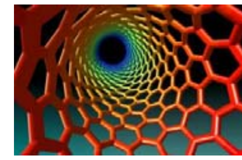
Inter-well and intra-well dynamics in a driven dissipative multilevel system

Francesco Nesi and Milena Grifoni

Institut für Theoretische Physik – Quanten Transport und Dissipation
Universität Regensburg
Universitätsstraße 31, D – 93053 Regensburg

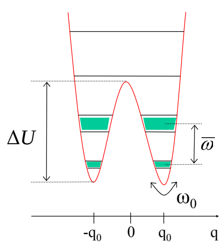


ABSTRACT

We investigate tunneling and vibrational relaxation in a driven dissipative double-well potential. We truncate the system's Hilbert space to the space spanned by the *M* lowest lying unperturbed eigenstates. A path-integral formalism is used to obtain an exact series expression for the reduced density matrix (RDM) of the system in the *discrete variable representation* (DVR) [1], being the basis in which the position operator is diagonal. By exploiting a separation of time scales between intra-well and inter-well tunneling dynamics, we wish to derive a set of coupled non-Markovian master equations for the RDM valid for low as well as high temperatures, and being *non-perturbative* in the dissipation strength.

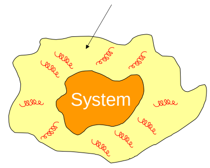
[1] M. Thorwart, M. Grifoni and P. Hänggi, Phys. Rev. Lett. **85**, 860 (2000).

1. Description of the system



$$V(q) = \frac{M^2\omega_0^4}{64\Delta U} q^4 - \frac{M\omega_0^2}{4} q^2$$

Reservoir composed of harmonic oscillators



$$H_{tot} = H_S + H_{S-Bath} + H_{Bath}$$

$$H_S|m\rangle = \mathcal{E}_m|m\rangle$$

$$H_{S-B} = q\zeta$$ stochastic force from the bath

$$\langle\zeta(t)\rangle_B = 0$$

spectral density of the bath

$$\langle\zeta(t)\zeta(0)\rangle_B = \frac{(2q_0)^2}{\hbar\pi}\int_0^\infty d\omega\, J(\omega)\left[\coth(\hbar\omega\beta/2)\ \cos(\omega t) - \mathbf{i}\sin(\omega t)\right]$$

2. Target

probability to find the system at time *t* in the right well — $P_R(t) = ?$

$$P_R(t_0) = 1$$

reduced density matrix — total density matrix

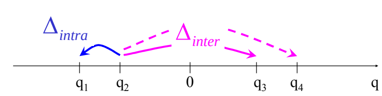
$$\rho(t) \equiv \mathrm{Tr}_B\{W_{tot}\}$$

3. DVR-basis

$$|u_m\rangle \equiv \sum_{m'=1}^{M} R_{mm'}|m'\rangle \qquad \langle u_m|\mathbf{q}|u'_m\rangle = q_m^{DVR}\delta_{mm'}$$

$$H_S = H_S(\Delta_{q_iq_j}) = H_S(\Delta_{inter}, \Delta_{intra})$$

Example: M=4



$$P_R(t) = \sum_{i=M/2+1}^{M} \rho_{ii}(t)$$

Feynman-Vernon influence functional

$$\rho_{\sigma_f\sigma_i}(t) = \int_{\sigma(t_0)=\sigma_i}^{\sigma(t)=\sigma_f} d\sigma\ A[\sigma] \int_{\sigma'(t_0)=\sigma_i}^{\sigma'(t)=\sigma_f} d\sigma'\, A^*[\sigma']\, F_{FV}[\sigma,\sigma']$$

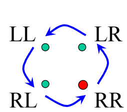
Master Equation

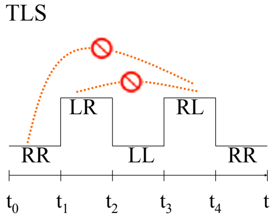
$$\dot\rho_{ii}(t) = \sum_j \int_{t_0}^{t} dt' K_{ij}(t,t')\rho_{jj}(t')$$

EXACT, but still too complex!

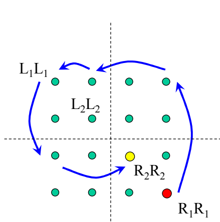
4. Approximation I

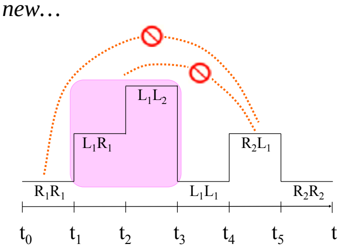
NIBA[1] (M=2), *standard* TLS





NICA[2] (M>2), what is *new*…





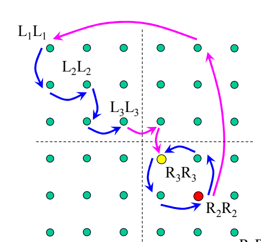
[1] A. O. Caldeira and A. J. Leggett, Phys. Rev. Lett. **46**, 211 (1981); Ann. Phys. (N.Y.) **149**, 374 (1983).

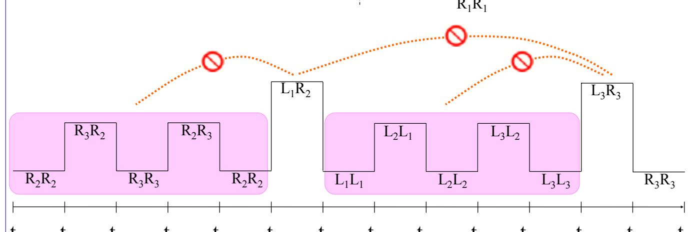
[2] R. Egger, C. H. Mak and U. Weiss, Phys. Rev. E **50**, R655 (1994); M. Thorwart, M. Grifoni and P. Hänggi, Phys. Rev. Lett. **85**, 860 (2000).

5. Approximation II

my work…

(M>2), *different* scales of time





Outlook

Application to *leakage* problem
($k_BT < \hbar\varpi$, M = 4)

francesco.nesi@physik.uni-regensburg.de   +49 941 943 2039