EUROPHYSICS LETTERS 1 June 2005

Europhys. Lett., **70** (5), pp. 642–648 (2005)
DOI: 10.1209/epl/i2004-10515-8

Study of a fluctuation-dissipation relation of a dissipative driven mesoscopic system

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received 13 October 2004; accepted in final form 8 April 2005
published online 27 April 2005

PACS. 72.10.-d – Theory of electronic transport; scattering mechanisms.
PACS. 73.23.-b – Electronic transport in mesoscopic systems.

Abstract. – We study the nonequilibrium dynamics of a mesoscopic metallic ring threaded by a time-dependent magnetic field and coupled to an electronic reservoir. We analyze the relation between the (nonstationary) real-time Keldysh and retarded Green functions and we argue that, in the linear-response regime with weak heat transfer to the environment, an effective temperature accounts for the modification of the equilibrium fluctuation-dissipation relation. We discuss possible extensions of this analysis.

Recent technical developments in nanoscience have renewed the interest in quantum transport in mesoscopic systems [1]. Heat transfer in these devices is a crucial issue which remains poorly understood.

A recent theoretical result in the field of glassy dynamics is that an "effective temperature", T_{eff}, controls the low-frequency linear response in the limit of small entropy production (long waiting time, weak drive) [2, 3]. T_{eff} is defined as the parameter replacing the environmental temperature, T, in the fluctuation-dissipation relation (FDR) evaluated at low frequencies [4–6]. This is not an arbitrary name given to a fitting parameter, since T_{eff} has the properties of a temperature in the sense that it can be measured with a thermometer, controls heat flows and partial equilibration, etc. [2, 3]. A similar phenomenon was found in the relaxation of quantum spin-glasses [7] and the Coulomb glass [8].

The question then arises as to whether the notion of T_{eff} plays a role in understanding some features of transport in quantum mesoscopic systems. To address it, we study the modification of the FDR in a very simple, exactly solvable, mesoscopic device that consists in a metallic ring connected by a lead to an external particle and thermal reservoir and driven out of equilibrium by a threading time-dependent magnetic field [9–13]. In this setting there is an electronic dc current along the wire and a heat flow towards the environment.

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We model the metallic wire with a system of noninteracting spin-less electrons described by a one-dimensional periodic tight-binding chain with length $L = Na$ (N is the number of sites and a the lattice spacing), hopping matrix element $w = W/4$ and bandwidth W:

$$H^{ring} = -w \sum_{i=1}^{N} \left(e^{-i\phi t} c_i^\dagger c_{i+1} + e^{i\phi t} c_{i+1}^\dagger c_i \right). \tag{1}$$

The time-dependent phase ϕt with $\phi \equiv \Phi/(\Phi_0 N)$ and $\Phi_0 = hc/e$ accounts for the external magnetic flux that we choose to depend linearly in time, $\Phi_M(t) = \Phi t$. The contact term between the lead and the ring is $H^c = -w_{1\alpha}(c_1^\dagger c_\alpha + c_\alpha^\dagger c_1)$. We model the lead and reservoir with a semi-infinite tight-binding chain with hopping amplitude $w_\alpha = W_\alpha/4$, bandwidth W_α, and spectral density $\rho_\alpha(\omega) = 4\sqrt{1-\omega^2/W_\alpha^2}\ \theta(W_\alpha - |\omega|)$. We assume that the reservoir is in equilibrium at temperature T and chemical potential μ and that its properties are not affected by the coupling to the small ring. The Hamiltonian of the full system is then $H = H^{ring} + H^c + H^\alpha$ [12]. We use a system of units such that $\hbar = k_B = \Phi_0 = 1$. All our results were obtained using a ring with $N = 20$ and $W = 1$, and a reservoir with $\mu = -1$ and $W_\alpha = 4$.

The dynamics of this problem is amenable to an exact treatment within the real-time nonequilibrium formalism. The retarded and Keldysh Green functions are

$$G_{ij}^R(t,t') \equiv -i\theta(t-t')\langle \left[c_i(t), c_j^\dagger(t')\right]_+ \rangle, \qquad G_{ij}^K(t,t') \equiv -i\langle \left[c_i(t), c_j^\dagger(t')\right]_- \rangle. \tag{2}$$

The angular brackets indicate an average in the grand-canonical ensemble, *i.e.* using $H - \mu\mathcal{N}$ in the statistical weight with $\mathcal{N} \equiv \sum_{i=1}^N c_i^\dagger c_i$. The exact evolution equations read [14]

$$\begin{aligned} -i\frac{\partial}{\partial t'} G_{ij}^R(t,t') - G_{ik}^R(t,t') w_{kj}(t') - \int \mathrm{d}t_1 G_{ik}^R(t,t_1)\Sigma_{kj}^R(t_1,t') &= \delta_{ij}\delta(t-t'), \\ -i\frac{\partial}{\partial t'} G_{ij}^K(t,t') - G_{ik}^K(t,t') w_{kj}(t') &= \int \mathrm{d}t_1 \left[G_{ik}^R(t,t_1)\Sigma_{kj}^K(t_1,t') + G_{ik}^K(t,t_1)\Sigma_{kj}^R(t_1,t') \right], \end{aligned} \tag{3}$$

with $w_{kj}(t') \equiv w\left(e^{i\phi t'}\delta_{k,j+1} + e^{-i\phi t'}\delta_{k,j-1}\right)$ and the summation rule for repeated indices.

We call $g_\alpha^{R,K}$ the Green functions of the bath,

$$g_\alpha^R(\tau) = -i\theta(\tau)\int \frac{\mathrm{d}\omega}{2\pi}\ \rho_\alpha^{gc}(\omega)\, e^{-i\omega\tau}, \qquad g_\alpha^K(\tau) = -i\int \frac{\mathrm{d}\omega}{2\pi}\ \tanh(\beta\omega/2)\ \rho_\alpha^{gc}(\omega)\, e^{-i\omega\tau}, \tag{4}$$

$\tau \equiv t - t'$, $\beta = 1/T$ and $\rho_\alpha^{gc}(\omega) = \rho_\alpha(\omega + \mu)$. These functions are stationary since the bath is assumed to be in equilibrium. The effect of the lead and reservoir is then captured by a correction at the contact site $i = 1$ [15]:

$$\Sigma_{kj}^{R,K}(t,t') = |w_{1\alpha}|^2 g_\alpha^{R,K}(t-t')\ \delta_{k1}\delta_{j1}\,. \tag{5}$$

If one assumes that the magnetic field and coupling to the reservoir had been switched on in the far past in such a way that any transient behaviour depending on the initial conditions died out at the working times (t,t'), eq. (3) reduces to

$$G_{ij}^K(t,t') = \int \mathrm{d}t_1 \mathrm{d}t_2\ G_{ik}^R(t,t_1)\Sigma_{kl}^K(t_1,t_2)G_{lj}^A(t_2,t'), \tag{6}$$

that yields G_{ij}^K once G_{ij}^R has been computed from eq. (3) [12]. $G_{lj}^A(t_2,t') = [G_{lj}^R(t_2,t')]^*$ is the advanced Green function. We then used a numerical algorithm to solve the exact dynamic equations (3)-(6) that are complex enough not to allow for a complete analytic solution.

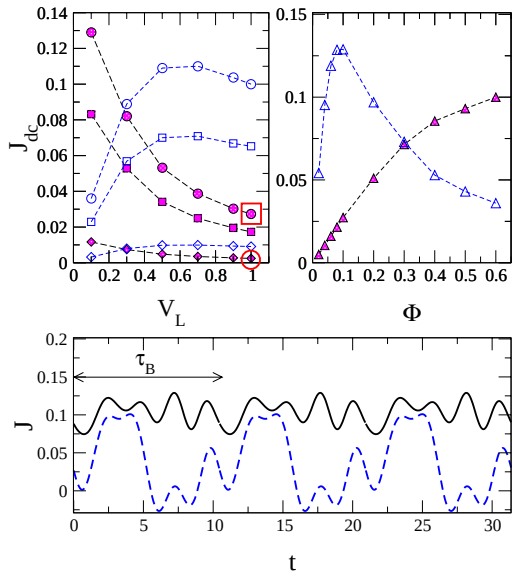

Fig. 1 – (Color online) Dependence of the current on time and various parameters. Upper-left panel: the dc current J_{dc} against the coupling to the lead V_L for $\Phi = 0.6$ (open blue symbols) and $\Phi = 0.1$ (filled magenta symbols). Different symbols correspond to $T = 0.05$ (circles), $T = 1$ (squares) and $T = 10$ (diamonds). The large circle and square indicate the values of J_{dc} that correspond to the data shown in figs. 2, 3 and 4. Upper-right panel: J_{dc} against Φ for $T = 0.05$. Open symbols with dashed blue line and solid symbols with dashed black line correspond to $V_L = 0.1$ and $V_L = 1$, respectively. Lower panel: $J_{12}(t)$ for $\Phi = 0.6$, $T = 0.05$, $V_L = 0.9$ (solid black line) and $V_L = 0.1$ (dashed blue line). The period $\tau_B \approx 10$ is indicated with an arrow.

In equilibrium a model-independent fluctuation-dissipation relation (FDR) between the retarded and Keldysh Green functions holds. Calling $G^{R,K}_{ij}(t,\omega)$ the Fourier transform with respect to τ, the FDR reads

$$G^K_{ij}(t,\omega) = \tanh(\beta\omega/2)\left(G^R_{ij}(t,\omega) - G^A_{ij}(t,\omega)\right), \tag{7}$$

where, for later convenience, we kept explicit a dependence on the observation time t that does not exist in equilibrium. Out of equilibrium, there is no reason why such a relation should hold, and the temperature and chemical potential of the system are not even defined. Our aim is to determine how should one modify (7) to account for the Green functions of the ring.

First, let us discuss the values of T, Φ and $V_L = |w_{1\alpha}|^2$ for which we may expect a simple generalization of the FDR. To this end we summarize the dependence of the current on time and these parameters in fig. 1 [12,13]. In the lower panel we show the time dependence of the current $J_{l,l+1}(t) \equiv 2ei\,\mathrm{Re}[we^{-i\phi t}\langle c^\dagger_l(t)c_{l+1}(t)\rangle]$ for $l = 1$, $\Phi = 0.6$, $T = 0.05$ and two values of the coupling to the lead, $V_L = 0.9$ (solid black line) and $V_L = 0.1$ (dashed, blue online, line). The current has the period $\tau_B = 2\pi/\Phi$ of Bloch oscillations. Their amplitude is diminished for large enough T and V_L and for small enough Φ as well as for very large $\Phi(> W)$.

Dissipation gives rise to a dc-component in the current, $J_{dc} = \tau_B^{-1}\int_0^{\tau_B} \mathrm{d}t\; J_{l,l+1}(t)$, that is related to the power at which energy is dissipated in the form of heat through $P = J_{dc}\Phi$ as has been verified exactly [13]. In the upper-left panel in fig. 1 we show the dependence of J_{dc} on the strength of the coupling to the reservoir, V_L, for several values of the electromotive

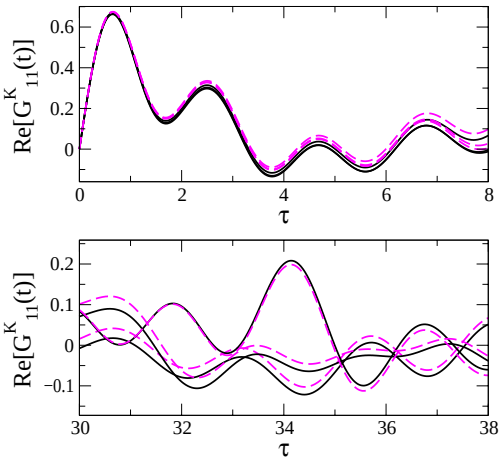

Fig. 2 – (Color online) Breakdown of stationarity and the FDR. Real part of $G^K_{11}(t, t-\tau)$ (solid black lines) and the inverse Fourier transform of the rhs of eq. (7) (dashed magenta lines) as a function of τ for three total times t equally spaced in the interval $[0, \tau_B]$. $V_L = 1$, $\Phi = 0.1$, $T = 0.05$ and $J_{dc} \approx 0.03$ (red square in fig. 1).

force (emf), Φ, and temperature. At fixed temperature J_{dc} is a nonmonotonic function of V_L with the boundary values $J_{dc}(0) = J_{dc}(\infty) = 0$ and $J_{dc} \propto V_L$ when $V_L \to 0$ [12,16]. For rather large values of the bias ($\Phi = 0.6$ open symbols), the maximum occurs at $V_L \approx 0.5$. For small values of the emf ($\Phi = 0.1$ filled symbols), the first increasing part of the curve is squeezed towards very low values of V_L and only the second decreasing regime is visible. For fixed Φ, the higher T the lower J_{dc}, as can be checked by comparing the curves with different symbols.

The upper-right panel in fig. 1 shows that J_{dc} is in approximate linear relation with Φ for small biases; deviations appear at a value Φ_m that increases with V_L, *e.g.* $\Phi_m \approx 0.075$ for $V_L = 0.1$ and $\Phi_m \approx 0.2$ for $V_L = 1$.

We now turn to the detailed study of the Green functions that we parametrize as $G^{R,K}_{ij}(t, t-\tau)$. In fig. 2 we illustrate the nontrivial dependence on t and $\tau \equiv t - t'$ by tracing, with solid black lines, $\mathrm{Re}\, G^K_{ij}$ for three values of the total time t equally spaced within τ_B. The two panels show the evolution on the intervals $0 \le \tau \le 8$ (upper) and $30 \le \tau \le 38$ (lower) [17]. Interestingly enough, all curves fall on top of each other for $\tau \le \tau^*(\Phi, \beta, V_L) \approx 1.5$, and they later deviate demonstrating the breakdown of stationarity. This trend can be understood by noting that $G^R_{ij}(t, \omega)$ contains a time-dependent structure within the spectral range of the free ring, *i.e.* in the interval $|\omega + \mu| \le W/2$, while the high-frequency part is dominated by the *stationary* spectral features of the reservoir which set the quick response in the time domain.

Figure 2 also shows a qualitative study of the FDR. The dashed lines are the inverse Fourier transform of the rhs of eq. (7) for the same values of t. The companion curves do not match and the FDR does not hold. We note, however, that for $\tau \le \tau^* \approx 1.5$ the behaviour is not only stationary but the FDR holds as well.

As fig. 2 demonstrates, the total time dependence is very complicated. Instead of studying the modification of the FDR for each value of t we found it natural to work with the averaged Green functions:

$$\langle G^{K,R}_{ij} \rangle(\tau) \equiv \frac{1}{\tau_B} \int_0^{\tau_B} \mathrm{d}t\, G^{K,R}_{ij}(t, \tau). \tag{8}$$

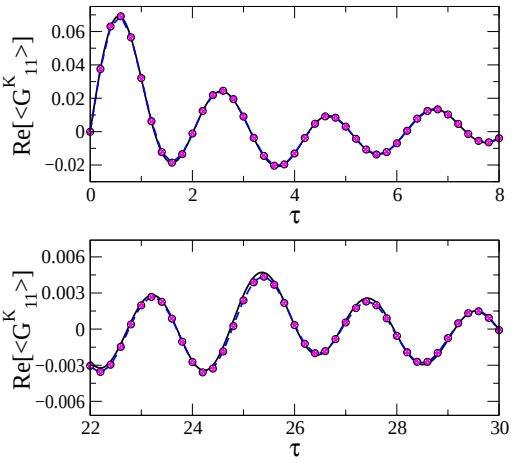

Fig. 3 – (Color online) Study of the FDR in the "classical" regime. Real part of $\langle G^K_{11}\rangle(\tau)$ (dashed blue line) and the inverse Fourier transform of the rhs of eq. (7) (solid black line) averaged over a period τ_B, see eq. (8), as a function of τ. The two curves are almost identical, apart from little deviations seen, *e.g.*, at $\tau \approx 25.5$. The symbols are obtained using the same functional form in the rhs of eq. (7) with T replaced by $T_{eff} = 10.02 \approx T = 10$. $V_L = 1$, $\Phi = 0.1$, $J_{dc} \approx 0.002$ (red circle in fig. 1).

In fig. 3 we show a quantitative test of the FDR in a "classical" regime (loosely) identified as the values of the environmental temperature T such that the classical limit of the FDR, $g^K_\alpha(\tau) = -i/(2T)\partial_\tau g^R_\alpha(\tau)$, $\tau \geq 0$, holds for the bath. We compare the left- and right-hand sides of the inverse Fourier transform of eq. (7) averaged over t as defined in eq. (8). In both intervals shown the accord between the two curves is rather good, proving that the FDR approximately holds when the driving force is weak and the temperature of the environment is high in such a way that P is extremely low.

In fig. 4 we test the FDR in the "quantum" regime, $T = 0.05$. The symbols represent a fit using the functional form in the rhs of eq. (7) with T replaced by $T_{eff} = 0.143$. For short time differences, say before the first minimum in the upper panel, the FDR holds —and the fit also falls on top of the original curves. Indeed, if $\beta_{eff}\omega \gg 1$, $\tanh(\beta_{eff}\omega/2) \approx 1$ and the Keldysh and retarded Green functions are in linear relation. For longer time differences the deviations are clear but the fit accounts well for the data.

Within the accuracy of our numerical solution, the effective temperature describes rather correctly the modification of the FDR whenever the dc current is in linear relation with the emf Φ (see fig. 1). Out of the linear-response regime, one cannot match the two sides of eq. (7) by simply using a single-valued T_{eff}. This limitation parallels the one observed in classical *strongly driven* glassy systems [5,6]. This is reasonable since the notion of an effective temperature was proposed to apply to a regime of small entropy production only [2, 3] and this, in our case, corresponds to low $P = J_{dc}\Phi$ values.

In all cases $T_{eff} > T$, as also found in glassy systems relaxing from a disordered initial configuration and in driven classical systems [4]. A heuristic argumement that explains this result is the following. The equations that govern the dynamics of the Hamiltonian H are the same as those of an effective Hamiltonian where the electrons are coupled to modes with energy quanta Φ [13]. It is natural to expect that such a coupling enables a mechanism for the electrons to spread out in energy, which can be interpreted as an effective increment of

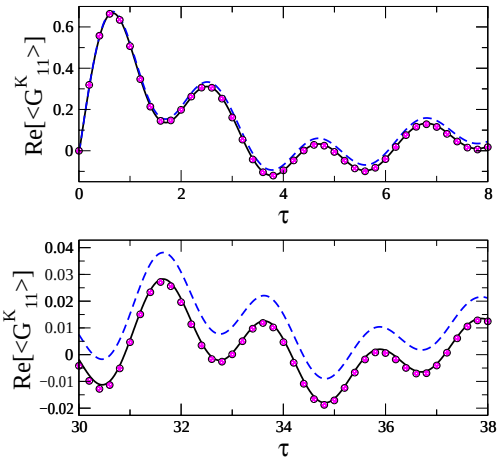

Fig. 4 – (Color online) FDR in the "quantum" regime, $T = 0.05$. $\mathrm{Re}\langle G^K_{11}\rangle$ (dashed blue line) and inverse Fourier transform of the rhs of eq. (7) (solid black line) averaged over a period τ_B against τ. The symbols correspond to the latter functional form with a fitting parameter $T_{eff} = 0.143$. $\Phi = 0.1$, $V_L = 1$ and $J_{dc} \approx 0.03$ (red square in fig. 1).

the electronic temperature. More quantitatively, we found that T_{eff} increases with the power dissipated, $P = J_{dc}\Phi$. Some rough estimates are shown in table I.

In conclusion, we managed to find a simple modification of the equilibrium FDR that holds in the limit of weak dissipation. The modification amounts to simply replacing the environmental temperature by a new *single* parameter T_{eff}. Remarkably enough, it describes the data *for all times explored*. We did not need to use a μ_{eff} since μ basically controls the period of the oscillations of the inverse Fourier transform of the rhs of eq. (7) that coincides with the period of $\mathrm{Re}\langle G^K_{11}\rangle(\tau)$, see figs. 3 and 4. In other nonequilibrium settings an upgrading of μ to μ_{eff} might be necessary.

Let us discuss some open questions. It remains to study whether we can associate T_{eff} to a *bona fide* temperature [2,3] for *nonequilibrium quantum systems with fermionic statistics*. We defined T_{eff} via the Green functions that are not, however, directly accessible experimentally. A similar description should apply to the current fluctuations [6] that can be measured in noise experiments [18]. Our problem bears some resemblance with a *classical ratchet* for which a

Table I – *Estimates of the effective temperature and dissipated power in the linear-response regime.*

V_L	Φ	T	T_{eff}	$(T_{eff} - T)/T$	$P(\times 10^{-3})$
1	0.1	0.05	0.143	1.84	2.7
1	0.1	0.1	0.167	0.67	2.6
1	0.1	0.2	0.264	0.32	2.5
1	0.1	1	1.052	0.052	1.7
1	0.1	10	10.02	0.002	0.3
0.1	0.06	0.05	0.769	14.38	7.1
0.1	0.06	0.1	0.8	7	7.0
0.1	0.06	0.2	0.833	3.16	6.9
0.1	0.06	1	1.43	0.43	4.6

T_{eff} could be defined in the strongly driven limit for long-wavelength observables [19]. It would be interesting to check whether this holds for quantum mesoscopic devices as well. Even if we have not found a site-dependent T_{eff} for weak forcings we cannot exclude such a dependence in a more general setting. Finally, it would be interesting to check the modifications of the FDR using different time-dependent magnetic fields, including disorder in the hopping rates, considering different dissipative mechanisms, etc.

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We thank SISSA, MPIPKS-Dresden and A. von Humboldt Stiftung (LA), ICTP and UBA (LFC) for hospitality. We acknowledge financial support from Ecos-Sud and ACI grants (LFC), CONICET and PICT 03-11609 (LA). We thank C. Chamon, B. Doucot, J. Kurchan, G. Lozano and Prof. Fulde for very helpful discussions.

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