Quantum Dissipation due to the Interaction with Chaos

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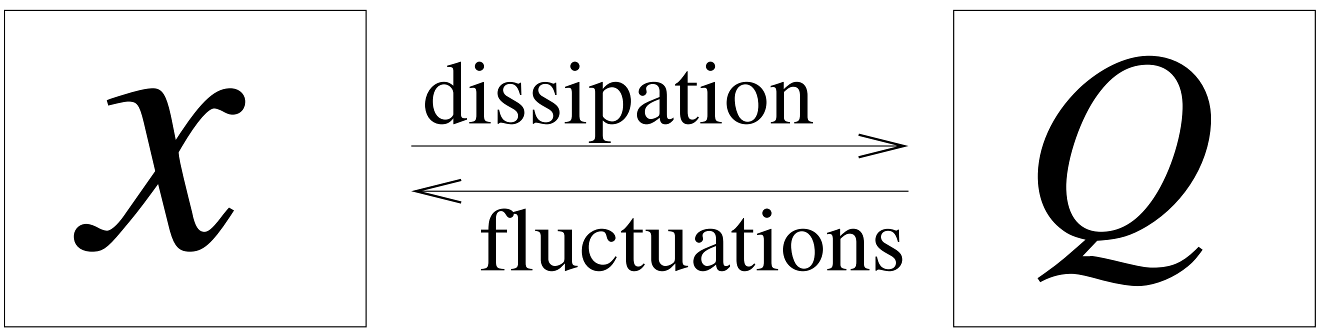
LANL cond-mat archive

$GIF, $ISF

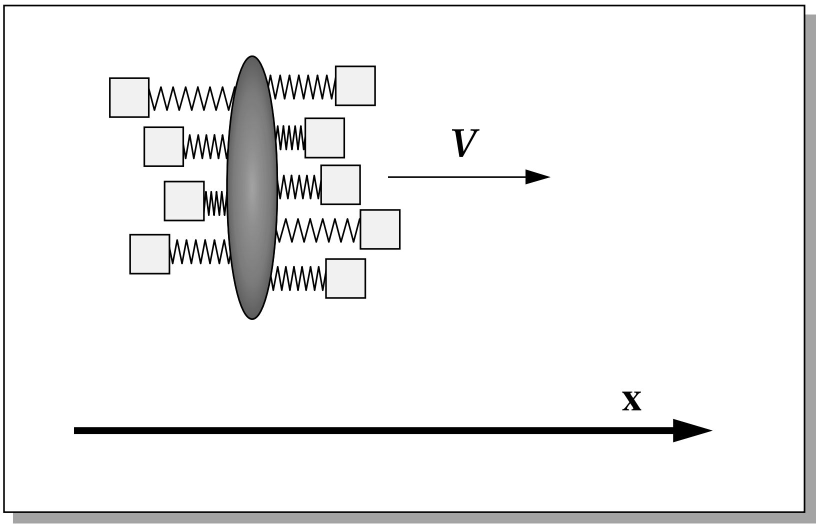
System - Environment

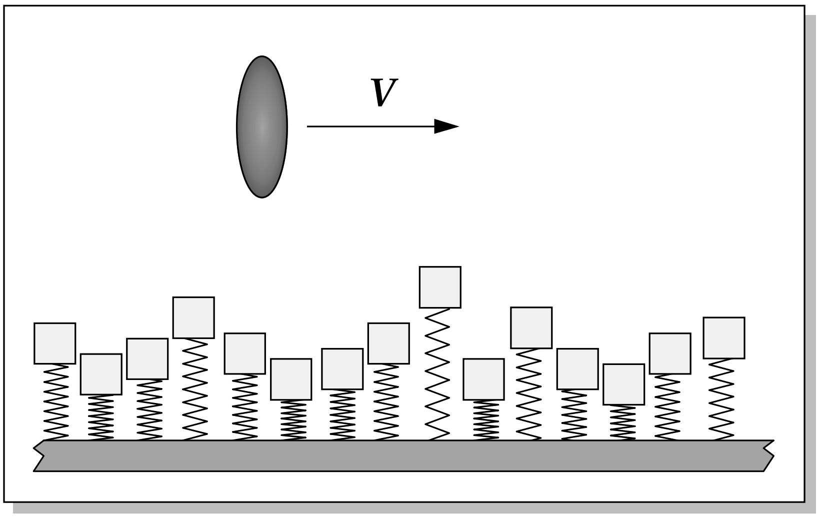
$$\mathcal{H}_{\text{total}} = \mathcal{H}_0(x,p) + \mathcal{H}(Q,P;x)$$



driving source | driven system
"slow" DoF | "fast" DoF
"system" | "environment"

Interaction with bath: ZCL/DLD models





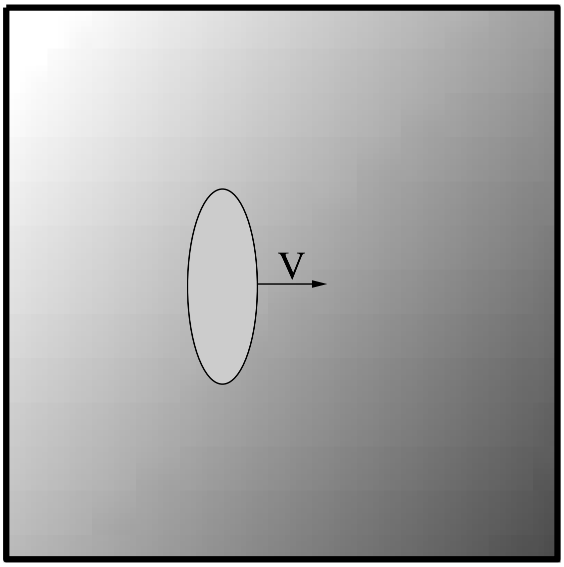
$$\mathcal{H}_{total} = \mathcal{H}_0(x,p) + \mathcal{H}(Q,P;x)$$

$$\mathcal{H}_0(x,p) = \frac{1}{2M}\, p^2$$

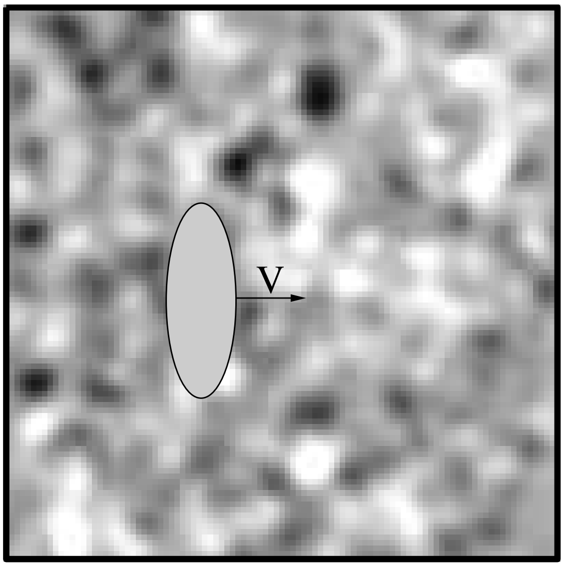
$$\mathcal{H}_{\rm ZCL} = \sum_\alpha \left(\frac{{P_\alpha}^2}{2\mathsf{m}_\alpha} + \frac{1}{2}\mathsf{m}_\alpha \omega_\alpha^2 {Q_\alpha}^2 \right) - x \sum_\alpha c_\alpha Q_\alpha$$

$$\mathcal{H}_{\rm DLD} = \sum_\alpha \left(\frac{{P_\alpha}^2}{2\mathsf{m}_\alpha} + \frac{1}{2}\mathsf{m}_\alpha \omega_\alpha^2 {Q_\alpha}^2 \right) - \sum_\alpha c_\alpha Q_\alpha u(x - x_\alpha)$$

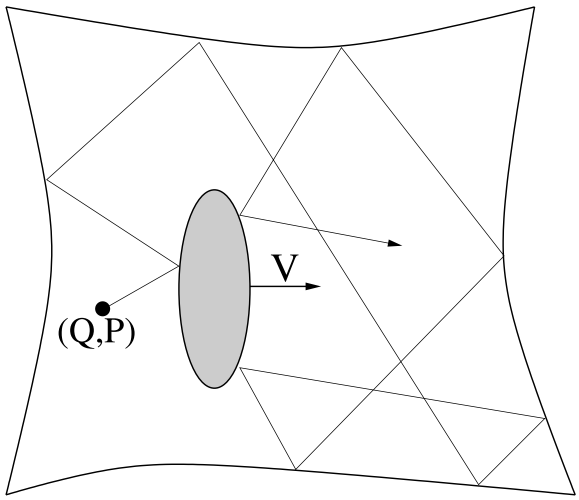
Brownian Motion modeling



ZCL model

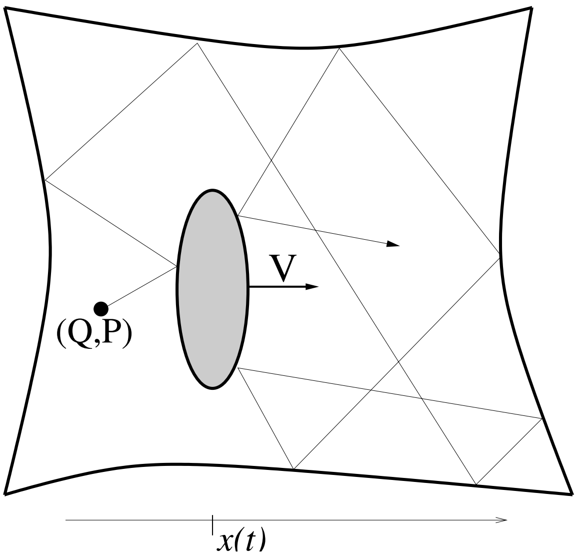


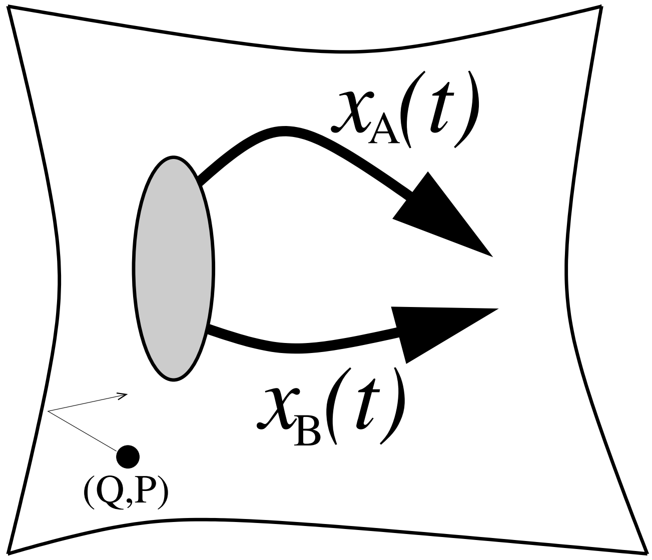
DLD model
(disorder)



piston model:
interaction
with
chaos

Interaction with chaos





$$\mathcal{H}_{total} = \mathcal{H}_0(x,p) + \mathcal{H}(Q,P;x)$$

$$\mathcal{H}_0(x,p) = \frac{1}{2M}\, p^2$$

$$\mathcal{H}(Q,P;x) = \frac{1}{2m} P^2 + U(Q;x)$$

[dephasing in this model: DC, PRE 2002]

"Spin" interacting with chaos

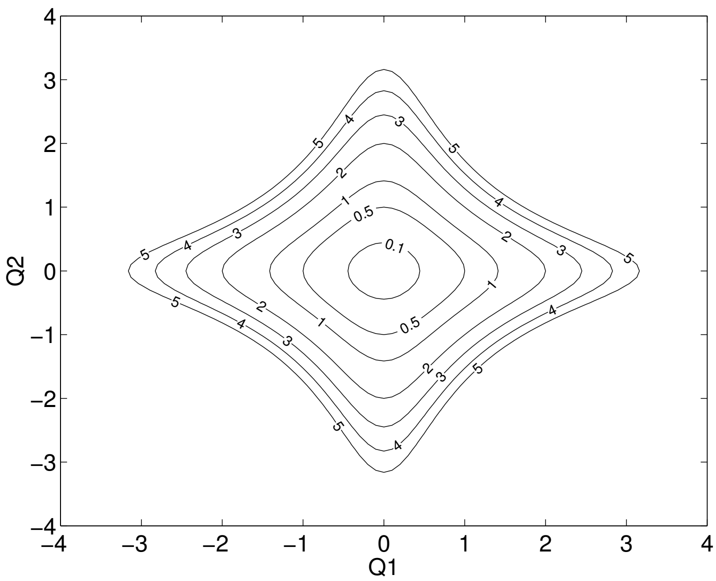
$$\mathcal{H}_{total} \;=\; \mathcal{H}_0 \;+\; \mathcal{H}(Q,P;x)$$

$x \;=\; v\sigma_3 \;=\;$ "position in the double well"

$$\mathcal{H}_0 \;=\; (\hbar\Omega/2)\sigma_1$$

The Hamiltonian of a nearby chaotic system:

$$\mathcal{H}(Q,P;x) = \frac{1}{2}(P_1^2{+}P_2^2 + Q_1^2{+}Q_2^2) + (1{+}x)\cdot Q_1^2 Q_2^2$$



Nuclear physics application:

boundary may have either of two shapes

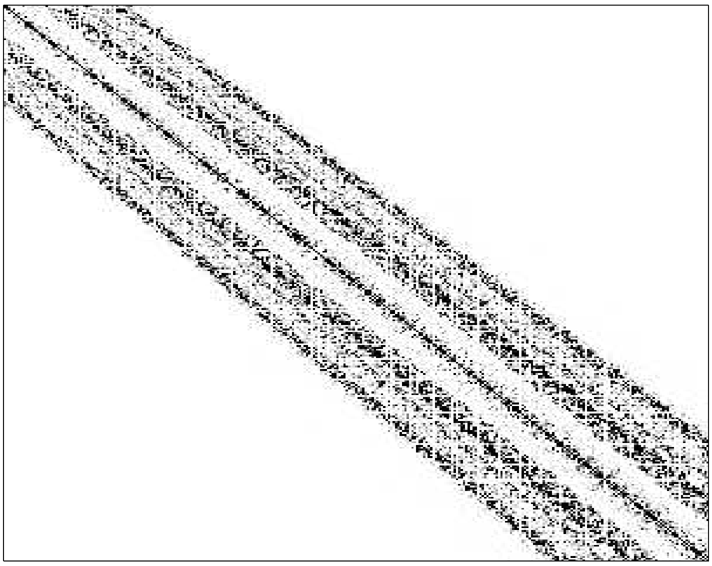
The Hamiltonian matrix
for interaction with chaos

$$\mathcal{H} = \frac{1}{2}(P_1^2+P_2^2 + Q_1^2+Q_2^2) + (1+x) \cdot Q_1^2 Q_2^2$$

$$\mathcal{H} = \boldsymbol{E} + x\boldsymbol{B}$$

It can be argued that $\boldsymbol{B}_{nm}$ is a banded matrix.

bandwidth $= \Delta_b = \hbar/\tau_{cl}$



$$\mathcal{H}_{total} = \frac{1}{2}\hbar\Omega\sigma_1 + \boldsymbol{E} + v\sigma_3\boldsymbol{B}$$

$$\mathcal{H}_{total} = \begin{bmatrix} \boldsymbol{E}+v\boldsymbol{B} & \Omega/2 \\ \Omega/2 & \boldsymbol{E}-v\boldsymbol{B} \end{bmatrix}$$

Simulations

$$|\Psi(t=0)\rangle \quad = \quad \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \ \otimes \ |\psi^{(E)}\rangle$$

basis: $\quad |\nu\rangle \otimes |n\rangle$

$$\rho_{\nu,\nu'}(t) \ = \ \sum_n \Psi_{\nu,n}(t)^* \Psi_{\nu',n}(t)$$

$$\rho(t) = \tfrac{1}{2}(1 + \vec{M}\cdot\vec{\sigma}) \mapsto \tfrac{1}{2}\begin{bmatrix} 1+M_3 & M_1 - iM_2 \\ M_1 + iM_2 & 1 - M_3 \end{bmatrix}$$

$$S(t) = (2\ \mathrm{trace}(\rho(t)^2) - 1) = \vec{M}\cdot\vec{M}$$

Pedagogical remark:

Given a basis ν for the representation of the spin, the wavefunction Ψ can always be written as

$$|\Psi\rangle = \sum_{\nu} |\nu\rangle \otimes |\psi^{(\nu)}\rangle$$

where the unnormalized wavefunction $\psi^{(\nu)}$ is called the relative state of the environment.

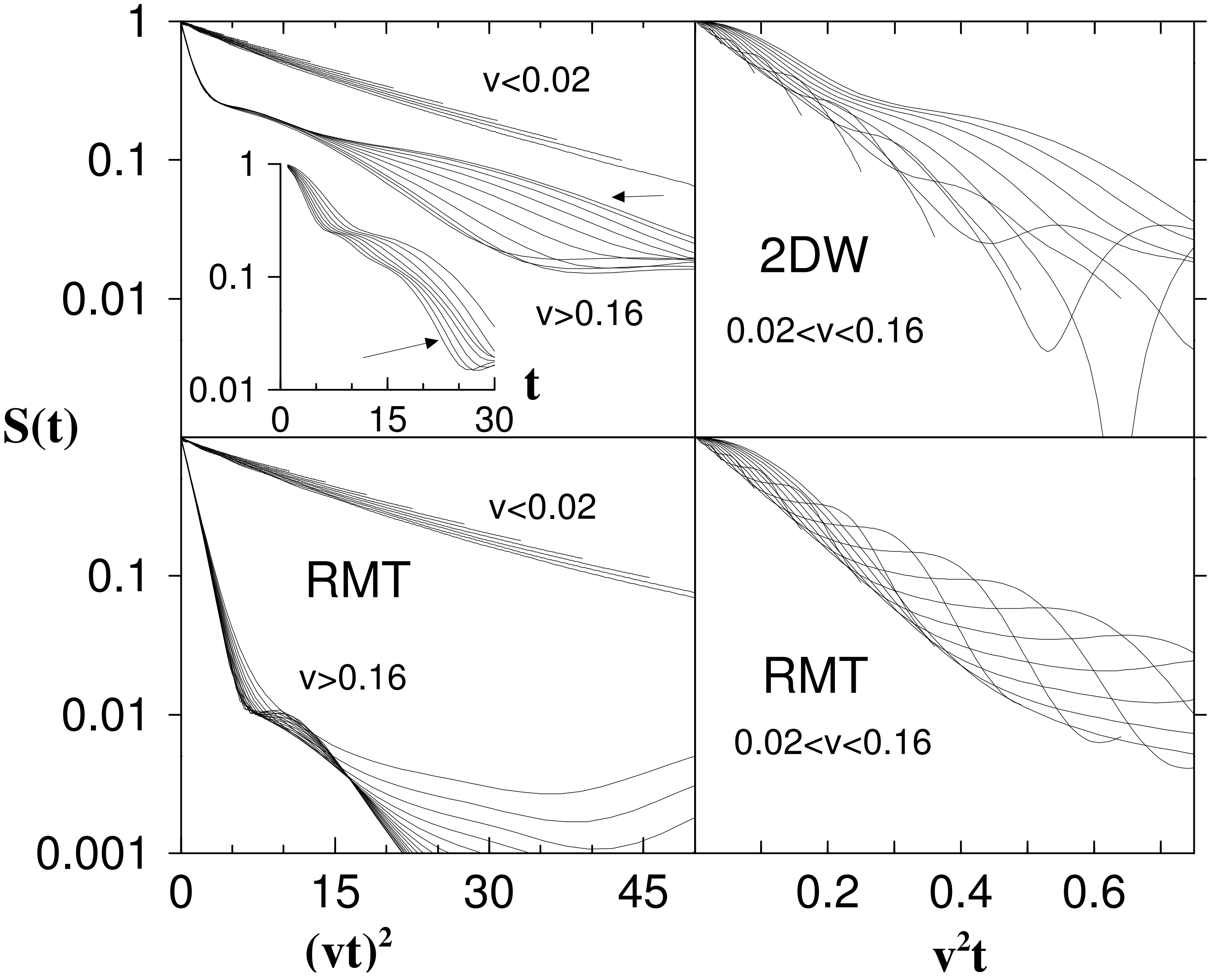
With this notation the elements of the reduced probability matrix are:

$$\rho_{\nu,\nu'} \;=\; \langle\psi^{(\nu)}|\psi^{(\nu')}\rangle$$

Hence the overlap of the relative states determines the purity of the spin state.

In particular orthogonality of the relative states implies a maximally mixed spin state.

Numerical observations



$2.8 < E < 3.2$

$T \sim 1.3$

$d_T \sim 2.4$

$10^{-4} < v < 0.3$

$\tau_{cl} \sim 1$

$\hbar = 0.03$

$\Delta_b \sim 0.2$

$\Delta \sim 0.004$

The Hamiltonian matrix for interaction with bath

$$\mathcal{H} = \sum_\alpha \left(\frac{P_\alpha^2}{2\mathsf{m}_\alpha} + \frac{1}{2}\mathsf{m}_\alpha \omega_\alpha^2 Q_\alpha^2 \right) \; - \; x \sum_\alpha c_\alpha Q_\alpha$$

The states of the bath are:

$$|\boldsymbol{n}\rangle \;=\; |\{n_\alpha\}\rangle = |n_1, n_2, n_3, ...\rangle$$

$$E_{\boldsymbol{n}} \;=\; \sum_\alpha \omega_\alpha n_\alpha$$

We can write:

$$\mathcal{H} = \boldsymbol{E} + x\boldsymbol{B}$$

$\boldsymbol{B}_{nm}$ is non-zero only for "one-photon" excitations.

For such excitations $|E_m - E_n| = \hbar\omega_\alpha$

Consequently $\boldsymbol{B}_{nm}$ is a sparse banded matrix.

bandwidth $= \Delta_b = \hbar\omega_c$

Fluctuations

$$\mathcal{H} \;=\; \mathcal{H}(Q, P; x)$$

$$\mathcal{F}(t) \;=\; -\frac{\partial \mathcal{H}}{\partial x}(Q(t), P(t); x)$$

The (asymmetrized) correlation function:

$$C(\tau) = \langle \mathcal{F}(\tau)\mathcal{F}(0) \rangle$$

The power spectrum of the fluctuations
(assuming preparation in the nth state):

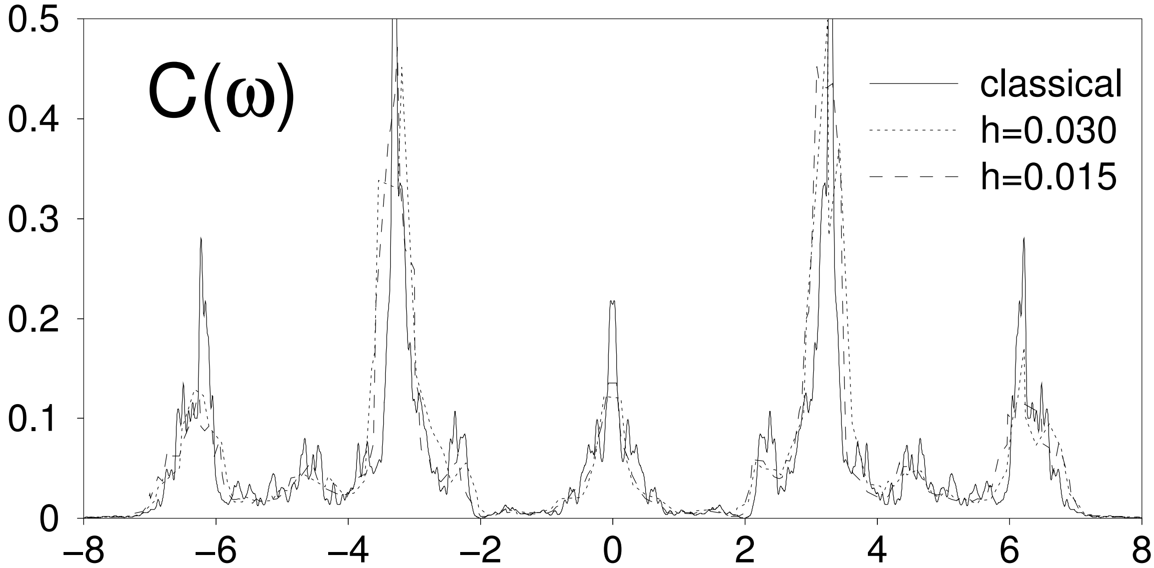
$$\tilde{C}(\omega) \;=\; \sum_m |\mathcal{F}_{mn}|^2 \;\; 2\pi\delta\left(\omega - \frac{E_m - E_n}{\hbar}\right)$$

Conclusion:
The bandprofile of the matrix $\mathcal{F}_{nm}$
is related to the power spectrum $\tilde{C}(\omega)$

Numerical example

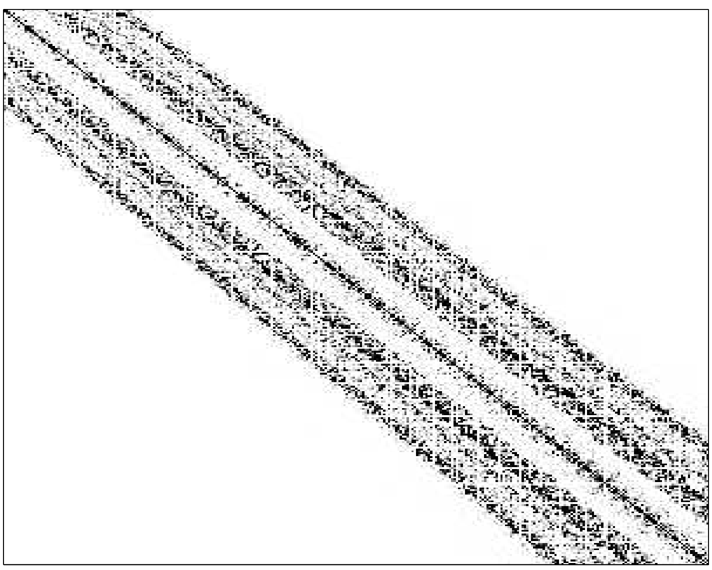
$$\mathcal{H} = \frac{1}{2}(P_1^2+P_2^2 + Q_1^2+Q_2^2) + (1+x)\cdot Q_1^2Q_2^2$$

$$\mathcal{F} \;=\; -Q_1^2Q_2^2$$



$$\mathcal{H} = \boldsymbol{E} + x\boldsymbol{B}$$

$$\boldsymbol{B} = \{-\mathcal{F}_{nm}\}$$



$$E \;\sim\; 3$$

$$\tau_{cl} \;\sim\; 1$$

$$\Delta \;\approx\; 4.3\cdot\hbar^2$$

$$\Delta_b \;\sim\; \hbar/\tau_{cl}$$

$$b \;\sim\; 1/\hbar$$

The bandprofile for bath

$$\mathcal{H} = \sum_\alpha \left(\frac{P_\alpha^2}{2\mathsf{m}_\alpha} + \frac{1}{2}\mathsf{m}_\alpha \omega_\alpha^2 Q_\alpha^2 \right) \; - \; x \sum_\alpha c_\alpha Q_\alpha$$

$$\mathcal{F} = \sum_\alpha c_\alpha Q_\alpha = \sum_\alpha c_\alpha \left(\frac{\hbar}{2\mathsf{m}_\alpha \omega_\alpha} \right)^{1/2} (a_\alpha + a_\alpha^\dagger)$$

For preparaion in state $\boldsymbol{n}$

$$\tilde{C}(\omega) = \sum_\alpha \sum_\pm c_\alpha^2 \; |\langle n_\alpha {\pm} 1 | Q_\alpha | n_\alpha \rangle|^2 \; 2\pi\delta(\omega \mp \omega_\alpha)$$

$$\tilde{C}(\omega) = \sum_\alpha \frac{\pi\hbar c_\alpha^2}{\mathsf{m}_\alpha \omega_\alpha} \Big[(1{+}n_\alpha)\delta(\omega - \omega_\alpha) + n_\alpha \delta(\omega + \omega_\alpha) \Big]$$

For canonical preparation

$$\tilde{C}_T(\omega) \;=\; 2J(\omega) \frac{1}{1 - \mathrm{e}^{-\beta\omega}} \;=\; \frac{J(\omega)}{\sinh(\omega/(2T))} \mathrm{e}^{\omega/(2T)}$$

where we define

$$J(\omega) \;=\; \frac{\pi}{2} \sum_\alpha \frac{c_\alpha^2}{\mathsf{m}_\alpha \omega_\alpha} \delta(\omega - \omega_\alpha) \;=\; \eta\omega \mathrm{e}^{-\omega/\omega_c}$$

(with anti-symmetric continuation)

Two notions of temperature

$$\frac{1}{T_{\text{EQLB}}} = \frac{d}{dE}\ln(g(E)) \qquad \rightsquigarrow \text{equilibrium}$$

$$\frac{1}{T_{\text{FLCT}}} = 2\frac{d}{d\omega}\ln(\tilde{C}(\omega))\Big|_{\omega\sim 0} \qquad \rightsquigarrow \text{dissipation}$$

which means that

$$g(E+\omega) \approx g(E)\exp\left[\frac{\omega}{T_{\text{EQLB}}}\right]$$

$$\tilde{C}(\omega) \approx \tilde{C}(\omega\sim 0)\exp\left[\frac{\omega}{2T_{\text{FLCT}}}\right]$$

For interaction with chaos

$$\tilde{C}_E(\omega) = \sum_m |\boldsymbol{B}_{mn}|^2 \; 2\pi\delta(\omega-(E_m-E_n)) = g(E+\omega)\;\sigma(E+\omega|E)^2$$

$$\frac{1}{T_{\text{FLCT}}} \geq \frac{2}{T_{\text{EQLB}}}$$

The FD relation

For canonical preparation

$$\mu \;=\; \text{friction coef} \;=\; \frac{1}{2T}\,\tilde{C}(\omega{\sim}0)$$

For interaction with microcanonical chaos

$$\mu \;=\; \frac{1}{2g(E)}\frac{d}{dE}\left[g(E)\tilde{C}_E(\omega{\sim}0)\right] \;=$$

$$=\; \frac{d}{d\omega}\tilde{C}_E(\omega)\Big|_{\omega\sim 0} \;=\; \frac{1}{2T_{\text{FLCT}}}\tilde{C}_E(\omega{\sim}0)$$

From now on we characterize the fluctuations by the symmetrized correlation function, and regard the temperature as an independent parameter.

$$\tilde{C}(\omega) \;=\; 2\pi\sigma^2\delta(\omega) \;+\; \frac{2\pi\hbar\sigma^2}{\Delta}R\left(\frac{\hbar\omega}{\Delta}\right)G\left(\frac{\hbar\omega}{\Delta_b}\right)$$

$G()$ = semiclassical envelope (bandprofile)

$R()$ = lower cutoff function (level repulsion)

$$\Delta_b \;=\; \frac{\hbar}{\tau_{\text{cl}}} \;=\; \hbar\omega_c \;=\; \text{bandwidth}$$

The parameters of the theory

$$\mathcal{H}_{\text{total}} = \mathcal{H}_0 + \boldsymbol{E} + x\boldsymbol{B}$$

parameter	*significance*
$\Delta \propto \hbar^d$	environment mean level spacing
$\Delta_b \propto \hbar$	environment bandwidth
T	environment temperature
d_{T}	environment heat capacity
ϵ	system energy
Γ	strength of coupling

$$d_{\text{T}} = \left(\frac{dT}{dE}\right)^{-1} = \text{heat capacity} \sim d$$

Assuming that x performs motion with amplitude A and velocity V, then Γ is related to $(\sigma A)^2$ and $(\sigma V)^2$.

$$\frac{\Gamma}{\Delta} = \text{minimum}\left(\left(\frac{\sigma}{\Delta}A\right)^2, \left(\frac{\hbar\sigma}{\Delta^2}V\right)^{2/3}\right)$$

The parameter Γ

$$\mathcal{H}_{nm} \;=\; E_n\delta_{nm} \;+\; x\boldsymbol{B}_{nm}$$

Δ = mean level spacing

Δ_b = bandwidth

$|\boldsymbol{B}_{nm}| \sim \sigma$ for $|E_n - E_m| < \Delta_b$

Assume a small constant perturbation $|x| = \delta x$

$$\Gamma(\delta x) \;\approx\; \left(\frac{\sigma\delta x}{\Delta}\right)^2 \Delta$$

Γ/Δ is the number of levels that are mixed non-perturbatively,

as implied by perturbation theory (to infinite order).

Re-write the Hamiltonian in the adiabatic basis:

$$\mathcal{H}_{nm} \;=\; E_n\delta_{nm} \;+\; \dot{x}\frac{i\hbar\boldsymbol{B}_{nm}}{E_n - E_m}$$

Assume a slow variation $\dot{x}$

$$\Gamma(\dot{x}) \;\approx\; \left(\frac{\hbar\sigma\dot{x}}{\Delta^2}\right)^{2/3} \Delta$$

The thermodynamic Limit

Parameters:

$T, \quad d_{\mathrm{T}}, \quad \Delta \propto \hbar^d, \quad \Delta_b \propto \hbar, \quad \epsilon, \quad \Gamma$

Mathematical definition of the Thermodynamic Limit:

$d \to \infty$ (infinitely many degrees of freedom).

Physical definition of the Thermodynamic Limit:

$\epsilon / d_{\mathrm{T}} \ll T$ (having well defined temperature).

In case of two level (spin) system:

$\Omega \ll d_{\mathrm{T}} \times T$

In case of d_0 dimensional system:

$d_0 \ll d_{\mathrm{T}}$

The High Temperature Limit

Parameters:

$T, \quad d_{\mathrm{T}}, \quad \Delta \propto \hbar^{d}, \quad \Delta_b \propto \hbar, \quad \epsilon, \quad \Gamma$

Mathematical definition of the high temperature limit:

$T \to \infty$ (vanishing friction effect in this limit)

Note: high temperature does not imply a lot of noise!

Physical definition of the high temperature limit:

$\hbar\omega/T \ll 1$ for the physically relvevnat frequencies

Sufficient condition: $T \gg \Delta_b$

In case of the Spin-Boson model: $T \gg \Omega, \Gamma$

$$K = \frac{1}{16\pi}\left(\frac{\Gamma}{T}\right) =$$ Kondo Parameter

The Semiclassical Limit

Parameters:

$T, \quad d_{\rm T}, \quad \Delta \propto \hbar^d, \quad \Delta_b \propto \hbar, \quad \epsilon, \quad \Gamma$

Mathematical definition of the semiclassical limit:

$\hbar \to 0$ (scaled planck constant).

Physical definition of the semiclassical limit:

$\Gamma > \Delta_b$ (the non-perturbative regime)

This should be contrasted with:

$\Gamma \ll \Delta_b$ (Fermi golden rule regime)

Note that the adiabatic / standard-prt regime is :

$\Gamma < \Delta$ (Born-Oppenheimer regime)

Feynman Vernon formalism

$$K(x_t, x'_t|x_0, x'_0) = \sum_{x,x'} F[x, x'] \; \mathrm{e}^{i(\mathcal{A}[x]-\mathcal{A}[x'])}$$

$$F[x^{\mathrm{A}}, x^{\mathrm{B}}] \; = \; \left\langle \; \psi^{(E)} \; \middle| \; U[x^{\mathrm{B}}]^{-1} \; U[x^{\mathrm{A}}] \; \middle| \; \psi^{(E)} \right\rangle$$

$$= \; \left\langle \; U[x^{\mathrm{B}}] \; \psi^{(E)} \; \middle| \; U[x^{\mathrm{A}}] \; \psi^{(E)} \; \right\rangle$$

$$U[x] = \mathcal{T} \exp\left(-\frac{i}{\hbar}(\boldsymbol{E} + x(t)\boldsymbol{B})\right)$$

Given a driving scheme we define

$$\mathcal{P}(t) \; = \; |F[x^{\mathrm{A}}, x^{\mathrm{B}}]|^2$$

FV picture and dephasing

Using the FV expression

$$\mathcal{P}(t) = \exp\left[-\frac{1}{\hbar^2}\int_0^t\int_0^t C(t'-t'')(x^{\mathrm{A}}(t')-x^{\mathrm{B}}(t''))^2 dt'dt''\right]$$

with $x = \pm v$ and the symmetrized

$$\tilde{C}(\omega) \;=\; 2\pi\sigma^2\delta(\omega) + \frac{2\pi\hbar\sigma^2}{\Delta} R\left(\frac{\hbar\omega}{\Delta}\right) G\left(\frac{\hbar\omega}{\Delta_b}\right)$$

then we get:

$$\mathcal{P}(t) = \exp(-4C(0)(vt/\hbar)^2)$$

$$\mathcal{P}(t) = \exp(-2\gamma t)$$ requires $\Delta \ll \Gamma \ll \Delta_b$

$$\mathcal{P}(t) = \exp(-(\sigma vt/\hbar)^2)$$

with:

$$\gamma \;=\; 2\left(\frac{v}{\hbar}\right)^2 \tilde{C}(\omega\sim 0) \;\approx\; \frac{1}{2}\frac{\Gamma}{\hbar}$$

which is identified as the $1/T_1$ rate

The adiabatic picture

$$\frac{d}{dt}|\psi\rangle \;=\; -\frac{i}{\hbar}\mathcal{H}(x(t))\;|\psi\rangle$$

$$|\psi\rangle \;=\; \sum_n a_n(t)\;|n(x(t))\rangle$$

$$\frac{da_n}{dt} = -\frac{i}{\hbar}E_n a_n + \frac{i}{\hbar}\sum_m \sum_j \dot{x}_j \boldsymbol{A}^j_{nm} a_m$$

$$\boldsymbol{A}^j_{nm}(x) = i\hbar\left\langle n(x)\left|\frac{\partial}{\partial x_j} m(x)\right.\right\rangle$$

$$\boldsymbol{A}^j_{nm}(x) = \frac{i\hbar}{E_m - E_n}\left(\frac{\partial \mathcal{H}}{\partial x_j}\right)_{nm} \qquad \text{for } n \neq m$$

$$\frac{da_n}{dt} = -\frac{i}{\hbar}(E_n - \dot{x}\boldsymbol{A}_n)a_n - \frac{i}{\hbar}\sum_m \boldsymbol{W}_{nm} a_m$$

$$\boldsymbol{W}_{nm} \equiv -\sum_j \dot{x}_j \boldsymbol{A}^j_{nm} \qquad \text{for } n{\neq}m\text{, else zero}$$

Linear Response Theory (Kubo)

$$\mathcal{H} \;=\; \mathcal{H}(\boldsymbol{r},\boldsymbol{p};\; x_1(t), x_2(t), x_3(t))$$

$$F^k \;=\; -\frac{\partial \mathcal{H}}{\partial x_k}$$

Generalized Ohm law:

$$\langle F^k \rangle = -\sum_j \boldsymbol{G}^{kj}\; \dot{x}_j$$

$$K^{kj}(\tau) \;=\; (i/\hbar)\langle [F^k(\tau), F^j(0)]\rangle$$

$$C^{kj}(\tau) \;=\; \tfrac{1}{2}(\langle F^k(\tau)F^j(0)\rangle + cc)$$

$$\boldsymbol{G}^{kj} \;=\; \lim_{\omega\to 0} \frac{\mathrm{Im}[\chi^{kj}(\omega)]}{\omega} \;=\; \int_0^\infty K_E^{kj}(\tau)\tau d\tau$$

$$=\; \frac{1}{g(E)}\frac{d}{dE}g(E)\; \int_0^\infty C_E^{kj}(\tau)d\tau$$

The Born-Oppenheimer picture

$$\mathcal{H}_{\text{total}} = \frac{1}{2M}\sum_j p_j^2 + \mathcal{H}(Q, P; x)$$

basis: $|x, n(x)\rangle = |x\rangle \otimes |n(x)\rangle$

$$|\Psi\rangle = \sum_{n,x} \Psi_n(x)\ |x, n(x)\rangle$$

$$\langle x, n(x)|\mathcal{H}|x_0, m(x_0)\rangle = \delta(x - x_0) \times \delta_{nm} E_n(x)$$

$$\begin{aligned}\langle x, n(x)|p_j|x_0, m(x_0)\rangle &= \\ &= (-i\partial_j \delta(x - x_0)) \times \langle n(x)|m(x_0)\rangle \\ &= -i\partial_j \delta(x - x_0)\delta_{nm} - \delta(x - x_0)\boldsymbol{A}^j_{nm}(x)\end{aligned}$$

hence: $p_j \mapsto -i\partial_j - \boldsymbol{A}^j_{nm}(x).$

$$\mathcal{H}_{\text{total}} = \frac{1}{2M}\sum_j (p_j - \boldsymbol{A}^j(x))^2 + \boldsymbol{E}(x)$$

$$\mathcal{H}_{\text{interaction}} \approx -\sum_j \dot{x}_j \boldsymbol{A}^j(x)$$