Recent developments in the theory of open quantum systems

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Open system S: connected to environment R
S = system of interest, e.g. a few spins

Environment R ("reservoir"): large compared to S
charact. by macroscopic quantities $(T, \mu, \rho, \ldots)$
R dissipative, irreversible processes (radiation to ∞)
irreversibility $\leftrightarrow$ size of R $\leftrightarrow$ large times

Coupling $S \leftrightarrow R$ induces irreversible processes of S
e.g. S approaches T of R

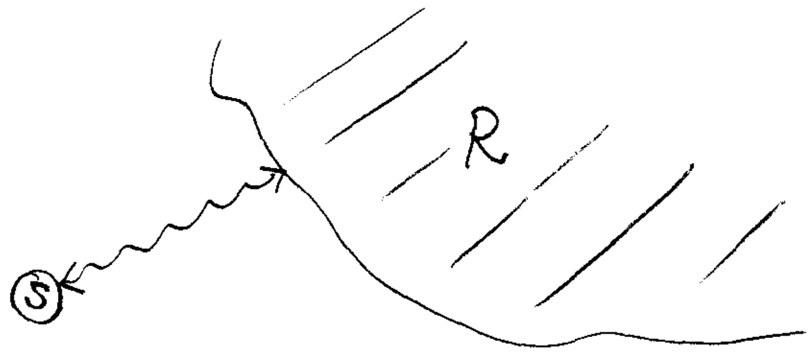
3 classes of systems built from R, S:

1) systems close to equilibrium

2) systems far from equilibrium

3) repeated interaction systems

1) S+R : syst. close to equilibrium



e.g. array of qubits (quantum register) interacting with a substrate

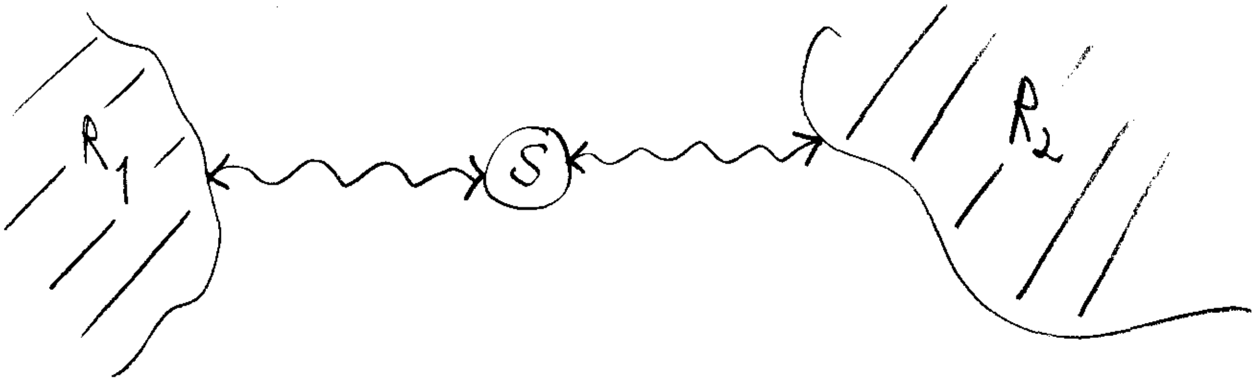
effects of R on S: thermalization & decoherence

thermalization: $S+R \xrightarrow{t\to\infty}$ equilibrium of coupled system

decoherence: phase relations of initial state disappear

$$\sum_{j,k} c_{j,k} \, |\psi_j\rangle\langle\psi_k| \xrightarrow{t\to\infty} \sum_n p_n \, |\psi_n\rangle\langle\psi_n|$$

2) $S + R_1 + R_2$: syst. far from equilibrium



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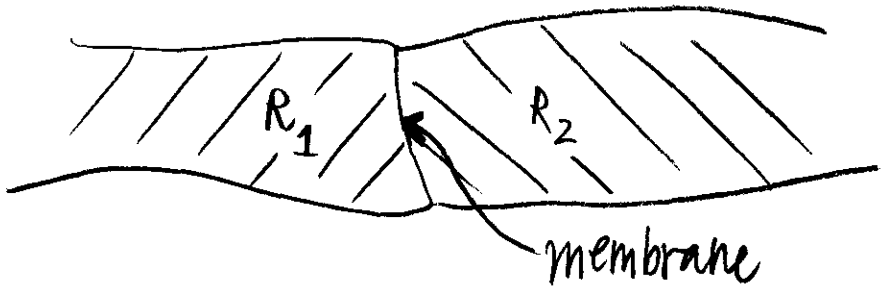


eg: junction of two pieces of metal

Phenomena:
- approach to Non-Equil. Steady State (NESS)
- fluxes of energy / matter, entropy prod.

driven by gradient in macroscopic parameters

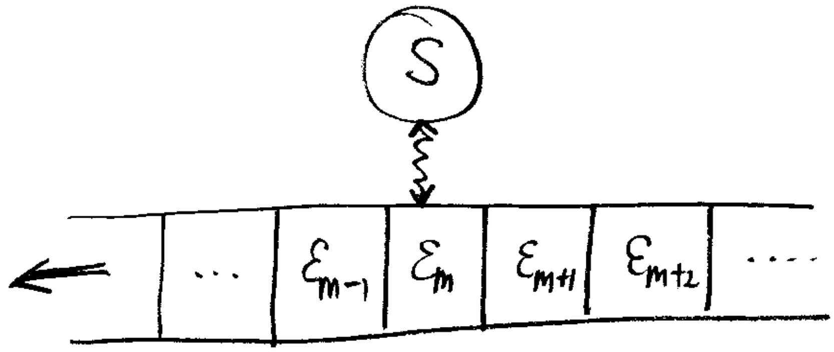
$$S + R_1 + R_2 \xrightarrow{t \to \infty} \text{NESS, stationary, but}$$

$$\langle \text{Entropy production} \rangle_{NESS} > 0$$

$$\langle \text{Energy flux} \rangle_{NESS} > 0 \quad \dots$$

3) $S + \mathcal{E}$, $\mathcal{E} = \mathcal{E}_1 + \mathcal{E}_2 + \cdots$: Repeated Interaction syst.

$\mathcal{E}_j$ ⟨ S, R



e.g. "One-Atom Maser"

Phenomena:

- approach of RIAS (rep. int. asympt state)
- control of S by variation of interaction

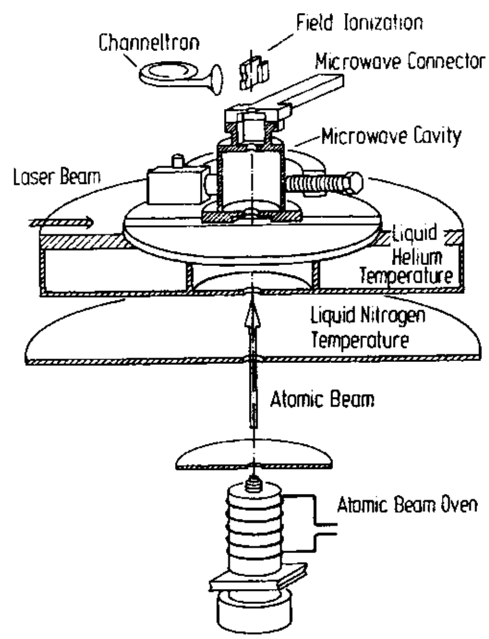


FIG. 1. Vacuum chamber with the atomic-beam arrangement and the microwave cavity. The upper part is cooled to liquid-helium temperature.

Fluctuations in chain:

$\mathcal{E}_j$ independent, random

→ state of S : Markov process with explicit ergodic mean limit.

Description of S

pure states : normalized vectors in $\mathcal{H}_S = \mathbb{C}^N$ (N spins)

mixed states : density matrices $\rho = \sum_n p_n \, |\psi_n\rangle\langle\psi_n|$

observables : A, self-adjoint operators on $\mathcal{H}_S$

dynamics : Hamiltonian H_S : matrix on $\mathcal{H}_S$

$$\mathrm{spec}\,(H_S) = \{ E_0, \ldots, E_{N-1} \}$$

$$A \mapsto A_t = e^{itH_S} A \, e^{-itH_S} \qquad (\hbar = 1)$$

averages : $\langle A_t \rangle = \mathrm{Tr}_{\mathcal{H}_S} (\rho A_t) = \mathrm{Tr}_{\mathcal{H}_S} (\rho_t A)$,

where $\rho_t = e^{-itH_S} \rho \, e^{itH_S}$

equilibrium : $\beta = 1/T > 0$ fixed

$$\rho_{S,\beta} = \frac{e^{-\beta H_S}}{\mathrm{Tr}_{\mathcal{H}_S} e^{-\beta H_S}} \qquad \text{Gibbs state.}$$

Representing any state as vector state on (enlarged) Hilbert space : "Gelfand-Naimark-Segal" constr.

$\rho \geq 0 \quad \rightarrow \quad \rho^{1/2}$

$$\langle A \rangle = \mathrm{Tr}_{\mathcal{H}_S}(\rho A) = \mathrm{Tr}_{\mathcal{H}_S}(\rho^{1/2}\rho^{1/2}A)$$

$$= \mathrm{Tr}_{\mathcal{H}_S}(\rho^{1/2} A \rho^{1/2})$$

$$= \langle \rho^{1/2}, A\rho^{1/2} \rangle_2 ,$$

where $\langle \cdot , \cdot \rangle$ is scalar product on space of all operators $\mathcal{O}$ on $\mathcal{H}_S$ s.t. $\mathrm{Tr}_{\mathcal{H}_S}(\mathcal{O}^*\mathcal{O}) < \infty$,

$$\langle \mathcal{O}_1, \mathcal{O}_2 \rangle = \mathrm{Tr}_{\mathcal{H}_S}(\mathcal{O}_1^* \mathcal{O}_2) .$$

$\Rightarrow$ ρ is represented on space of such operators by the <u>vector</u> $\rho^{1/2}$.

Space of operators $\cong \mathcal{H}_S \otimes \mathcal{H}_S$

$$\rho^{1/2} = \sum_n p_n^{1/2} \, |\psi_n\rangle\langle\psi_n|$$

$$\cong \sum_n p_n^{1/2} \, \psi_n \otimes \mathcal{C}\psi_n =: \Omega \in \mathcal{H}_S \otimes \mathcal{H}_S,$$

where $\mathcal{C}$ is antilinear, $\mathcal{C}^2 = \mathbb{1}$. Then

$$\langle A\rangle = \langle \rho^{1/2}, A\rho^{1/2}\rangle_2 = \langle \Omega, (A\otimes\mathbb{1})\Omega\rangle_{\mathcal{H}_S\otimes\mathcal{H}_S} .$$

$\Rightarrow$ every mixed state on $\mathcal{H}_S$ can be described by a vector state on $\mathcal{H}_S \otimes \mathcal{H}_S$

E.g. Gibbs state $\Omega_{S,\beta} = Z_{S,\beta}^{-1/2} \sum_{n=0}^{N-1} e^{-\beta E_n/2} \, \varphi_n \otimes \varphi_n$

(where $H_S \varphi_n = E_n \varphi_n$)

How does dynamics look in $\mathcal{H}_S \otimes \mathcal{H}_S$?

$$\langle A\rangle_t = \langle \Omega, \left(e^{itH_S} A e^{-itH_S} \otimes \mathbb{1}\right)\Omega\rangle$$

$$= \langle \Omega, \left[e^{itH_S} \otimes e^{itH_S'}\right] (A\otimes\mathbb{1}) \left[e^{-itH_S} \otimes e^{-itH_S'}\right]\Omega\rangle$$

where H_S' is anything !

Eg. can choose H_S' s.t. $\Omega_{S,\beta}$ is invariant : $H_S' = -H_S$,

$$\left(e^{itH} \otimes e^{-itH}\right) \varphi_n \otimes \varphi_n = \varphi_n \otimes \varphi_n$$

$$\Rightarrow \qquad L_S = H_S \otimes \mathbb{1} - \mathbb{1} \otimes H_S$$

"standard Liouville operator"

<u>Sum up:</u>

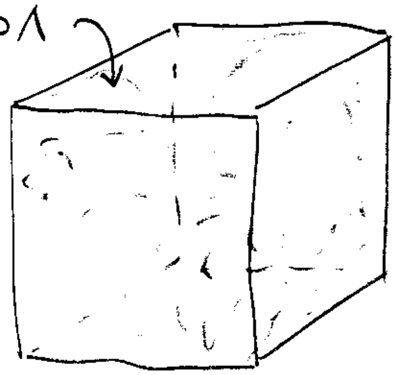
$$\mathrm{Tr}_{\mathcal{H}_S}(\rho A) \longrightarrow \langle \Omega, (A \otimes \mathbb{1}) \Omega \rangle$$

$$e^{itH_S} A e^{-itH_S} \longrightarrow e^{itL_S} (A \otimes \mathbb{1}) e^{-itL_S}$$

Description of R

Thermodynamic limit of ideal quantum gas.

$\mathbb{R}^3 \supset \Lambda$



$|\Lambda| < \infty$ $\quad \rho = \frac{N}{|\Lambda|}$ density, fixed.

$N, |\Lambda| \to \infty$

N non-interacting Bosons in box

$$\begin{cases} \mathcal{H}_\Lambda = L^2_{sym}\left(\Lambda^{3N}, d^{3N}x\right) \\ H_\Lambda = \sum_{j=1}^{N} -\frac{\hbar^2}{2m_j}\Delta_j = -\sum_{j=1}^{N}\Delta_j \end{cases}$$

Second quantization description

f^j_Λ = eigenstate of $-\Delta$ with momentum k_j

(e.g. periodic bndry cond. $f^j_\Lambda(x) = \frac{1}{\sqrt{|\Lambda|}} e^{ik_j x}$)

Fix $\rho_j = \frac{n_j}{|\Lambda|}$ density of mode j, $j = 1, \dots, p$

$$\psi_\Lambda = \frac{1}{\sqrt{n_1! \cdots n_p!}} \; a^*(f^1_\Lambda)^{n_1} \cdots a^*(f^p_\Lambda)^{n_p}\, \Omega$$

where a^* are creation operators, Ω is vacuum.

Fundamental "observable": Weyl operator

$$W(f) = e^{i\varphi(f)} = e^{\frac{i}{\sqrt{2}}[a^*(f)+a(f)]}$$

expectation functional $E_\Lambda(f) = \langle \Psi_\Lambda, W(f)\Psi_\Lambda \rangle$

As $|\Lambda| \to \infty$, $\{\rho_j\} \to$ continuous distribution $\rho(k)$, $k \in \mathbb{R}^3$,

one finds $E_\Lambda(f) \to E(f) = \exp\left\{-\frac{1}{4}\langle f, (1+16\pi^3\rho)f\rangle\right\}$

Hilbert space and vector therein corresponding to this ∞-volume state?

$$\mathcal{H}_\rho = \mathcal{F}(L^2(\mathbb{R}^3, d^3k)) \otimes \mathcal{F}(L^2(\mathbb{R}^3, d^3k))$$

$$\Omega_\rho = \Omega \otimes \Omega$$

$$W(f) \to W_\rho(f) = W(\sqrt{1+\mu}\, f) \otimes W(\sqrt{\mu}\, \bar{f})$$

$$\mu = 8\pi^3\rho$$

Then $\langle \Omega_\rho, W_\rho(f)\Omega_\rho \rangle = E(f)$.

∞-volume representation!

Equilibrium : $\rho(k) = \frac{1}{e^{\beta\omega(k)} - 1}$ Planck's black body radiation law

particle density : $0 < \bar{n} = \int_{\mathbb{R}^3} \rho(k)\, d^3k$.

$\Rightarrow$ the ∞-volume equilibrium state is given by vector $\Omega \otimes \Omega$ on $\mathcal{F} \otimes \mathcal{F}$, and expectation of $a^{\#}(f)$ is

$$\langle a^{\#}(f) \rangle_\beta = \langle \Omega \otimes \Omega,\ a_\beta^{\#}(f)\, \Omega \otimes \Omega \rangle,$$

where
$$\begin{cases} a_\beta(f) = a\left(\sqrt{1+\mu}\, f\right) \otimes \mathbb{1} + \mathbb{1} \otimes a^*\left(\sqrt{\mu}\, \bar{f}\right) \\ a_\beta^*(f) = a^*\left(\sqrt{1+\mu}\, f\right) \otimes \mathbb{1} + \mathbb{1} \otimes a\left(\sqrt{\mu}\, \bar{f}\right) \end{cases}$$

(thermal creation / annihilation operators)

Dynamics: $a^{\#}(f) = a^{\#}\left(e^{i\omega(k)t} f\right)$

$$\Rightarrow \quad a_\beta^{\#}\left(e^{i\omega t} f\right) = e^{itL}\, a_\beta^{\#}(f)\, e^{-itL},$$

$$L = H \otimes \mathbb{1} - \mathbb{1} \otimes H \qquad \left(H = \int \omega(k)\, a^*(k) a(k) \right)$$

$$L\, \Omega \otimes \Omega = 0$$ standard Liouville operator.

Interactions

S+R, uncoupled system : $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_S \otimes \mathcal{F} \otimes \mathcal{F}$

$$L_0 = L_S + L_R$$

$$\begin{cases} L_S = H_S \otimes \mathbb{1} - \mathbb{1} \otimes H_S \\ L_R = H_R \otimes \mathbb{1} - \mathbb{1} \otimes H_R \end{cases}$$

coupling : operator λV $\qquad$ λ = coupling constant.

typical example $\qquad V = G \otimes \varphi(g) \qquad \left(\leftrightarrow G \otimes \mathbb{1}_{\mathcal{H}_S} \otimes \varphi_\beta(g) \right)$

where $\begin{cases} G : \text{symmetric matrix on } \mathcal{H}_S \\ \varphi(g) : \text{field operator smoothed out} \\ \qquad \text{with } \underline{\text{form factor}} \ g(k),\ k \in \mathbb{R}^3 \end{cases}$

Choice of Liouville operator

$L_\lambda = L_0 + \lambda V - \lambda V'$

V': any operator that commutes with all observables $\mathcal{O}$:

$$e^{it(L_0+\lambda V)}\, \mathcal{O}\, e^{-it(L_0+\lambda V)} = e^{itL_\lambda}\, \mathcal{O}\, e^{-itL_\lambda}$$

(observables of S are $A \otimes \mathbb{1}_{\mathcal{H}_S}$ on $\mathcal{H}_S \otimes \mathcal{H}_S$, similarly for R)

Given a reference state $\psi \in \mathcal{H}$, can choose V' s.t.

$$L_\lambda \psi = 0$$

(V' has explicit form involving V & "modular data" of ψ)

Results

1) Systems close to equilibrium

reference state $\Omega_{\beta,\lambda}$: equil. state of coupled system.

(normal) initial state $\psi \sim B'\Omega_{\beta,\lambda}$, B' commutes with all observables

$$\langle \psi, e^{itL_\lambda} \mathcal{O} e^{-itL_\lambda} \psi \rangle$$
$$= \langle \psi, B' e^{itL_\lambda} \mathcal{O} \Omega_{\beta,\lambda} \rangle \xrightarrow{t\to\infty} \langle \psi, B' P_\lambda \mathcal{O} \Omega_{\beta,\lambda} \rangle$$

P_λ : projection onto kernel of L_λ.

Spectral analysis of L_λ (complex deformations, positive commutators, Mourre theory)

If λ is small & system is well coupled, then
$$\ker L_\lambda = \mathbb{C}\,\Omega_{\beta,\lambda}$$

Corollary: $P_\lambda = |\Omega_{\beta,\lambda}\rangle\langle\Omega_{\beta,\lambda}|$, so

$$\langle \psi, e^{itL_\lambda} \mathcal{O} e^{-itL_\lambda} \psi \rangle \xrightarrow{t\to\infty} \langle \Omega_{\beta,\lambda}, \mathcal{O}\, \Omega_{\beta,\lambda} \rangle$$

Rem: Starting point for dynamical resonance theory!

2) Systems far from equilibrium

reference state $\Omega_{R_1,\beta_1} \otimes \Omega_S \otimes \Omega_{R_2,\beta_2} = \Omega_0$

associated Liouville operator : $L_\lambda \Omega_0 = 0$.

It turns out : L_λ is <u>not</u> a <u>symmetric</u> operator

$$\langle \Omega_0, e^{itL_\lambda} \mathcal{O} e^{-itL_\lambda} \Omega_0 \rangle = \langle \Omega_0, e^{itL_\lambda} \mathcal{O} \Omega_0 \rangle$$

spectral analysis of L_λ : $\ker L_\lambda = \{0\}$, but there is a "generalized state" (vector) $\chi \notin \mathcal{H}$, s.t.

$$e^{itL_\lambda} \xrightarrow{t\to\infty} |\Omega_0\rangle\langle\chi|$$

in a weak sense : If $\mathcal{O}$ is sufficiently nice (e.g. energy flux), then

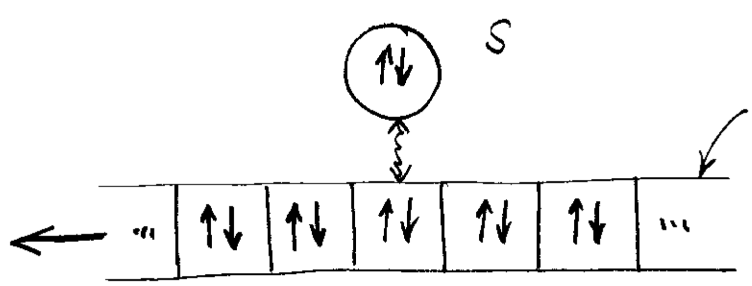
$$\langle \Omega_0, e^{itL_\lambda} \mathcal{O} e^{-itL_\lambda} \Omega_0 \rangle \xrightarrow{t\to\infty} \langle \chi_\lambda, \mathcal{O} \Omega_0 \rangle =: \omega_{NESS}(\mathcal{O})$$

examine χ_λ by perturbation theory :

$$\omega_{NESS}\left(\frac{d\,(\text{Energy } R_1)}{dt} \right) \propto \lambda^2 (T_2 - T_1) + O(\lambda^2)$$

3) Repeated interaction systems

concrete example : spin-spin



$\mathcal{E}$ chain at inv. temperature β

$$H_S = \begin{bmatrix} 0 & 0 \\ 0 & E_S \end{bmatrix}, \quad H_\mathcal{E} = \begin{bmatrix} 0 & 0 \\ 0 & E_\mathcal{E} \end{bmatrix}$$

interaction $S \leftrightarrow \mathcal{E}$: $\quad \lambda v$, where

$$v = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \otimes \underbrace{\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}}_{a^* \text{ creation op.}} + h.c.$$

<u>Deterministic system</u> $\quad v, \tau$ fixed, same in each interaction step. If $\tau \notin \mathcal{R}$ ("a resonance set") and λ small ($\neq 0$), then S approaches a limiting state $\rho_{+,\lambda}$, as $t \to \infty$ (expon. fast)

$$\rho_{+,\lambda}(A) = \frac{\alpha_1}{\alpha_1+\alpha_2}\left\langle \begin{bmatrix}1\\0\end{bmatrix}, A\begin{bmatrix}1\\0\end{bmatrix}\right\rangle + \frac{\alpha_2}{\alpha_1+\alpha_2}\left\langle \begin{bmatrix}0\\1\end{bmatrix}, A\begin{bmatrix}0\\1\end{bmatrix}\right\rangle$$

$$+ O(\lambda^2),$$

where $$\alpha_1 = |b|^2 \operatorname{sinc}^2\left[\frac{\tau(E_\mathcal{E}-E_S)}{2}\right] + e^{-\beta E_\mathcal{E}}|c|^2 \times \operatorname{sinc}^2\left[\frac{\tau(E_\mathcal{E}+E_S)}{2}\right]$$

$$\alpha_2 = e^{-\beta E_\mathcal{E}}|b|^2 \operatorname{sinc}^2\left[\frac{\tau(E_\mathcal{E}-E_S)}{2}\right] + |c|^2 \operatorname{sinc}^2\left[\frac{\tau(E_\mathcal{E}+E_S)}{2}\right]$$

$\left(\operatorname{sinc}(x) = \frac{\sin x}{x}\right)$

<u>Corollary</u> $\rho_{+,\lambda} = p_1 \left|\begin{bmatrix}1\\0\end{bmatrix}\right\rangle\left\langle\begin{bmatrix}1\\0\end{bmatrix}\right| + p_2 \left|\begin{bmatrix}0\\1\end{bmatrix}\right\rangle\left\langle\begin{bmatrix}0\\1\end{bmatrix}\right| + O(\lambda^2),$

where $0 \le p_{1,2} \le 1$, $p_1 + p_2 = 1$, and by varying the interaction (a, b, c, d) we can achieve any values of $p_{1,2} \in [0,1]$ (control of S)

Mechanism of process:

independence of the $\mathcal{E}_j$ in $\mathcal{C}$

$$\Rightarrow \quad \rho_0\left(\alpha_{RI}^{n}(A)\right) \sim \langle \psi_0, M^n A \psi_0 \rangle ,$$

where M is discrete-time propagator, reduced to system S; $\quad M = P e^{i\tau K} P$, $\quad M\psi_S = \psi_S$ (ref. state)

Spectral properties of matrix M determines $\lim_{n\to\infty} M^n$.

Random system $\quad \tau = \tau(\omega)$ random variable. If $p\left(\,|\tau - \mathcal{R}| \geq \eta > 0\right) \neq 0$, where $\mathcal{R}$ is a "resonance set" and if λ $(\neq 0)$ is small, then the system approaches an asymptotic state:

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \rho_0\left(A_{t=n,\omega}\right) = \langle \theta, A\psi_S \rangle ,$$

for almost all ω, and where $\theta = \left(P_{1,\mathbb{E}[M]}\right)^* \psi_S$.

Literature

Syst. close to equil.

RtE:

- Jakšić – Pillet — Comm. Math. Phys. 178, 627 (1996)
- Bach – Fröhlich – Sigal — J. Math. Phys. 41, 3985 (2000)
- Fröhlich – Merkli — Comm. Math. Phys. 251, 235 (2004)

therm. & decoh.:

- Merkli – Sigal – Berman
  - Phys. Rev. Lett 98, 130401 (2007)
  - Ann. Physics, to appear quant-ph/0702207

Syst. far from equil.

- Jakšić – Pillet — Comm. Math. Phys. 226, 131 (2002)
- Merkli – Mück – Sigal — J. Funct. Anal. 243, 87 (2007)
- Fröhlich – Merkli – Ueltschi — Ann. H. Poincaré 4, 897 (2003)

Repeated int. syst.

- Wellens et al — Phys. Rev. Lett. 85 3391 (2000)
- Bruneau – Joye – Merkli
  - J. Funct. Anal. 239, 310 (2006)
  - math.PR/0703675