eta}(t,t')\!=\!-i\langle T_C b(t)\,\eta(t')\rangle$ where T_C is the time ordering along the Keldysh contour C^{22} . Then the time-dependent current is given by $I(t)\!=\!-(\gamma/2)G_{b\eta}(t\!+\!0^+,t)$ where by abuse of notation $G_{b\eta}(t,t')$ 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 γ and resummation of the series one can show that the following reduction is valid: 22

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

 $D_{bb}(t,t')$ = $-i\langle T_C b(t)b(t')\rangle$ is the *exact* homogeneous b-Majorana GF. $g_{\xi\eta}(t,t')$ = $-i\langle T_C \xi(t)\,\eta(t')\rangle$ are zero order in tunneling GFs. Remarkably, all its Keldysh components are equal and given by $g_{\xi\eta}(\omega)$ = $(n_L-n_R)/2$ 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 ρ_0 . In the resonant-level TLL setup ρ_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

$$I(t) = i\frac{\Gamma T}{2} \int_0^\infty dt' D_{bb}^R(t, t') \frac{\sin[V(t'-t)]}{\sinh[\pi T(t'-t)]},$$
 (12)

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

$$\begin{split} D_{bb}^{R}(t,t') &= D_{bb}^{(0)R}(t-t') \\ &+ \int_{0}^{\infty} dt_{1} dt_{2} D_{bb}^{(0)R}(t,t_{1}) \Sigma^{R}(t_{1}-t_{2}) D_{bb}^{R}(t_{2},t'), \end{split} \tag{13}$$

where the self-energy is due to the tunneling only and is up to a prefactor identical to the homogeneous η GF. It is most compact in the energy representation

$$\Sigma^{R}(\omega) = -i\Gamma, \quad \Sigma^{<}(\omega) = -i\Gamma(n_L + n_R),$$

$$\Sigma^{>}(\omega) = -i\Gamma(n_I + n_R - 2). \tag{14}$$

To make progress we use

$$D_{bb}^{(0)R}(t,t') = -i\Theta(t-t')\cos[\Delta(t-t')],$$
 (15)

for the GF in the absence of coupling, which is valid at $J_{\pm} = 0.^{23}$ It can be shown, that the solution of Eq. (13) 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

$$f(t) = f^{(0)}(t) - \Gamma \int_0^t d\tau f^{(0)}(t - \tau) f(\tau), \tag{16}$$

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.²⁴ 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

$$D_{bb}^{R}(\omega) = \frac{\omega}{\omega^2 - \Delta^2 + i\omega\Gamma}.$$
 (17)

Transformed back it yields

$$f(t) = \frac{e^{-\Gamma t/2}}{2\Omega} [2\Omega \cosh(t\Omega) - \Gamma \sinh(t\Omega)], \qquad (18)$$

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 Eq. (12)

$$I(t) = \frac{\Gamma T}{2} \int_0^t d\tau f(\tau) \frac{\sin(V\tau)}{\sinh(\pi T\tau)}.$$
 (19)

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

$$I_{\text{stat}} = \frac{\Gamma}{4\pi\Omega} \text{Im} \sum_{p=\pm} (\Omega + p\Gamma/2) \Psi\left(\frac{1}{2} + \frac{iV + p\Omega + \Gamma/2}{2\pi T}\right),$$
(20)

where Ψ denotes the digamma function. The transient part is given by

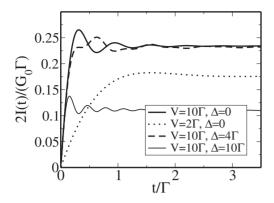


FIG. 1. Full current through the constriction at zero temperature for different voltages V and dot offset energies Δ . The current is measured in units of $G_0\Gamma/2$ where $G_0=2e^2/h$ is the conductance quantum.

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

$$\times_{2} \mathbf{F}_{1} \left(1, \frac{1}{2} - \frac{iV + p\Omega - \Gamma/2}{2\pi T}; \frac{3}{2} - \frac{iV + p\Omega - \Gamma/2}{2\pi T}; e^{-2\pi Tt}\right), \tag{21}$$

where ${}_2{\bf F}_1$ 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 Ω 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, see 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 $D_{ab}^<(t,t')=-i\langle a(t)b(t')\rangle$. The calculation of this GF is accomplished using the Dyson equation in the time domain (multiplication corresponds to time integrations): $D_{ab}=D_{ab}^{(0)}+D_{ab}^{(0)}\Sigma D_{bb}$ where the self-energy is proportional to the unperturbed GF for the ξ Majoranas $\Sigma=\Gamma g_{\xi\xi}$. After the Keldysh disentanglement we obtain

$$D_{ab}^{<} = D_{ab}^{(0)<} + D_{ab}^{(0)R} \Sigma^{R} D_{bb}^{<} + D_{ab}^{(0)R} \Sigma^{<} D_{bb}^{A} + D_{ab}^{(0)<} \Sigma^{A} D_{bb}^{A}. \tag{22} \label{eq:22}$$

Thus the calculation of the inhomogeneous D_{ab} GF is now reduced to the calculation of the homogeneous D_{bb} . The necessary zero-order GFs are

$$D_{ab}^{(0)<}(t) = -(\kappa/2)e^{i\kappa\Delta t}, \quad D_{ab}^{(0)R}(t) = -i\Theta(t)\sin(\Delta t),$$

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

$$D_{bb}^{R} = D_{bb}^{(0)R} + D_{bb}^{(0)R} \Sigma^{R} D_{bb}^{R}.$$

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

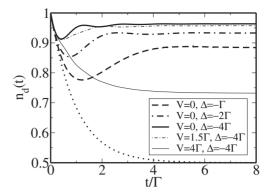


FIG. 2. Population of the dot at zero temperature for different voltages V and dot offset energies Δ . The dotted line corresponds to the resonant case $\Delta=0$.

$$n_d(t) = (1 + \kappa e^{-\Gamma t})/2.$$
 (23)

This is a very remarkable result since the relaxation of the dot occupation/magnetization is independent of both temperature and applied voltage and is only governed by the time scale $1/\Gamma$.

In the off-resonant case the calculations are more complex since we need the full homogeneous $D_{hb}^{<}$. It is given by 25

$$D_{bb}^{<} = (1 + D_{bb}^{R} \Sigma^{R}) D_{bb}^{(0) <} (1 + \Sigma^{A} D_{bb}^{A}) + D_{bb}^{R} \Sigma^{<} D_{bb}^{A}.$$

Putting the result into Eq. (22) we obtain for weak detuning

$$\begin{split} n_d(t) &= \frac{1}{2} (1 + \kappa e^{-\Gamma t}) - \frac{\Gamma \Delta}{2\Omega^2} \int \frac{d\omega}{2\pi} \frac{4\Omega n_L}{(\Delta^2 - \omega^2)^2 + \omega^2 \Gamma^2} \\ &\quad \times \{\Omega \omega (1 + e^{-\Gamma t}) - e^{-\Gamma t/2} [(\omega^2 + \Delta^2) \sinh(\Omega t) \sin(\omega t) \\ &\quad + 2\omega \Omega \cosh(\Omega t) \cos(\omega t)] \}. \end{split}$$

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 of 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 Δ vanishes toward 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 [Eq. (23)] 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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