Program on
« QUANTUM DYNAMICS OUT OF EQUILIBRIUM »
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Pierre GASPARD

Center for Nonlinear Phenomena and Complex Systems,

Université Libre de Bruxelles,

Brussels, Belgium

1) **SEMICLASSICS AND PERIODIC-ORBIT QUANTIZATION OF CHAOTIC SCATTERING**

2) **SLOWING DOWN OF QUANTUM DECAYS IN CLASSICALLY CHAOTIC SCATTERING**

3) **DECAY OF QUANTUM STATISTICAL MIXTURES IN CLASSICALLY CHAOTIC SCATTERING**

4) **NONEQUILIBRIUM TRANSIENTS AND TRANSPORT IN LARGE QUANTUM SYSTEMS**

NONEQUILIBRIUM TRANSIENTS AND TRANSPORT IN LARGE QUANTUM SYSTEMS

Pierre GASPARD
Brussels, Belgium

M. Nagaoka, *Japan*
M. Esposito, *Brussels & San Diego USA*

- **REDUCED DESCRIPTION & MASTER EQUATION**

- **LIOUVILLIAN RESONANCES**

- **STOCHASTIC SCHRÖDINGER EQUATION**

REDUCED DESCRIPTION IN MANY-BODY SYSTEMS

quantum subsystem coupled to a heat reservoir:
description in terms of a reduced density matrix $\hat{\rho}_s(t)$ obeying some master equation.

Ex: spin-boson model in the weak-limit coupling: Bloch-Redfield equations

density matrix $$\hat{\rho} = \sum_j \left|\psi_j\right\rangle P_j \left\langle\psi_j\right|$$

Landau-von Neumann eq. $$\partial_t \hat{\rho} = \frac{1}{\mathrm{i}\hbar}[\hat{H}, \hat{\rho}] \equiv \hat{\hat{L}}\, \hat{\rho} \qquad \hat{\rho}_t = \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar} \hat{\rho}_0\, \mathrm{e}^{+\mathrm{i}\hat{H}t/\hbar}$$

observable of the subsystem: $$\hat{A} = \hat{A}_s \otimes \hat{I}_b$$

statistical average: $$\left\langle \hat{A}(t) \right\rangle = \mathrm{tr}_s\, \hat{A}_s\, \mathrm{tr}_b\, \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar} \hat{\rho}_0\, \mathrm{e}^{+\mathrm{i}\hat{H}t/\hbar} = \mathrm{tr}_s\, \hat{A}_s\, \hat{\rho}_s(t)$$

coarse-graining by tracing out the bath degrees of freedom

QUANTUM SUBSYSTEM
WEAKLY COUPLED TO AN ENVIRONMENT

Ex: spin-boson model in the weak-limit coupling

Hamiltonian $\hat{H}_{\text{tot}} = \hat{H}_s + \hat{H}_b + \lambda \hat{V}$ $\qquad \hat{V} = \sum_\alpha \hat{S}_\alpha \hat{B}_\alpha$

Landau-von Neumann eq. $\partial_t \hat{\rho} = \frac{1}{\mathrm{i}\hbar}[\hat{H}_{\text{tot}}, \hat{\rho}] \equiv \hat{\hat{L}}\,\hat{\rho}$

initial density matrix:

$$\hat{\rho}(0) = \hat{\rho}_s(0) \otimes \frac{\mathrm{e}^{-\beta \hat{H}_b}}{Z_b}$$

perturbative expansion:

$$\hat{\rho}_I(t) = \hat{\rho}(0) + \int_0^t dt_1 \hat{\hat{L}}_I(t_1)\hat{\rho}(0) + \int_0^t dt_1 \int_0^{t_1} dt_2 \hat{\hat{L}}_I(t_1)\hat{\hat{L}}_I(t_2)\hat{\rho}(0) + O(\lambda^3)$$

tracing out the bath degrees of freedom

$$\hat{\rho}_s(t) = \mathrm{e}^{\hat{\hat{L}}_s t}\hat{\rho}_s(0) + \int_0^t dT \int_0^T d\tau \left\langle \hat{\hat{L}}_I(0)\hat{\hat{L}}_I(-\tau) \right\rangle_b \mathrm{e}^{\hat{\hat{L}}_s T}\hat{\rho}_s(0) + O(\lambda^3)$$

$$\frac{d\hat{\rho}_s(t)}{dt} = \left[\hat{\hat{L}}_s + \int_0^t d\tau \left\langle \hat{\hat{L}}_I \mathrm{e}^{\hat{\hat{L}}_0 \tau} \hat{\hat{L}}_I \mathrm{e}^{-\hat{\hat{L}}_0 \tau} \right\rangle_b + O(\lambda^3) \right] \hat{\rho}_s(t)$$

Redfield master equation: Markovian approximation $t >> t_b$

$$\frac{d\hat{\rho}_s^R(t)}{dt} = \left[\hat{\hat{L}}_s + \int_0^\infty d\tau \left\langle \hat{\hat{L}}_I \mathrm{e}^{\hat{\hat{L}}_0 \tau} \hat{\hat{L}}_I \mathrm{e}^{-\hat{\hat{L}}_0 \tau} \right\rangle_b + O(\lambda^3) \right] \hat{\rho}_s^R(t)$$

SLIPPAGE OF INITIAL CONDITIONS

autocorrelation function of bath coupling operators:

$$C(t) = \left\langle \hat{B}(t)\hat{B}(0) \right\rangle_b \qquad \text{(a)}$$

non-Markovian evolution:

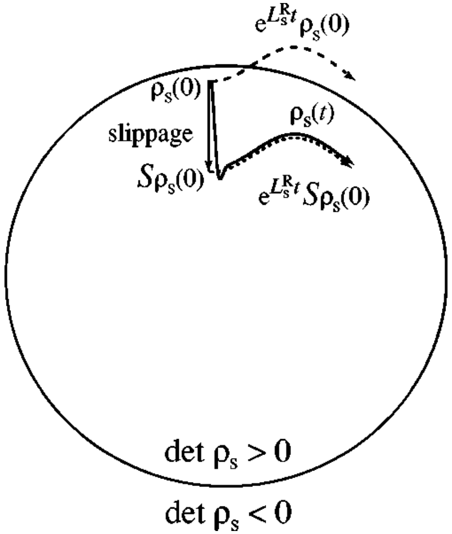
$$\hat{\rho}_s(t) = \mathrm{e}^{\hat{\hat{L}}_s t}\hat{\rho}_s(0) + \int_0^t dT \int_0^T d\tau \left\langle \hat{\hat{L}}_I(0)\hat{\hat{L}}_I(-\tau) \right\rangle_b \mathrm{e}^{\hat{\hat{L}}_s T}\hat{\rho}_s(0) + O(\lambda^3) \qquad \text{(b)}$$

Markovian evolution:

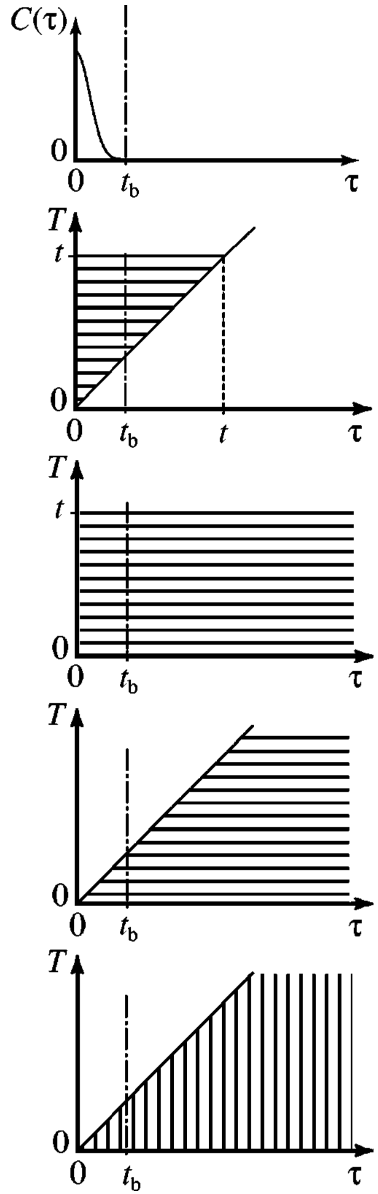
$$\hat{\rho}_s^R(t) = \mathrm{e}^{\hat{\hat{L}}_s t}\hat{\rho}_s(0) + \int_0^t dT \int_0^\infty d\tau \left\langle \hat{\hat{L}}_I(0)\hat{\hat{L}}_I(-\tau) \right\rangle_b \mathrm{e}^{\hat{\hat{L}}_s T}\hat{\rho}_s(0) + O(\lambda^3) \qquad \text{(c)}$$

slippage of initial conditions:

$$\hat{\rho}_s(t) \approx \mathrm{e}^{\hat{\hat{L}}_s^R t}\hat{\hat{S}}\hat{\rho}_s(0)$$



(a) (b) (c) (d) (e)



SPIN-BOSON MODEL

Hamiltonian $\hat{H}_{\text{tot}} = -\frac{\Delta}{2}\hat{\sigma}_z + \hat{H}_b + \lambda\hat{\sigma}_x\hat{B}$ $\qquad \hat{H}_b = \frac{1}{2}\sum_\alpha\left(\hat{p}_\alpha^2 + \omega_\alpha^2\hat{q}_\alpha^2\right)$ $\qquad \hat{B} = \sum_\alpha c_\alpha\hat{q}_\alpha$

spectral strength $J(\omega) = \sum_\alpha \frac{c_\alpha^2}{2\omega_\alpha}\delta(\omega - \omega_\alpha) = K\omega^s \exp(-\omega/\omega_c)$

autocorrelation function: $C(t) = \left\langle \hat{B}(t)\hat{B}(0)\right\rangle_b = \int_0^\infty d\omega J(\omega)\left(\coth\frac{\beta\hbar\omega}{2}\cos\omega t - i\sin\omega t\right)$

Bloch-Redfield Markovian master equation:

$$\begin{cases} x = \langle\hat{\sigma}_x\rangle \\ y = \langle\hat{\sigma}_y\rangle \\ z = \langle\hat{\sigma}_z\rangle \end{cases} \qquad \begin{cases} \dot{x} = \Delta y \\ \dot{y} = -(\Delta + h)x - gy \\ \dot{z} = -f - gz \end{cases}$$

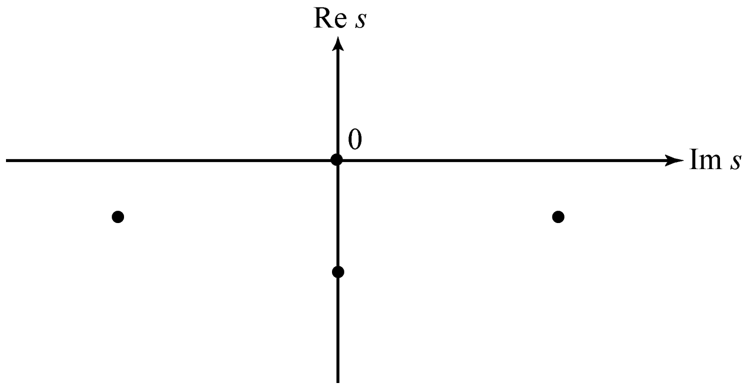
$$\begin{cases} f = 4\lambda^2\int_0^\infty \sin\Delta t \ \operatorname{Im}C(t)\ dt \\ g = 4\lambda^2\int_0^\infty \cos\Delta t \ \operatorname{Re}C(t)\ dt \\ h = 4\lambda^2\int_0^\infty \sin\Delta t \ \operatorname{Re}C(t)\ dt \end{cases}$$

Liouvillian resonances:

$s = 0$ invariant equilibrium state

$s = -g$ population relaxation

$s = -\frac{g}{2} \pm i\left(\Delta + \frac{h}{2}\right)$ decoherence



QUANTUM MODEL OF DIFFUSION

Hamiltonian: tight-binding electronic Hamiltonian coupled to a bath of bosons

Ohmic spectral strength $$J(\omega) = \sum_\alpha \frac{c_\alpha^2}{2\omega_\alpha}\delta(\omega - \omega_\alpha) = K\omega \exp(-\omega/\omega_c)$$

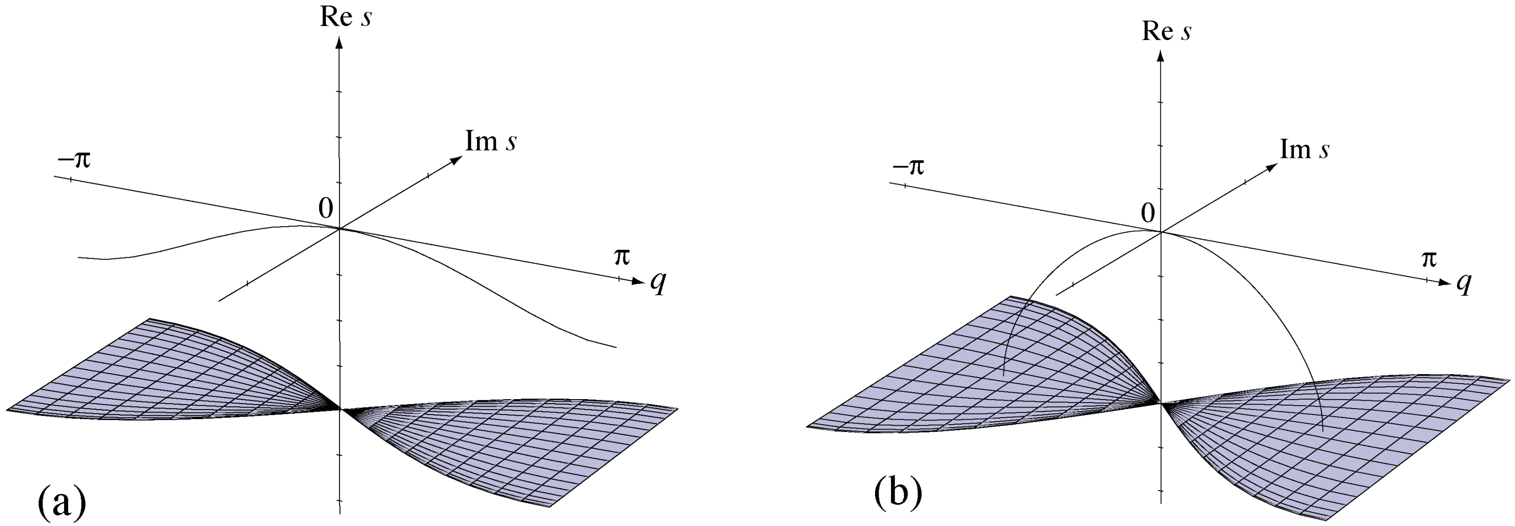
autocorrelation function: $$C(t) = \left\langle \hat{B}(t)\hat{B}(0)\right\rangle_b = Q\delta(t)$$

tunneling amplitude of electrons: A

Liouvillian resonances: diffusive branch:

$$s = -2Q\lambda^2 + 2\sqrt{Q^2\lambda^4 - (2A\sin q/2)^2} = -Dq^2 + O(q^4)$$

diffusive coefficient: $$D = \frac{A^2}{Q\lambda^2} = \frac{A^2}{\pi K\lambda^2 k_B T}$$ conductivity: $$\sigma = \frac{e^2 n}{k_B T}D$$



STOCHASTIC SCHRÖDINGER EQUATION

Hamiltonian: $$\hat{H}_{\text{tot}} = \hat{H}_s + \hat{H}_b + \lambda \hat{V} \qquad \hat{V} = \sum_\alpha \hat{S}_\alpha \hat{B}_\alpha$$

Schrödinger eq. $$\mathrm{i}\hbar\, \partial_t \Psi(x_s, x_b; t) = \hat{H}_{\text{tot}} \Psi(x_s, x_b; t)$$

bath orthonormal basis: $$\hat{H}_b \chi_n(x_b) = \varepsilon_n \chi_n(x_b)$$

expansion of the total wave function: $$\Psi(x_s, x_b; t) = \sum_n \psi_n(x_s; t)\, \chi_n(x_b)$$

a typical subsystem wave function $\psi_n(x_s;t)$ obeys the stochastic Schrödinger equation:

$$\mathrm{i}\partial_t \psi(x_s;t) = \hat{H}_s \psi(x_s;t) + \lambda \sum_\alpha \eta_\alpha(t) \hat{S}_\alpha \psi(x_s;t) - \mathrm{i}\lambda^2 \int_0^t d\tau \sum_{\alpha\beta} C_{\alpha\beta}(t-\tau) \hat{S}_\alpha \mathrm{e}^{-\mathrm{i}\hat{H}_s(t-\tau)} \hat{S}_\beta \psi(x_s;t) + O(\lambda^3)$$

Gaussian noises:
$$\overline{\eta_\alpha(t)} = 0$$
$$\overline{\eta_\alpha(t)\eta_\beta(t')} = 0$$
$$\overline{\eta^*_\alpha(t)\eta_\beta(t')} = C_{\alpha\beta}(t-t')$$

This stochastic Schrödinger equation is associated with the non-Markovian master equation.

CONCLUSIONS & PERSPECTIVES

The concept of Liouvillian resonances extends to many-body quantum systems where they describe the properties of relaxation and decoherence.

The quantum Liouvillian resonances are given as the eigenvalues of the quantum master equations such as the Bloch-Redfield master equation.

As the Pollicott-Ruelle resonances in classical dynamical systems, the quantum Liouvillian resonances give the dispersion relations of transport properties such as diffusion (as well as the associated decoherence).

In the same way, a stochastic Langevin equation is associated to the Fokker-Planck master equation, it is possible to associate a stochastic Schrödinger equation to quantum master equations. In the present setting, they concern typical « subsystem wave functions », i.e., the coefficients of the expansion of the total wave function on an orthonormal basis of the bath.
Such stochastic Schrödinger equations provide us with a framework to understand how stochasticity can manifest itself, e.g. in quantum measurement processes.
In this sense, they are complementary to the master equations describing the process of decoherence.

Dynamical randomness can be characterized by quantities such as the KS entropy per unit time.