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Open Quantum Systems

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Abstract

These notes give an informal introduction to open quantum systems. Starting from Schrödinger's equation, we are lead to density matrices and then to states which are positive, normalized linear functionals on observable algebras. We then go through the notions of KMS states and C^*-, W^*-, and quantum dynamical systems and mathematically formulate the property of return to equilibrium, which we then demonstrate to hold true for a spin-boson model. Finally, we give an application to decoherence of qubits of a quantum computer.

These notes are based on articles whose precise reference is appended. (Particularly useful were Pillet's article in [2] and [10].)

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I Quantum Statistical Mechanics

I.1 Schrödinger's Equation

We begin by reviewing the principal notions of quantum mechanics. The **state vector** of a system at a given time $t \in \mathbb{R}$ is determined by a normalized vector $\psi_t \in \mathcal{H}$ in a (separable, complex) **Hilbert space** $\mathcal{H}$.

The dynamics of the system is generated by the selfadjoint **Hamiltonian** $H = H^*$ on $\mathcal{H}$, i.e., given the initial value $\psi_0 \in \mathcal{H}$, Schrödinger's equation

$$\forall t \in \mathbb{R}: \quad \dot{\psi}_t \;=\; -iH\psi_t, \qquad \psi_{t=0} \;=\; \psi_0 \tag{I.1}$$

is the equation of motion in quantum mechanics.

Note that H is unbounded in many interesting situations. So, it is not defined for all vectors in $\mathcal{H}$, but only on a dense domain $\mathcal{D}(H) \subseteq \mathcal{H}$, $\overline{\mathcal{D}(H)} = \mathcal{H}$, on which it is closed. The existence and uniqueness of the solution to (I.1) is guaranteed by

Theorem 1 (Stone's theorem) *Let $\mathcal{H}$ be a Hilbert space.*

(i) Suppose that $(U_t)_{t\in\mathbb{R}} \subseteq B(\mathcal{H})$ is a ***strongly continuous unitary group****, i.e.,*

(a) $\forall t \in \mathbb{R}$: U_t is unitary, $U_0 = \mathbf{1}$,

(b) $\forall t, s \in \mathbb{R}$: $U_t U_s = U_{t+s}$,

(c) $\forall \psi \in \mathcal{H}$: $\lim_{t\to 0} ||U_t\psi - \psi|| = 0$.

Then there exists a selfadjoint operator $H = H^*$ on a dense domain $\mathcal{D}(H) \subseteq \mathcal{H}$ such that

$$\forall \psi \in \mathcal{D}(H): \qquad \lim_{t\to 0} \left\{ \frac{1}{t}(U_t\psi - \psi) \right\} \;=\; H\psi. \tag{I.2}$$

Moreover $U_t[\mathcal{D}(H)] \subseteq \mathcal{D}(H)$, and for all $\psi \in \mathcal{D}(H)$, $\psi_t = U_t\psi$ is the unique solution of

$$\forall t \in \mathbb{R}: \quad \dot{\psi}_t \;=\; -iH\psi_t, \qquad \psi_0 \;:=\; \psi. \tag{I.3}$$

(ii) Conversely, if $H = H^*$ is a selfadjoint operator on a dense domain $\mathcal{D}(H)$ then the initial value problem

$$\forall t \in \mathbb{R}: \quad \dot{\psi}_t \;=\; -iH\psi_t, \qquad \psi_0 \;=\; \psi \in \mathcal{D}(H) \tag{I.4}$$

has a unique solution $(\psi_t)_{t\in\mathbb{R}} \subseteq \mathcal{D}(H)$, and the family $(U_t)_{t\in\mathbb{R}} \subseteq B(\mathcal{H})$ of operators given by $U_t\psi := \psi_t$ defines a strongly continuous unitary group on $\mathcal{H}$.

Actually, Stone's theorem is a special case of the

Theorem 2 (Hille-Yosida theorem) *Let X be a Banach space over $\mathbb{C}$.*

(i) If $\{U_t\}_{t\geq 0} \subseteq B(X)$ is a C_0-semigroup, i.e.,

  (a) $U_0 = \mathbf{1}$,

  (b) $\forall t, s \geq 0$: $U_t U_s = U_{t+s}$,

  (c) $\forall x \in X$: $\lim_{t\to 0} \|U_t x - x\| = 0$,

then there exists a densely defined, closed operator $G \in \mathcal{L}(\mathrm{dom}(G),\ X)$, $\overline{\mathrm{dom}(G)} = X$, such that

$$\exists \beta > 0,\ M < \infty\ \forall\, \mathrm{Re}\,\lambda > \beta : \quad \|(\lambda - \beta G)^{-n}\|_{op} \ \leq \ \frac{M}{(\mathrm{Re}\,\lambda - \beta)^n} \tag{I.5}$$

and that

$$\forall x \in \mathrm{dom}(G) : \quad \lim_{t\to 0} \left\{ \frac{1}{t}(U_t x - x) \right\} \ = \ Gx, \tag{I.6}$$

i.e., G is the generator of $U_{(.)}$.

(ii) Conversely, if G obeys (I.3) *then, for all $x \in \mathrm{dom}(G)$, the initial value problem*

$$\forall t > 0 : \quad \dot{x}_t \ = \ Gx, \qquad x_0 = x \tag{I.7}$$

has a unique solution $x_{(.)} \in C^1(\mathbb{R}_0^+;\ X)$, and the operator $U_t :\ \mathrm{dom}(G) \to X$, $U_t x := x_t$ extends by continuity to a C^0-semigroup.

The unitary operator U_t in Theorem 1 is usually denoted $U_t = e^{-itH}$, so

$$\psi_t \ = \ e^{-itH} \psi_0. \tag{I.8}$$

Given an observable $A \in B(\mathcal{H})$, its expectation value in a vector state $\psi \in \mathcal{H}$ is given as

$$\langle A \rangle_\psi \ := \ \langle \psi | A \psi \rangle. \tag{I.9}$$

Hence, defining $\alpha_t : B(\mathcal{H}) \to B(\mathcal{H})$ by

$$\alpha_t(A) \ := \ e^{itH} A e^{-itH}, \tag{I.10}$$

$\alpha := (\alpha_t)_{t\in\mathbb{R}}$ defines a family of automorphisms (= bijective linear operators) on $B(\mathcal{H})$ such that

$$\langle \psi_t | A \psi_t \rangle \ = \ \langle \psi | \alpha_t(A) \psi \rangle. \tag{I.11}$$

The **Heisenberg equation of motion** is then

$$\forall t \in \mathbb{R} : \quad \frac{\mathrm{d}}{\mathrm{d}t} \, [\alpha_t(A)] \;=\; i[H, \alpha_t(A)], \quad \alpha_0(A) \;=\; A. \tag{I.12}$$

This ODE, however, is less innocent as it may seem. Namely, the limit involved in differentiating $t \mapsto \alpha_t(A)$ is not a norm limit, but rather a weak limit:

$$\forall \varphi, \psi \in \mathcal{D}(H) : \; \frac{\mathrm{d}}{\mathrm{d}t} \, \langle \varphi | \alpha_t(A) \psi \rangle \;=\; \langle \varphi | i[H, \; \alpha_t(A)] \psi \rangle. \tag{I.13}$$

Also, $\alpha_t(A) \in B(\mathcal{H})$ which is not a Hilbert space, but usually a non-separable Banach space (i.e., its norm is not given by a scalar product and it does not contain a countable dense subset like, e.g., $L^\infty([0,1])$).

I.2 Density matrices

In quantum mechanics, we are always simplifying the description of the evolution of the universe by focusing on a small part of it (e.g., all observables which can be realized on earth). In principle, when describing a system by a state $\psi \in \mathcal{H}$ in a Hilbert space $\mathcal{H}_{syst}$, we should always have in the back of our mind that there is the rest of the world (=everything but the system) evolving in a Hilbert space $\mathcal{H}_{rest}$ which is likely to be much bigger (whatever that may mean) than $\mathcal{H}_{syst}$, so that actually the total wave function Ψ^{univ} of the entire universe is a vector in

$$\mathcal{H}_{universe} \;=\; \mathcal{H}_{syst} \otimes \mathcal{H}_{rest}. \tag{I.14}$$

Measuring observables $A \in B(\mathcal{H}_{syst})$ amounts to measuring

$$\langle A \rangle_{syst} \;:=\; \langle \Psi^{univ} | (A \otimes \mathbf{1}_{rest}) \Psi^{univ} \rangle_{universe} \;=\; \mathrm{Tr}_{syst}\{\rho A\}, \tag{I.15}$$

where $\rho_{syst} \in B(\mathcal{H}_{syst})$ is defined by

$$\langle \varphi | \rho_{syst} \tilde{\varphi} \rangle_{syst} \;:=\; \big\langle \Psi^{univ} \big| \, \big(|\tilde{\varphi}\rangle\langle\varphi| \otimes \mathbf{1}_{rest} \big) \Psi^{univ} \big\rangle_{universe}. \tag{I.16}$$

Obviously, ρ_{syst} is a positive operator of trace one. Spectral theory implies that there is an ONB $\{\varphi_n\}_{n=1}^\infty \subseteq \mathcal{H}_{syst}$ of eigenvectors of ρ, i.e.,

$$\rho_{syst} \;=\; \sum_{n=1}^\infty \lambda_n \; |\varphi_n\rangle\langle\varphi_n|, \quad 0 \le \lambda_n, \quad \sum_{n=1}^\infty \lambda_n \;=\; 1. \tag{I.17}$$

Trace class operators obeying (I.17) are called **density matrices**. States given by single wave functions ψ, as in (I.1), correspond to density matrices of rank one,

$$\rho_\psi := |\psi\rangle\langle\psi| \quad \Longrightarrow \quad \langle A\rangle_\psi = \langle\psi|A\psi\rangle = \mathrm{Tr}\{\Big(|\psi\rangle\langle\psi|\Big)A\} = \mathrm{Tr}\{\rho A\}, \tag{I.18}$$

so-called **pure** states.

Going back to $\mathcal{H}_{syst} \otimes \mathcal{H}_{rest}$, we observe that

$$\rho \text{ is pure, } \rho = |\psi_{syst}\rangle\langle\psi_{syst}| \quad \Longleftrightarrow \quad \exists\psi_{rest}: \ \Psi^{univ} = \psi_{syst} \otimes \psi_{rest}. \tag{I.19}$$

This will hardly ever be the case if the system interacts with the rest of the universe.

Some textbooks on quantum mechanics introduce density matrices by invoking a necessity to study "statistical mixtures" due to an "uncertainty" (not the Heisenberg uncertainty principle) that seems to relate to the Copenhagen interpetation of the meaning of the wave function - I never understood this. So, as far as I am concerned, the main physical reason for considering density matrices, as opposed to mere wave function, lies in (I.19) and the fact that any physical system is likely to be a subsystem of a yet bigger one. Mathematically, one may argue that density matrices naturally arise as the closed convex hull of pure states, forming a subspace of the dual of all observables (which would here be identified with all bounded operators on the physical Hilbert space).

We thus have to be prepared to change our viewpoint to translating the Schrödinger equation (I.1) for wave functions into one for density matrices. Namely, for $\psi_t = e^{-itH}\psi_0$ we have

$$\rho_t \;=\; |\psi_t\rangle\langle\psi_t| \;=\; e^{-itH}|\psi_0\rangle\langle\psi_0|e^{itH} \;=\; e^{-itH}\rho_0 e^{itH}, \tag{I.20}$$

and hence

$$\forall t > 0: \qquad \dot\rho_t \;=\; -i[H,\, \rho_t], \quad \rho_0 \;=\; \rho_{t=0}. \tag{I.21}$$

If we define $\eta_t := \sqrt{\rho_t} \in \mathcal{L}^2(\mathcal{H})$ then we observe that

$$\eta_t \;=\; \sqrt{U_t\rho_0U_t^*} \;=\; U_t\sqrt{\rho_0}U_t^* \;=\; U_t\eta_0U_t^* \tag{I.22}$$

and hence

$$\forall t \in \mathbb{R}: \qquad \dot\eta_t \;=\; -iL(\eta_t),\ \eta_0 \;=\; \sqrt{\rho_0}, \tag{I.23}$$

where $L(\eta_t) := [H,\, \eta_t]$. In fact, $L = L^*$ on a suitable domain $\mathcal{D}(L) \subseteq \mathcal{L}^2(\mathcal{H})$.

We introduce the **(von Neumann) entropy** $S(\rho)$ of a density matrix $\rho = \sum_{k=1}^\infty \lambda_k|\varphi_k\rangle\langle\varphi_k|$ (where $\langle\varphi_k|\,\varphi_l\rangle = \delta_{kl}$, $\lambda_k \geq 0$, $\sum_k \lambda_k = 1$) by

$$S(\rho) := -\mathrm{Tr}\{\rho\ln\rho\} \;=\; \sum_{k=1}^\infty \lambda_k \ln\left(\frac{1}{\lambda_k}\right) \geq 0, \tag{I.24}$$

if the series is summable and $S(\rho) := \infty$ otherwise.

The *maximum entropy principle* asserts that the equilibrium state ρ_* of a system for a fixed energy expectation value $E = \mathrm{Tr}\{\rho H\}$ is determined by the maximal entropy, i.e., for

$$\mathcal{S}_E := \sup \big\{ S(\rho) \big| \ \rho \text{ is a density matrix, } \mathrm{Tr}\{\rho H\} \ = \ E \big\}, \tag{I.25}$$

it holds true that

$$\mathcal{S}_E \ = \ S(\rho_*). \tag{I.26}$$

From this requirement it follows that

$$\mathcal{S}_E < \infty \quad \iff \quad \exists \beta > 0 : \ \mathrm{Tr}\{e^{-\beta H}\} < \infty, \ \mathrm{Tr}\{H e^{-\beta H}\} \ = \ E, \tag{I.27}$$

and in this case

$$\rho_* \ = \ Z^{-1} \, e^{-\beta H}, \quad Z := \mathrm{Tr}\{e^{-\beta H}\}. \tag{I.28}$$

We are now going to determine $e^{-\beta H}$ and $Z = \mathrm{Tr}\{e^{-\beta H}\}$. In view of (I.28), we study the condition that $e^{-\beta H} \in \mathcal{L}^1(\mathcal{H})$.

Suppose that $\mathfrak{h}$ is the one-particle Hilbert space of the system (e.g., $L^2(\Lambda)$, $\Lambda \subseteq \mathbb{R}^d$ or $l^2(\Lambda)$, $\Lambda \subseteq \mathbb{Z}^d$), and $h = h^*$ is the self-adjoint 1-particle Hamiltonian.

If the spectrum of h is not purely discrete, i.e., for some $E \in \mathbb{R}$ and all $\varepsilon > 0$,

$$\mathrm{Tr}\{ \ \mathbf{1}[E - \varepsilon < h < E + \varepsilon] \ \} \ = \ \infty \tag{I.29}$$

then, by the functional calculus,

$$\begin{aligned} \mathrm{Tr}\{e^{-\beta H}\} \ &\geq \ \mathrm{Tr}\{ \ e^{-\beta H} \ \mathbf{1}[E - \varepsilon < h < E + \varepsilon] \ \} \\ &\geq \ e^{-\beta H} \ \mathrm{Tr}\{ \ \mathbf{1}[E - \varepsilon < h < E + \varepsilon] \ \} \ = \ \infty, \end{aligned}$$

and $e^{-\beta H}$ is not trace class and hence not a density matrix. So, the notion of a density matrix representing $e^{-\beta H}$ necessarily requires that $\sigma(h) = \sigma_d(h)$.

If this is fulfilled, $\sigma(h) = \sigma_d(h)$, then we consider the second quantization

$$\mathbb{H} := d\Gamma(h) := \sum_{k=1}^{\infty} \ h_k \ a_k^* a_k. \tag{I.30}$$

on bosonic Fock space $\mathcal{F}_b(\mathfrak{h}) =: \mathcal{H}$, where $h = \sum_{k=1}^{\infty} h_k \, |\varphi_k\rangle \, \langle\varphi_k|$ and $a_k^{\#} := a^{\#}(\varphi_k)$. By replacing h_k by $h_k - \inf_k h_k - 1$, if necessary, we may assume w.l.o.g. that $h_k \geq 1$. We observe that

$$e^{-\beta \mathbb{H}} \ = \ \Gamma(e^{-\beta h}) \ = \ \bigoplus_{N=0}^{\infty} \left(\underbrace{e^{-\beta h} \otimes \ldots \otimes e^{-\beta h}}_{N \text{ factors}} \right), \tag{I.31}$$

hence

$$\begin{aligned}\mathrm{Tr}\{e^{-\beta\mathbb{H}}\} &= \sum_{N=0}^{\infty} \mathrm{Tr}\{e^{-\beta h}\otimes\ldots\otimes e^{-\beta h}\} \\ &= \sum_{N=0}^{\infty} \sum_{\substack{(n_k)_{k=1}^{\infty}\subseteq\mathbb{N}_0,\\ \sum_k n_k=N}} e^{-\beta\sum_{k=1}^{\infty} h_k n_k} \\ &= \prod_{k=1}^{\infty}\Big(\sum_{n=0}^{\infty}\big(e^{-\beta h_k}\big)^n\Big) = \prod_{k=0}^{\infty}\frac{1}{1-e^{-\beta h_k}}.\end{aligned}$$

Therefore

$$\begin{aligned}\mathrm{Tr}\{e^{-\beta\mathbb{H}}\}<\infty \quad &\Longleftrightarrow \quad \sum_{k=1}^{\infty} 1-\frac{1}{1-e^{-\beta h_k}} = \sum_{k=1}^{\infty}\frac{e^{-\beta h_k}}{1-e^{-\beta h_k}} < \infty \\ &\Longleftrightarrow \quad \sum_{k=1}^{\infty} e^{-\beta h_k} < \infty,\end{aligned}$$

additionally using that $1 \geq 1-e^{-\beta h_k} \geq 1-e^{-\beta}$.

As a concrete example, we study the discrete Laplacian $h = -\Delta = \sum_{|e|=1}(1-T^e)$ on $l^2(\mathbb{Z}^d)$ and its restriction $\Delta_L = \mathbf{1}_{\Lambda_L}\Delta\mathbf{1}_{\Lambda_L}$ to $l^2(\Lambda_L)$, with $\Lambda_L = \mathbb{Z}^d \cup [-L/2, L/2)$ and $L \in 2\mathbb{Z}$ even and where $(T^k\varphi)(x) := \varphi(x-k)$. For $1 \ll L < \infty$, we have that

$$\begin{aligned}\mathrm{Tr}\{e^{-\beta h_L}\} &= \Big(\frac{L}{2\pi}\Big)^d \Big(\frac{2\pi}{L}\Big)^d \sum_{\xi\in\frac{2\pi}{L}\mathbb{Z}_L^d} e^{-\beta\omega_L(\xi)} \\ &\overset{L\gg 1}{\sim} \Big(\frac{L}{2\pi}\Big)^d \int_{[-\pi,\pi]^d} e^{-\beta\omega(\xi)}\,\mathrm{d}^d\xi, \qquad \text{(I.32)}\end{aligned}$$

where ω_L and ω denote the spectral values of $-\Delta_L$ and of $-\Delta$, respectively.

Without deriving it in detail, we remark that establishing (I.32) goes through the discrete Laplacian $-\Delta_L^{per}$ on $l^2(\Lambda_L)$ with periodic boundary conditions and eigenvalues ω_L^{per}, because the corresponding Schrödinger equation $-\Delta_L^{per}\varphi_\xi = \omega_L^{per}(\xi)\varphi_\xi$ can be solved explicitly. Indeed, the spectrum of $-\Delta_L^{per}$ is given as

$$\begin{aligned}\sigma(-\Delta_L^{per}) &= \big\{\omega_L^{per}(\xi)\ \big|\ \xi\in 2\pi L^{-1}\mathbb{Z}_L^d\big\}, \quad \omega_L^{per}(\xi) = \sum_{\nu=1}^{d}\big(1-\cos(\xi_\nu)\big), \qquad \text{(I.33)} \\ 2\pi L^{-1}\mathbb{Z}_L^d &\cong \big\{-\pi(L-2)L^{-1}, -\pi(L-4)L^{-1},\ldots,\pi(L-2)L^{-1},\pi\big\}^d.\end{aligned}$$

One then shows that

$$\lim_{L\to\infty} \frac{\mathrm{Tr}\{\exp[-\beta(-\Delta_L)]\}}{\mathrm{Tr}\{\exp[-\beta(-\Delta_L^{per})]} \;=\; 1, \tag{I.34}$$

which follows from the fact that the difference of $-\Delta_L$ and $-\Delta_L^{per}$ is bounded in norm by 1 and of rank $\#\{\partial\Lambda_L\} \leq 2dL^{d-1}$. Hence its contribution to the partition function $\mathrm{Tr}\{\exp[-\beta(-\Delta_L)]$ is negligible in the limit $L \to \infty$.

Returning to Eq. (I.32), we observe that

$$\lim_{L\to\infty} \mathrm{Tr}\{e^{-\beta h_L}\} \;=\; \infty. \tag{I.35}$$

So, while $\rho_L := Z_L^{-1}\, e^{-\beta \mathbb{H}_L} \in \mathcal{L}^1(\mathcal{H})$ defines a density matrix, for any $L < \infty$ and with $\mathbb{H}_L := d\Gamma(h_L)$ being the second quantization of h_L, we conclude that the limit of the sequence $(\rho_L)_{L=1}^{\infty} \subseteq \mathcal{L}^1(\mathcal{H})$ of density matrices, if existent at all, is *not* a density matrix. Nor is $e^{-\beta\mathbb{H}_\infty} \in \mathcal{L}^1(\mathcal{H})$.

This shows that the set of density matrices is not closed under taking thermodynamic limits. The example also shows that this has nothing to do with the boundedness or unboundedness of h_L (which is the discrete Laplacian is chosen, rather than the usual differential operator). It also shows that the convergence of h_L to h_∞ or of $\mathbb{H}_L$ to $\mathbb{H}_\infty$(in a suitable sense) is of no help, either.

I.3 Local Observables and KMS-Condition

From the previous section it is clear that density matrices are not suitable for studying systems right away in the thermodynamic limit. This insight leads us to local observables $\mathcal{A}_{loc} \subseteq B(\mathcal{H})$, where $\mathcal{H} = \mathcal{F}_b(\mathfrak{h})$ is the bosonic Fock space over $\mathfrak{h} = \ell^2(\mathbb{Z}^d)$.

In order to introduce $\mathcal{A}_{loc}$, we remark that, for any partition $\mathbb{Z}^d = \Lambda \cup \Lambda^c$, we have $\mathfrak{h} = \mathfrak{h}_\Lambda \oplus \mathfrak{h}_{\Lambda^c}$, with $\mathfrak{h}_\Lambda = \ell^2(\Lambda)$ and $\mathfrak{h}_{\Lambda^c} = \ell^2(\Lambda^c)$. For $x_1, x_2, \ldots, x_M \in \Lambda$ and $y_1, y_2, \ldots, y_N \in \Lambda^c$ we define

$$J\big[a_{x_1}^* a_{x_2}^* \cdots a_{x_M}^*\, a_{y_1}^* a_{y_2}^* \cdots a_{y_N}^* \Omega\big] \;:=\; a_{x_1}^* a_{x_2}^* \cdots a_{x_M}^* \Omega_\Lambda \,\otimes\, a_{y_1}^* a_{y_2}^* \cdots a_{y_N}^* \Omega_{\Lambda^c}. \tag{I.36}$$

Then, extending J to $\mathcal{H}$ by linearity and continuity, we see that

$$\mathcal{H} \;\cong\; \mathcal{F}(\mathfrak{h}_\Lambda) \otimes \mathcal{F}(\mathfrak{h}_\Lambda^\perp) \tag{I.37}$$

are isomorphic. Moreover there is a natural injection $j : \mathcal{F}(\mathfrak{h}_\Lambda) \to \mathcal{H}$, namely

$$j\big[a_{x_1}^* a_{x_2}^* \cdots a_{x_M}^* \Omega_\Lambda\big] \;:=\; a_{x_1}^* a_{x_2}^* \cdots a_{x_M}^* \Omega_\Lambda \otimes \Omega_{\Lambda^c}. \tag{I.38}$$

While $\mathcal{F}(\mathfrak{h}_\Lambda)$ is clearly the subspace of vectors supported on Λ, the injection j in (I.38) yields a useful characterization of $\mathcal{F}(\mathfrak{h}_\Lambda) \cong j[\mathcal{F}(\mathfrak{h}_\Lambda)] \subseteq \mathcal{H}$ as a subspace: it contains all vectors with zero particle number (expectation) in Λ^c. This leads us to define the observables supported on a given set $\Lambda \subseteq \mathbb{Z}^d$ as follows,

$$\mathcal{A}(\Lambda) \ := \ \big\{ A \in B(\mathcal{H}) \ \big| \ \forall x \in \Lambda^c : A a_x^* a_x = a_x^* a_x A = 0 \quad \big\}. \qquad \text{(I.39)}$$

The **local observables** are then defined as the norm closure of all observables of bounded support,

$$\mathcal{A}_{loc} \ := \ \overline{\bigcup \big\{ \mathcal{A}(\Lambda) \ \big| \ \Lambda \subseteq \mathbb{Z}^d, \ |\Lambda| < \infty \big\}}, \qquad \text{(I.40)}$$

or, equivalently, $A \in \mathcal{B}[\mathcal{H}]$ is a local observable if, for any $\varepsilon > 0$, there exist a finite subset $\Lambda \subseteq \mathbb{Z}^d$ and an observable $\widetilde{A} \in \mathcal{A}(\Lambda)$ supported on Λ, such that

$$\|A - \widetilde{A}\|_{op} \ < \ \varepsilon. \qquad \text{(I.41)}$$

We come to introducing the Kubo-Martin-Schwinger (KMS) boundary condition. Let $\Lambda \subset \mathbb{Z}^d$ be a bounded subset, $A, B \in \mathcal{A}(\Lambda)$ two observables supported in Λ, and $L \gg 1$ sufficiently large so that $\Lambda_L \supset \Lambda$. Using the density matrix

$$\rho_L \ := \ Z_L^{-1} \, e^{-\beta \mathbb{H}_L} \qquad \text{(I.42)}$$

to define a state on $\mathcal{A}(\Lambda_L)$ by

$$\omega_L(A) := \mathrm{Tr}\{\rho_L \, A\} \qquad \text{(I.43)}$$

and a time evolution automorphism group $(\alpha_L^t)_{t \in \mathbb{R}}$ on $\mathcal{A}(\Lambda_L)$ by

$$\alpha_L^t(A) := e^{it\mathbb{H}_L} A e^{-it\mathbb{H}_L}, \qquad \text{(I.44)}$$

where $\mathbb{H}_L := d\Gamma(\Delta_L)$. We then observe that the cyclicity of the trace implies

$$\begin{aligned} \omega_L(A\alpha_L^t(B)) \ &= \ Z_L^{-1} \ \mathrm{Tr}\big\{ \ e^{-\beta\mathbb{H}_L} A \ e^{it\mathbb{H}_L} B e^{-it\mathbb{H}_L} \ \big\} \\ &= \ Z_L^{-1} \ \mathrm{Tr}\big\{ \ e^{i(-t+i\beta)\mathbb{H}_L} A e^{-i(-t+i\beta)\mathbb{H}_L} \ e^{-\beta\mathbb{H}_L} B \ \big\} \\ &= \ Z_L^{-1} \ \mathrm{Tr}\Big\{ e^{\ -\beta\mathbb{H}_L} B \alpha_L^{-t+i\beta}(A) \ \Big\} \\ &= \ \omega_L(B\alpha_L^{-t+i\beta}(A)), \end{aligned} \qquad \text{(I.45)}$$

which is called **KMS Condition** and holds for all $L < \infty$.

Moreover, for $A \in \mathcal{A}_{loc}$

$$\alpha_L^t(A) \stackrel{L\to\infty}{\longrightarrow} \alpha^t(A) \quad \text{strongly}, \qquad \text{(I.46)}$$

where $\alpha^t = e^{it\mathbb{H}} \ \cdot \ e^{-it\mathbb{H}}$ and $\mathbb{H} := d\Gamma(\Delta)$. It is the KMS Condition (I.45) and Eq. (I.46) which survive the thermodynamic limit $L \to \infty$. To understand this, we introduce the notion of C^*-, W^*-Algebras.

II C^*- and W^*-Algebras

II.1 Definitions

Definition 3

(i) *A $\mathbb{C}$-vector space $\mathcal{A}$ equipped with distributive multiplication $\mathcal{A}\times\mathcal{A}\to\mathcal{A}$ is called an **algebra**.*

(ii) *An algebra $\mathcal{A}$ which is also a Banach space with $\|AB\| \le \|A\| \cdot \|B\|$ is called a **Banach algebra**.*

(iii) *A Banach algebra $(\mathcal{A}, \|\cdot\|)$ with an involution $*: \ \mathcal{A}\to\mathcal{A}$, such that $A** = A$ and $\|A^*A\| = \|A\|^2$, for all $A \in \mathcal{A}$, is called a C^***-algebra**.*

(iv) *A C^*-algebra $(\mathcal{A}, \|\cdot\|)$, which is the dual space of some Banach space $\mathcal{A}_*$, is called a W^***-Algebra**. In this case, $\mathcal{A}_*$ is called **predual of** $\mathcal{A}$.*

Examples:

- $\mathrm{Mat}(N, \mathbb{C})$ is a C^*-algebra w.r.t. the norm induced by the unitary scalar product.
- $B(\mathcal{H})$ is a C^*-algebra.
- The compact operators $\mathrm{Com}(\mathcal{H}) \subseteq B(\mathcal{H})$ on $\mathcal{H}$ is a C^*-(sub)algebra of $B(\mathcal{H})$.
- $B(\mathcal{H})$ is W^*-algebra with $B(\mathcal{H})_* = \mathcal{L}^1(\mathcal{H})$.
- The GNS construction below shows that any C^*-Algebra is $\subseteq B(\mathcal{H})$, for some $\mathcal{H}$.

Definition 4 *Let $\mathcal{A}$ be a C^*-Algebra.*

(i) *$(\mathcal{H}, \pi)$ is called a **representation of** $\mathcal{A}$ $:\Longleftrightarrow$ $\mathcal{H}$ is a Hilbert space and $\pi: \ \mathcal{A}\to B(\mathcal{H})$ is a $*$-automorphism, i.e., for all A, B $\mathcal{A}$,*

$$\pi(A+\lambda B) = \pi(A) + \lambda\pi(B), \ \pi(AB) = \pi(A)\pi(B), \ \pi(A^*) = \pi(A)^*. \tag{II.1}$$

*If $\ker \pi = 0$ then $(\mathcal{H}, \pi)$ is called **faithful**.*

(ii) *Let $(\mathcal{H}, \pi)$ be a representation of $\mathcal{A}$.*
*$\Omega \in \mathcal{H}$ is called **cyclic** $:\Longleftrightarrow$ $\overline{\pi(\mathcal{A})\Omega} = \mathcal{H}$.*
*$\Omega \in \mathcal{H}$ is called **separable** $:\Longleftrightarrow$ $\pi(A)\Omega = 0$ implies $\pi(A) = 0$.*

(iii) $(\mathcal{H}, \pi, \Omega)$ *is called a* ***cyclic representation of*** $\mathcal{A}$
$:\iff$ $(\mathcal{H}, \pi)$ *is a representation and* Ω *is cyclic in* $\mathcal{H}$.

(iv) *A linear functional* $\omega \in \mathcal{A}^*$ *is called a* ***state on*** $\mathcal{A}$
$:\iff$ $\|\omega\| = 1$ *and* $\omega(A^*A) \geq 0$*, for all* $A \in \mathcal{A}$.
Moreover, if $\omega(A^*A) = 0$ *implies* $A = 0$ *then* ω *is called* ***faithful***.

<u>Remarks:</u>

- If $(\mathcal{H}, \pi)$ is a representation then $\pi(A) \subseteq B(\mathcal{H})$ is a C^*-subalgebra.
- The cyclicity $\overline{\pi(\mathcal{A})\Omega} = \mathcal{H}$ of Ω means that $\pi(\mathcal{A})\Omega$ is dense in $\mathcal{H}$, i.e., for all $\psi \in \mathcal{H}$ and any $\varepsilon > 0$ there exists an $A \in \mathcal{A}$ such that $\|\psi - \pi(A)\Omega\| < \varepsilon$.
- If $\mathcal{A} = B(\mathcal{H})$ and $\rho \in \mathcal{L}^1(\mathcal{H})$ a density matrix, i.e., $\rho \geq 0$, $\mathrm{Tr}\rho = 1$, then
$$\omega_\rho(A) := \mathrm{tr}\{\rho A\} \tag{II.2}$$
defines a state.
- But not all states are of this form, we have
$$B(\mathcal{H})_* \;=\; \mathcal{L}^1(\mathcal{H}) \subsetneq B(\mathcal{H})^*. \tag{II.3}$$
This is much like
$$L^1(\mathbb{R}^d)^{**} \;=\; L^\infty(\mathbb{R}^d)^* \supsetneq L^1(\mathbb{R}^d). \tag{II.4}$$

Theorem 5 (GNS) *Let* $\mathcal{A}$ *be a* C^**-Algebra and* ω *a state on* $\mathcal{A}$.

(i) *There exists a cyclic representation* $(\mathcal{H}, \pi, \Omega)$ *of* $\mathcal{A}$ *such that*
$$\omega(A) \;=\; \langle \Omega |\, \pi(A)\Omega \rangle\,, \tag{II.5}$$
$(\mathcal{H}, \pi, \Omega)$ *is called* ***GNS representation of*** $(\mathcal{A}, \omega)$.

(ii) $(\mathcal{H}, \pi, \Omega)$ *is unique up to unitary equivalence, i.e., if* $(\widetilde{\mathcal{H}}, \widetilde{\pi}, \widetilde{\Omega})$ *is another cyclic representation of* $\mathcal{A}$ *then* $\exists U : \mathcal{H} \to \widetilde{\mathcal{H}}$ *unitary:* $\widetilde{\pi} = U\pi U^*$, $\widetilde{\Omega} = U\Omega$.

(iii) ω *is faithful* $\iff$ π *is faithful and* Ω *is separable.*

Corollary 6 *Let* $\alpha^t : \mathcal{A} \to \mathcal{A}$ *be a* $*$*-automorphism leaving* ω *invariant, i.e.,* $\omega(\alpha^t(A)) = \omega(A)$*, for all* $A \in \mathcal{A}$*. Then there exists a family of unitary operators* $(U_t)_{t\in\mathbb{R}}$ *such that* $\pi(\alpha^t(A)) = U_t \pi(A) U_t^*$, $U_t\Omega = \Omega$*, for all* t.

Exercise: Let $\mathcal{A} = B(\mathfrak{h})$ and $\rho \in \mathcal{L}^1(\mathfrak{h})$ a density matrix with $\ker(\rho) = 0$. Construct a (the GNS) cyclic representation $(\mathcal{H}, \pi, \Omega)$ of $\mathcal{A}$.
Hint: Observe that $(A, B) := \mathrm{Tr}\{\rho A^* B\}$ defines a scalar product.

Definition 7 *Let $\mathcal{A}$ be a C^*-Algebra, ω a state on $\mathcal{A}$, and $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ the GNS representation. A state $\widetilde{\omega} \in \mathcal{A}^*$ is called **normal with respect to** ω $:\Longleftrightarrow$ $\widetilde{\omega}$ is a density matrix in $B(\mathcal{H}_\omega)$, i.e., there exist an ONB $\{\psi_k\}_{k=1}^\infty \subseteq \mathcal{H}$ and a sequence $(\lambda_k)_{k=1}^\infty$ of nonnegative number with $\sum_k \lambda_k = 1$ such that*

$$\widetilde{\omega}(A) = \sum_{k=1}^{\infty} \lambda_k \langle \psi_k | \, \pi_\omega(A) \psi_k \rangle \, , \tag{II.6}$$

for all $A \in \mathcal{A}$.

Remark: Normality defines an equivalence relation, equivalence classes are "small perturbations of ω".

II.2 Dynamics on Operator Algebras

Definition 8 *$(\mathcal{A}, \alpha)$ is a **C^*-dynamical system** $:\Longleftrightarrow$
$\mathcal{A}$ is a C^*-Algebra and $\alpha = (\alpha^t)_{t \in \mathbb{R}}$ is a strongly continuous group of $*$-automorphisms on $\mathcal{A}$, i.e., $\alpha^{t=0} = \mathbf{1}$, $\alpha^t \alpha^s = \alpha^{t+s}$, and*

$$\forall A \in \mathcal{A} : \quad \lim_{t \to 0} \| \alpha^t(A) - A \| \; = \; 0. \tag{II.7}$$

Remark: Let $\mathcal{A} = B(\mathcal{H})$, $H = H^*$ on $\mathcal{H}$ and $\alpha^t := e^{itH} A e^{-itH}$. Then

$$(\mathcal{A}, \alpha) \text{ is a } C^*\text{-dynamical system} \iff H \text{ is bounded.} \tag{II.8}$$

Thus, the notion of C^*-dynamical systems is only of limited value.

Definition 9 *$(\mathcal{A}, \alpha)$ is a **W^*-dynamical system** $:\Longleftrightarrow$
$\mathcal{A}$ is a W^*-Algebra and $\alpha = (\alpha^t)_{t \in \mathbb{R}}$ a σ-weakly continuous group of $*$-automorphisms, i.e., $\alpha^{t=0} = \mathbf{1}$, $\alpha^t \alpha^s = \alpha^{t+s}$, and*

$$\forall \omega \in \mathcal{A}_*, \; A \in \mathcal{A} : \; \lim_{t \to 0} \omega(\alpha^t(A)) = \omega(A). \tag{II.9}$$

Definition 10 *$(\mathcal{A}, \alpha, \omega)$ is a **quantum dynamical system** $:\Longleftrightarrow$
$\mathcal{A}$ is a C^*-Algebra (with $\mathbf{1}$), $\alpha = (\alpha^t)_{t \in \mathbb{R}}$ a $*$-automorphism group, and ω an α-invariant state on $\mathcal{A}$, i.e., $\omega \circ \alpha^t = \omega$, so that $\forall A \in \mathcal{A}$: $t \mapsto \omega(A^* \alpha^t(A))$ is continuous.*

Theorem 11 *If $(\mathcal{A}, \alpha)$ is a C^*-dynamical system or W^*-dynamical system then there exists an α-invariant state ω on $\mathcal{A}$.*

Idea of Proof: Let μ be a state on $\mathcal{A}$ and define

$$\mu_T(A) := \frac{1}{T} \int_0^T \mu\big(\alpha^t(A)\big)\, dt. \tag{II.10}$$

Then $(\mu_T)_{T>0}$ is a family of states (normalized, positive and, in particular, bounded linear functionals on $\mathcal{A}$), $\mu_T \in \mathcal{A}^*$, $\|\mu_T\|_{\mathcal{A}^*} = 1$, $\mu_T(A^*A) \geq 0$. The Banach-Alaoglu theorem now guarantees the existence of a weak-$*$-limit point ω and, passing to a subsequence, if necessary, we have

$$\forall A \in \mathcal{A}: \quad \omega(A) = \lim_{T\to\infty} \mu_T(A). \tag{II.11}$$

Then $\omega(A^*A) \geq^0$, $\omega \in \mathcal{A}^*$, $\|\omega\| = 1$. Moreover

$$\begin{aligned} |\mu_T(\alpha^t(A)) - \mu_T(A)| &\leq \frac{1}{T} \int_0^\infty |\mu(\alpha^s(A))| \mathrm{d}s + \frac{1}{T} \int_T^{T+t} |\mu(\alpha^s(A))| \mathrm{d}s \\ &\leq \frac{2t\,\|A\|}{T} \quad \overset{T\to\infty}{\longrightarrow} 0 \end{aligned} \tag{II.12}$$

so $\omega(\alpha^t(A)) = \lim_{T\to\infty} \mu_T(\alpha^t(A)) = \lim_{T\to\infty} \mu_T(A) = \omega(A)$. $\square$

Remarks:

- The limit state ω may not be normal w.r.t. μ.
- Thus, every C^*-dynamical system and W^*-dynamical system is a quantum dynamical system, because stationary states always exist (but might not be unique).

Theorem 12 *Let $(\mathcal{A}, \alpha, \omega)$ be a quantum dynamical system and $(\mathcal{H}, \pi, \Omega)$ its GNS representation. There exists a unique self-adjoint operator $L = L^*$ on $\mathcal{H}$, the* ***standard Liouvillean****, such that*

$$\begin{aligned} (i) \quad \pi\big(\alpha^t(A)\big) &= e^{itL}\, \pi(A)\, e^{-itL} \quad , \\ (ii) \quad L\,\Omega &= 0. \end{aligned}$$

Remark: Conversely, for a C^*-Algebra $\mathcal{A}$ and a state ω on $\mathcal{A}$ with GNS representation $(\mathcal{H}, \pi, \Omega)$, there exists a natural self-adjoint operator $\mathscr{L}$, the *modular Liouvillean*, and a natural $*$-automorphism group $\tau = (\tau^t)_{t\in\mathbb{R}}$ on $\mathcal{A}$, the *modular automorphism group*, such that (i) and (ii) hold true for $(\mathcal{A}, \tau, \omega)$. This is a result of *Tomita-Takesaki theory* which I completely suppress here.

Definition 13 *Let $(\mathcal{A}, \alpha)$ be a C^*-dynamical system or W^*-dynamical system, $\beta > 0$, and $\mathcal{S}_\beta := \{z \in \mathbb{C} | 0 < \operatorname{Im} z < \beta\} \subseteq \mathbb{C}$ a strip on the upper half plane. A state ω on $\mathcal{A}$ is called an (α, β)-**KMS state** :$\Longleftrightarrow$*
For all $A, B \in \mathcal{A}$ there exists a function $F^{(\beta)}_{A,B} : \mathcal{S}_\beta \to\to \mathbb{C}$, which is analytic on $\mathcal{S}_\beta$, continuous on $\overline{\mathcal{S}_\beta}$, and obeys

$$\forall t \in \mathbb{R} : \ F^{(\beta)}_{A,B}(t) = \omega(A\alpha^t(B)), \quad F^{(\beta)}_{A,B}(t + i\beta) = \omega(\alpha^t(B)A). \tag{II.13}$$

Theorem 14 *Let $(\mathcal{A}, \alpha)$ be a C^*-dynamical system or W^*-dynamical system, $\beta > 0$, and ω an (α, β)-KMS state. Then ω is α-invariant.*

III KMS states and Return to Equilibrium

III.1 The Araki-Woods Representation

The definition of (α, β)-KMS states leaves the question open whether such states exist in concrete situations.

Suppose we study an N-level atom, $\mathcal{K}_{at} = \mathbb{C}^N$ is the Hilbert space of atomic vector states of energies $E_1 < E_2 < \ldots < E_N$ (in particular, we assume that no eigenvalue is degenerate), so $H = \sum_{i=1}^N E_i |\varphi_i\rangle \langle\varphi_i| = H^*$, $\langle\varphi_i| \varphi_j\rangle = \delta_{ij}$ is the Hamiltonian, $\rho_{at} = Z_\beta^{-1} \cdot \sum_{i=1}^N e^{-\beta E_i} |\varphi_i\rangle \langle\varphi_i|$ is its density matrix at temperature $\beta > 0$, so that $\omega_{at}(A) = \operatorname{Tr}\{\rho_{at} A\}$ defines an (α, β)-KMS state on $B(\mathcal{K}_{at})$, where $\alpha^t_{at}(A) = e^{itH_{at}} A e^{-itH_{at}}$.

The GNS representation is $(\mathcal{H}_{at} = \mathcal{K}_{at} \otimes \mathcal{K}_{at}, \pi_{at}, \Omega_{at})$ with $\pi_{at}(A) = A \otimes \mathbf{1}$ and

$$\Omega_{at} := \sum_{i=1}^N Z_\beta^{-1}\, e^{-\beta E_i}\, \varphi_i \otimes \overline{\varphi_i}. \tag{III.1}$$

Note that $\pi'_{at}(A) := \mathbf{1} \otimes A^*$ is another representation commuting with π_{at}.

Next, suppose we consider a free scalar quantum field on a Fock space $\mathcal{K}_{ph} = \mathcal{F}(L^2(\mathbb{R}^d))$ with field Hamiltonian $H_{ph} = \int \varepsilon(k)\, a_k^* a_k \,\mathrm{d}^d k$ and an automorphism group $\alpha_{ph} = (\alpha^t_{ph})_{t\in\mathbb{R}}$ on the Weyl algebra $\mathcal{W}$ (actually, not the Weyl algebra over all of $L^2(\mathbb{R}^d)$, but a suitable subalgebra, depending on the dispersion relation ε), such that, for all $A \in \mathcal{W}$

$$\alpha^t_{ph}(A) := e^{itH_{ph}} A e^{-itH_{ph}}, \tag{III.2}$$

i.e.,

$$\alpha^t_{ph}(a^\#(f)) = a^\#(e^{it\varepsilon} f). \tag{III.3}$$

Araki and Woods gave an explicit construction of the GNS-representation of the corresponding (α_{ph}, β)-KMS state as follows, the GNS representation is $(\mathcal{H}_{ph}, \pi_{ph}, \Omega_{ph})$ with

$$\mathcal{H}_{ph} = \mathcal{K}_{ph} \otimes \mathcal{K}_{ph} \cong \mathcal{F}\left[L^2(\mathbb{R}^d \times \{l, r\})\right], \tag{III.4}$$

$$\Omega_{ph} = \text{ vacuum in } \mathcal{H}_{ph} \ , \tag{III.5}$$

$$\pi_{ph}(a(f)) := a_l(\sqrt{1+\rho_\beta}\ f) + a_r^*(\sqrt{\rho_\beta}\ \overline{f}), \tag{III.6}$$

(there is a commuting representation $\pi'_{ph}(a(f)) := a_l^*(\sqrt{\rho_\beta}\,\overline{f}) + a_r(\sqrt{1+\rho_\beta}\,f)$) where

$$\rho_\beta(k) := \frac{1}{e^{\beta\varepsilon(k)} - 1}. \tag{III.7}$$

Then $\omega_{ph}(A) := \langle \Omega_{ph} |\ \pi_{ph}(A)\Omega_{ph}\rangle$ is an (α_{ph}, β)-KMS state. Moreover,

$$\pi_{ph}(\alpha_{ph}^t(A)) = e^{itL_{ph}} \pi_{ph}(A) e^{-itL_{ph}} \tag{III.8}$$

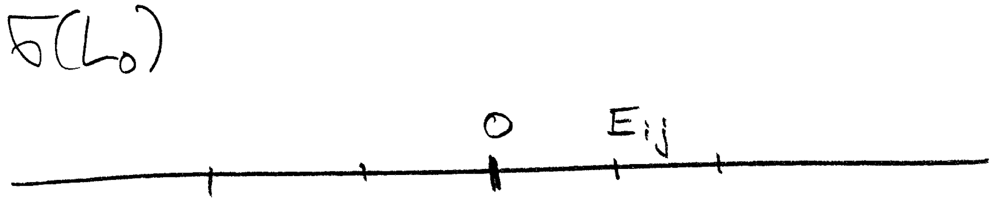
where the Liouvillean is

$$L_{ph} = \int \varepsilon(k) \left(a_{l,k}^* a_{l,k} - a_{r,k}^* a_{r,k}\right) \mathrm{d}^d k. \tag{III.9}$$

Note that $\ker L_{ph} = \mathbb{C} \cdot \Omega_{ph}$ and $\sigma(L_{ph}) \setminus \{0\} = \sigma_{ac}(L_{ph}) \setminus \{0\}$.

If we study a system of an atom and the scalar field at temperature $\beta^{-1} > 0$ but without interaction, then $\mathcal{A} = \mathcal{A}_{at} \otimes \mathcal{A}_{ph}$, $\alpha_0 := \alpha_{at} \otimes \alpha_{ph}$, $\omega_0 = \omega_{at} \otimes \omega_{ph}$ is an (α_0, β)-KMS state, $\alpha_0^t(A) = e^{itL_0} A e^{-itL_0}$, with $L_0 = L_{at} \otimes \mathbf{1}_{ph} + \mathbf{1}_{at} \otimes L_{ph}$ on $\mathcal{H}_0 = \mathcal{H}_{at} \otimes \mathcal{H}_{ph}$, and the GNS representation of $(\mathcal{A}, \omega_0)$ is given by

$$(\mathcal{H}_0, \quad \pi_0 = \pi_{at} \otimes \pi_{ph}, \quad \Omega_0 = \Omega_{at} \otimes \Omega_{ph}). \tag{III.10}$$



<u>Remarks:</u>

- Note that
$$\sigma(L_{at}) = \{E_{ij} := E_i - E_j |\ 1 \le i, j \le N\} \tag{III.11}$$
and so E_{ij} are also eigenvalues of L_0

- In particular $0 = \{E_{ii} |\ i = 1, \ldots, N\}$ is an N-fold degenerate eigenvalue.

- All states

$$\omega_{ij}(A) := \langle \varphi_i \otimes \overline{\varphi_j} \otimes \Omega_{ph} |\, \pi_0(A)\, (\varphi_i \otimes \overline{\varphi_j} \otimes \Omega_{ph}) \rangle \tag{III.12}$$

are α_0-invariant, but only

$$\omega_0 = Z^{-1} \sum_{i=1}^{N} e^{-\beta E_i} \omega_{ii} \tag{III.13}$$

is KMS.

Theorem 15 (Return to Equilibrium) *Suppose that $(\mathcal{A}, \alpha_0)$ is a W^*-dynamical system, ω_0 an (α_0, β)-KMS state, and $(\mathcal{H}_0, \pi_0, \Omega_0)$ the GNS representation of $(\mathcal{A}, \omega_0)$. Let $(\mathcal{A}, \alpha_g)$ be a W^*-dynamical system and $L_g = L_g^*$ on $\mathcal{H}_0$ such that*

$$\forall A \in \mathcal{A} : \; \pi_0(\alpha_g^t(A)) = e^{itL_g} \pi_0(A) e^{-itL_g} \tag{III.14}$$

and that 0 is the only and a simple eigenvalue of L_g,

$$\ker L_g = \mathbb{C} \cdot \Omega_g, \quad \|\Omega_g\| = 1, \tag{III.15}$$

and

$$\sigma(L_g) \setminus \{0\} = \sigma_{ac}(L_g) \setminus \{0\}. \tag{III.16}$$

Then

(i)

$$\omega_g(A) := \langle \Omega_g |\, \pi_0(A) \Omega_g \rangle_{\mathcal{H}_0} \tag{III.17}$$

defines the unique (β, α_g)-KMS state $\omega_g \in \mathcal{A}^*$.

(ii) For all $\widetilde{\omega}$, which are normal w.r.t. ω_g (or ω_0, resp.) and all $A \in \mathcal{A}$:

$$\lim_{t\to\infty} \widetilde{\omega}(\alpha_g^t(A)) = \omega_g(A). \qquad \text{(R-to-E)} \tag{III.18}$$

Sketch of Proof for (i) ⇒ (ii): Suppose that $A, B, C \in \mathcal{A}$ (actually, they are taken from a dense subset of $\mathcal{A}$ of analytic vectors) and consider

$$\begin{aligned}
&\langle \Omega_g |\, \pi_0(B)^* \; \pi_0(\alpha_g^t(A)) \; \pi_0(C) \; \Omega_g \rangle \\
&= \omega_g\big([B^* \alpha_g^t(A)] C\big) \;=\; \omega_g\big(\alpha^{-i\beta}(C)[B^*\alpha_g^t(A)]\big) \\
&= \langle \Omega_g |\, \pi_0(\alpha^{-i\beta}(C) B^*) e^{itL_g} \; \pi_0(A) \; e^{-itL_g} \; \Omega_g \rangle \\
&= \langle \Omega_g |\, \pi_0(\alpha^{-i\beta}(C) B^*) \; e^{itL_g} \pi_0(A) \; \Omega_g \rangle \\
&\xrightarrow{t\to\infty} \langle \Omega_g |\, \pi_0(\alpha^{-i\beta}(C) B^*) \; \Omega_g \rangle \langle \Omega_g |\, \pi_0(A) \; \Omega_g \rangle \\
&= \omega_g(\alpha^{-i\beta}(C) B^*) \cdot \omega_g(A) \\
&= \omega_g(B^* C) \; \omega_g(A) \;=\; \omega_g(A) \cdot \langle \Omega_g |\, \pi_0(B) \pi_0(C) \; \Omega_g \rangle .
\end{aligned} \tag{III.19}$$

So $\forall A, B, C$:

$$\lim_{t\to\infty} \langle \pi_0(B)\Omega_g | \, \pi_0(\alpha_g^t(A))\pi_0(C)\Omega_g \rangle = \langle \pi_0(B)\Omega_g | \, \pi_0(C)\Omega_g \rangle \cdot \omega_g(A). \quad \text{(III.20)}$$

Thus for all $B_1, \ldots, B_N \in \mathcal{A}$ and $\lambda_1, \ldots, \lambda_N \geq 0$ with $\sum_{k=1}^N \lambda_k \leq 1$,

$$\lim_{t\to\infty} \sum_{k=1}^{N} \langle \Psi_k | \, \pi_0(\alpha_g^t(A))\psi_k \rangle \; = \; \omega_g(A) \cdot \left(\sum_{k=1}^{N} \lambda_k \, \|\psi_k\|^2 \right), \quad \text{(III.21)}$$

where $\psi_k := B_k \Omega_g$. If $\widetilde{\omega}$ is ω_g normal w.r.t. ω_0 then $\widetilde{\omega}$ can be approximated by such finite rank density matrices, and the result follows. □

IV Applications

In this section we assume that $\mathcal{A} = \mathcal{A}_{at} \otimes \mathcal{A}_{ph}$ is a suitable algebra of observables of an atom (or an array of these) and a scalar quantum field. The atom is assumed to have only N levels, each of which are nondegenerate. $N < \infty$ is a crucial assumption, unfortunately, and also the nondegeneracy of the atomic eigenvalues helps a lot. The scalar character of the field, however, is chosen merely for notational convenience.

Recall the Hilbert space $\mathcal{K} = \mathcal{K}_{at} \otimes \mathcal{K}_{ph}$ of the atom-photon system, where $\mathcal{K}_{at} = \mathbb{C}^N$ and $\mathcal{K}_{ph} = \mathcal{F}_b[L^2(\mathbb{R}^d)]$. The interacting Hamiltonian H_g, where g is a coupling constant, is given by

$$H_g \;=\; H_0 + gI, \quad \text{(IV.1)}$$

$$H_0 \;=\; H_{at} \otimes \mathbf{1} + \mathbf{1} \otimes H_{ph}, \quad \text{(IV.2)}$$

$$I \;=\; \int (G_k \otimes a_k^* + G_k^* \otimes a_k) \, d^d k =: a^*(G) + a(G). \quad \text{(IV.3)}$$

Here, $G_k \in B(\mathcal{K}_{at})$ represents the transition matrix of the atom in a dipole approximation and is of the form

$$G_k^{dip}(i,j) = \int_{\mathbb{R}^3} \overline{\varphi_i^{at}(x)} \left(\frac{\kappa(k/\Lambda)}{\sqrt{k}} x \right) \varphi_j^{at}(x) \, d^3x \quad \text{(IV.4)}$$

or

$$G_k^{mc}(i,j) = \int_{\mathbb{R}^3} \overline{\varphi_i^{at}(x)} \left(\frac{\kappa(k/\Lambda)}{\sqrt{k}} e^{-ikx} \; \vec{\varepsilon}_k \cdot \frac{1}{i} \vec{\nabla}_x \varphi_j^{at}(x) \right) \, d^3x. \quad \text{(IV.5)}$$

The function $\kappa(\frac{\cdot}{\Lambda})$ is an analytic UV cutoff. To be specific, we choose

$$\kappa(k) := e^{-k^2}. \quad \text{(IV.6)}$$

The dynamics α_g generated by H_g at temperature $\beta^{-1} > 0$,

$$\alpha_g^t(A) = e^{itH_g} A e^{-itH_g}, \tag{IV.7}$$

is implemented in the Araki-Woods representation (III.4)-(III.10) as

$$\pi_0(\alpha_g^t(A)) \;=\; e^{itL_g}\, \pi_0(A)\, e^{-itL_g} \tag{IV.8}$$

with

$$\begin{aligned} L_g &= L_0 + g\,(\pi_0(I) - J\pi_0'(I)J) \\ &=: L_0 + g\,W, \end{aligned} \tag{IV.9}$$

$$\begin{aligned} W &= a_l^*\left(\sqrt{1+\rho_\beta}G_l - \sqrt{\rho_\beta}\overline{G_r^*}\right) + a_l\left(\sqrt{1+\rho_\beta}G_l - \sqrt{\rho_\beta}\overline{G_r^*}\right) \\ &\quad + a_r^*\left(\sqrt{\rho_\beta}G_l^* - \sqrt{1+\rho_\beta}\overline{G_r}\right) + a_r\left(\sqrt{\rho_\beta}G_l^* - \sqrt{1+\rho_\beta}\overline{G_r}\right) \\ &=: a_l^*(F_l) + a_l(F_l) + a_r^*(F_r) + a_r(F_r), \end{aligned} \tag{IV.10}$$

where, for $k \in \mathbb{R}^d$, $F_{l/r,k}$ are the $N^2 \times N^2$-Matrices

$$F_{l,k} \;=\; \sqrt{1+\rho_\beta(k)} \cdot G_k \otimes \mathbf{1} - \sqrt{\rho_\beta(k)} \cdot \mathbf{1} \otimes G_k^{tr}, \tag{IV.11}$$

$$F_{r,k} \;=\; \sqrt{\rho_\beta(k)} \cdot G_k^* \otimes \mathbf{1} - \sqrt{1+\rho_\beta(k)} \cdot \mathbf{1} \otimes \overline{G_k}. \tag{IV.12}$$

IV.1 Complex Deformations

Studying perturbations L_g of L_0 is difficult because the unperturbed operator is not semibounded and the eigenvalues are embedded in continuous spectrum. One overcomes these problems by using, e.g., complex deformations (or positive commutator methods). There are two main types of complex deformations: complex translations or complex dilations. Both use the form

$$\varepsilon(k) = |k| \tag{IV.13}$$

in an essential way.

If we have a self-adjoint $A = A^*$ (possibly unbounded) on $\mathfrak{h} = L^2(\mathbb{R}^n)$ then

$$\mathbb{R} \ni \theta \;\mapsto\; U_\theta = e^{i\theta A} \;\in B(\mathfrak{h}) \tag{IV.14}$$

defines a unitary C_0-group. For an analytic vector $\psi \in \mathcal{M} \subseteq \mathfrak{h}$, the map

$$\mathbb{R} \ni \theta \;\mapsto\; \psi_\theta := U_\theta \psi \in \mathfrak{h} \tag{IV.15}$$

has an analytic continuation to a strip $\mathcal{S}_{\theta_0} = \{-\theta_0 < \operatorname{Im}\theta < \theta_0\}$, $\theta_0 > 0$, about the real axis,

$$\mathcal{S}_{\theta_0} \ni \theta \ \mapsto \ \Psi_\theta \in \mathfrak{h}. \tag{IV.16}$$

In many situations, also

$$\mathbb{R} \ni \theta \ \mapsto \ L_g(\theta) = U_\theta L_g U_\theta^{-1} \in B(\mathcal{D}(L_0); \mathfrak{h}) \tag{IV.17}$$

allows for an analytic continuation in θ, i.e., $\theta \mapsto L_g(\theta)$ is an analytic function on $\mathcal{S}_{\theta_0}$ with values in the (Banach space of) bounded operators from $\mathcal{D}(L_0)$ to $\mathfrak{h}$.

Remarks:

- Note that we wrote $L_g(\theta) = U_\theta L_g U_\theta^{-1}$, and not $L_g(\theta) = U_\theta L_g U_\theta^*$ (which cannot have an analytic continuation because $\theta \mapsto U_\theta^*$ is not analytic but antianalytic).
- The domain $\mathcal{D}(L_0)$ of $L_g(\theta)$ neither depends (locally) on g nor on θ.
- Such maps $\mathcal{S}_{\theta_0} \ni \theta \mapsto L_g(\theta) \in B(\mathcal{D}(L_0); \mathfrak{h})$ are called analytic families.
- Eigenvalues are invariant under $L_g(0) \to L_g(\theta)$. In particular, if E is not an eigenvalue of $L_g(\theta)$ then E is not an eigenvalue of $L_g(0)$, either.

Jaksic-Pillet glueing ($d = 3$)**:** Observe that, in spherical coordinates,

$$\mathbb{R}^3 \ \cong \ \mathbb{R}^+ \times \mathbb{S}^2, \tag{IV.18}$$

$$\mathbb{R}^3 \times \{r, l\} \ \cong \ \mathbb{R}^+ \times \{r, l\} \times \mathbb{S}^2 \cong \mathbb{R} \times \mathbb{S}^2. \tag{IV.19}$$

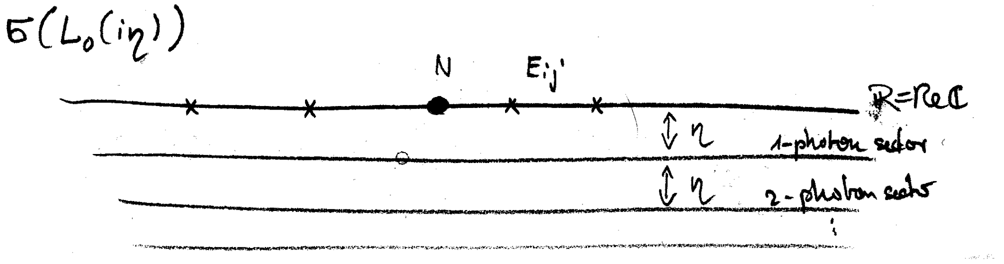
In other words, we consider the momenta of the l-photons to have positive magnitude and the momenta of the r-photons to be of negative magnitude. Implementing this coordinate change leads to

$$L_{ph} = \int_{\mathbb{R}\times\mathbb{S}^2} k \ b^*(k,\sigma) b(k,\sigma) \, dk \mathrm{d}^2\sigma, \tag{IV.20}$$

i.e., L_{ph} may be regarded as the second quantization of the one-dimensional momentum operator. It turns out that translations $k \mapsto k + \xi$

$$L_{ph}(\xi) := \int_{\mathbb{R}\times\mathbb{S}^2} (k + \xi) \ b^*(k,\sigma) b(k,\sigma) \, dk \mathrm{d}^2\sigma, \tag{IV.21}$$

allow for analytic continuation and lead to an analytic family $(L_g(\xi))_\xi$. In particular, for $\xi = i\eta$ with $\eta > 0$, we have



The N^2 eigenvalues

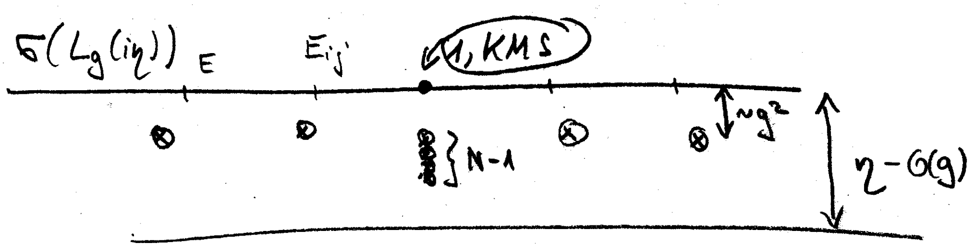
$$E_{ij}(0) := E_{ij} = E_i - E_j, \quad i,j \in \{1,\ldots,N\} \tag{IV.22}$$

are isolated and of finite multiplicity. The nondegeneracy of $E_1 < E_2 < \ldots < E_N$ ensures that the degeneracy of 0, as an eigenvalue of $L_0(i\eta)$, is N, namely

$$E_{11} = E_{22} = \cdots = E_{NN} = 0, \tag{IV.23}$$

$$\forall i \neq j: \; E_{ij} \neq 0. \tag{IV.24}$$

The eigenvalues E_{ij} of $L_0(i\eta)$ are isolated, and the eigenvalues of $L_g(i\eta)$ can be computed by standard perturbation theory. The result is



0 is a simple eigenvalue of $L_g(i\eta)$, corresponding to the KMS state and there are $N^2 - 1$ complex eigenvalues

$$\begin{aligned} E_{mm}(g) &= -ig^2\gamma_{mm}, \quad m \in \{2,3,\ldots,N\}, \\ E_{mn}(g) &= E_{mn} + g^2\delta_{mn} - ig^2\gamma_{mn}, \quad m,n \in \{1,\ldots,N\}, m \neq n, \end{aligned} \tag{IV.25}$$

where $\{\gamma_{mn}\}_{m+n\geq 3} \subseteq \mathbb{R}^+$ are positive numbers (their positivity actually requires a genericity assumption on G_k ensuring that there are no forbidden transitions) resulting from second-order perturbation theory. We set

$$\Gamma := \min_{\substack{1\leq m,n\leq N \\ m+n\geq 3}} \{\gamma_{mn}\} > 0 \tag{IV.26}$$

noting that $\Gamma > 0$ requires $\underline{N < \infty}$ (!). Moreover,

$$\sigma_{disc}(L_g(i\eta)) = \{0\} \cup \{E_{mn}(g) | \quad 1 \leq m,n \leq N, \; m+n \geq 3\}, \tag{IV.27}$$

with corresponding projections

$$\begin{aligned} L_g(i\eta)\ P_{mn}(g,\eta) &= E_{mn}(g)P_{mn}(g,\eta), \\ \text{rank } P_{mn}(g,\eta) &= 1, \quad P_{mn}(g,\eta) = P^2_{mn}(g,\eta), \end{aligned} \tag{IV.28}$$

and

$$\sigma_{ess}(L_g(i\eta)) \subseteq \mathbb{R} + i(-\infty, \eta - cg). \tag{IV.29}$$

For an analytic vector $\varphi \in \mathcal{H}_0$, we obtain

$$\begin{aligned} &\langle \varphi|\ e^{-itL_g}\varphi \rangle \\ &= \lim_{\varepsilon \searrow 0} \operatorname{Im} \left\{ \frac{-1}{2\pi i} \int e^{-itE} \langle \varphi|\ (L_g - E - i\vec{\varepsilon})^{-1} \varphi \rangle\ dE \right\} \\ &= \lim_{\varepsilon \searrow 0} \operatorname{Im} \left\{ \frac{-1}{2\pi i} \int e^{-itE} \langle \varphi_{-i\eta}|\ (L_g(i\eta) - E - i\vec{\varepsilon})^{-1} \varphi_{i\eta} \rangle\ dE \right\} \\ &= \operatorname{Im} \left\{ \frac{-1}{2\pi i} \int_{\mathbb{R}} e^{-itz} \langle \varphi_{-i\eta}|\ (L_g(i\eta) - z)^{-1} \varphi_{i\eta} \rangle\ \mathrm{d}z \right\} \\ &= \operatorname{Im} \left\{ \frac{-1}{2\pi i} \int_{\mathbb{R} - i(\eta - cg)} e^{-itz} \langle \varphi_{-i\eta}|\ (L_g(i\eta) - z)^{-1} \varphi_{i\eta} \rangle\ \mathrm{d}z \right\} \\ &\quad + \langle \varphi_{-i\eta}|\ \Omega_{g,i\eta} \rangle \langle \Omega_{g,-i\eta}|\ \varphi_{i\eta} \rangle \\ &\quad + \sum_{m+n \geq 3} \langle \varphi_{-i\eta}|\ P_{mn}(g,\eta) \varphi_{i\eta} \rangle \cdot e^{-iE_{mn}(g)t}. \end{aligned} \tag{IV.30}$$

Using that $|e^{-itz}| = e^{\operatorname{Im} z \cdot t}$ and the fact that

$$\langle \varphi_{-i\eta}|\ \Omega_{g,i\eta} \rangle \langle \Omega_{g,-i\eta}|\ \varphi_{i\eta} \rangle = \langle \varphi|\ \Omega_g \rangle \langle \Omega_g|\ \varphi \rangle, \tag{IV.31}$$

we obtain by analytic continuation $i\eta \to 0$ that

$$\begin{aligned} \left| \langle \varphi|\ e^{-itL_g} \varphi \rangle - |\langle \varphi|\ \Omega_g \rangle|^2 \right| &\leq C \cdot \left(e^{-(\eta - cg)t} + e^{-g^2 \Gamma t} \right) \\ &= \tilde{C} \cdot \left(e^{-g^2 \Gamma t} \right), \end{aligned} \tag{IV.32}$$

i.e., the return to equilibrium is, in fact, exponentially fast.

Moreover, we observe from (IV.30) that

$$\begin{aligned} &\left| \langle \varphi|\ e^{-itL_g} \varphi \rangle - |\langle \varphi|\ \Omega_g \rangle|^2 - \sum_{m+n \geq 3} \langle \varphi_{-i\eta}|\ P_{mn}(g,\eta) \varphi_{i\eta} \rangle \cdot e^{-iE_{mn}(g)t} \right| \\ &\qquad \leq C \cdot e^{-(\eta - cg) \cdot t}, \end{aligned} \tag{IV.33}$$

where the validity of the analytic continuation requires, in particular, that

$$g \ll \eta \ll \frac{1}{\beta}. \tag{IV.34}$$

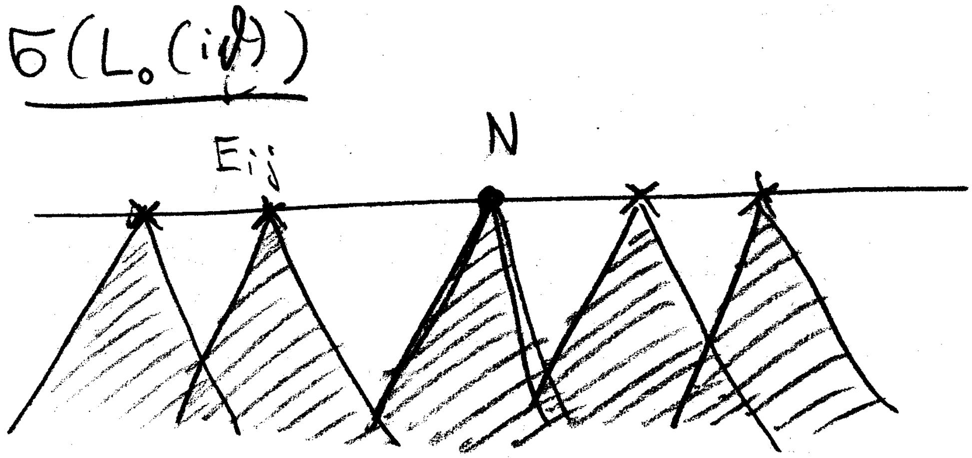
Complex Dilations: Alternatively to Jaksic-Pillet glueing, we can use dilations

$$\mathbb{R} \ni \theta \ \mapsto \ e^{-\frac{d\theta}{2}} \ a^*_{l,e^{\theta}k}, \quad e^{\frac{d\theta}{2}} \ a^*_{r,e^{-\theta}k}, \tag{IV.35}$$

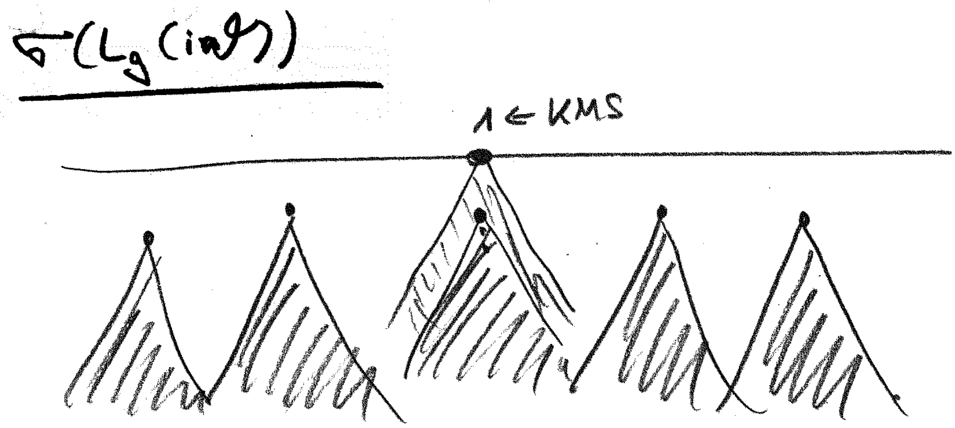
which leads to

$$L_{ph}(\theta) = \int \left(e^{-\theta} \, |k| \ \ a^*_{l,k} a_{l,k} - e^{\theta} \, |k| \ \ a^*_{r,k} a_{r,k} \right) \, d^d k, \tag{IV.36}$$

and, for $\theta = i\vartheta$, $\vartheta > 0$, we obtain



and then



Let us compare these two complex deformations:

Complex translations and J.-P. glueing:

+ elegant idea
+ result on $\sigma(L_g(i\eta))$ can be computed by standard perturbation theory
− very restrictive analycity requirements on the matrix elements $G_k(i,j)$ at $k=0$
− requires large temperatures/resp. small coupling: $g \ll \eta \ll \frac{1}{\beta}$

Complex dilations:

+ minimal analycity requirements on $G_k(i,j)$ at $k=0$
+ uniformity in g: applies $\forall 0 \le g \le g_0$, $0 < \beta \le \beta_0$. (still, zero temperature limit is not allowed [and should not be allowed])
− result on $L_g(i\vartheta)$ makes use of (involved) RG theory necessary
− does not yield exponentially fast R-to-E.

IV.2 Decoherence

For simplicity, we henceforth assume $N=2$, i.e., we study a single qubit, $\mathbb{C}^2$, coupled to the photon field at temperature $\beta^{-1} > 0$.

We assume that

$$G_k = \begin{pmatrix} a & c \\ \bar{c} & b \end{pmatrix} \cdot \widehat{G}(k), \quad \widehat{G}(k) = \frac{\kappa(k/\Lambda)}{\sqrt{|k|}}. \tag{IV.37}$$

We introduce as initial qubit states

$$\varphi_{ij} := \varphi_i \otimes \overline{\varphi_j} \otimes \Omega_{ph}, \quad 1 \le i,j \le 2, \tag{IV.38}$$

and

$$\rho_{ij}(t) := \langle \varphi_{ij} | \, e^{-itL_g} \varphi_{ij} \rangle \tag{IV.39}$$

noting that Ω_0 is an analytic vector (in fact, $\Omega_{0,\pm i\eta} = \Omega_0$). $\rho_{ij}(t)$ measures the time-decay of qubits in states $E^{ij} \cdot (ij$-th matrix unit), e.g.,

$$\rho_{12}(t) \quad \text{corresponds to} \quad \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \in B(\mathbb{C}^2). \tag{IV.40}$$

Note that perturbative arguments yield

$$\langle \varphi_{ij} | \, \Omega_g \rangle = \langle \varphi_{ij} | \, \Omega_0 \rangle + \mathcal{O}(g^2), \tag{IV.41}$$

$$\begin{aligned}\langle \varphi_{ij} | \, \Omega_0 \rangle &= Z^{-1} \sum_{m=1}^{2} e^{-\beta E_m} \langle \varphi_i \otimes \overline{\varphi_j} | \, \varphi_m \otimes \overline{\varphi_m} \rangle \\ &= \left(\frac{e^{-\beta E_1}}{e^{-\beta E_1} + e^{-\beta E_2}} \right) \delta_{i1} \delta_{j1} + \left(\frac{e^{-\beta E_2}}{e^{-\beta E_1} + e^{-\beta E_2}} \right) \delta_{i2} \delta_{j2},\end{aligned}$$

and, for $m \neq n$,

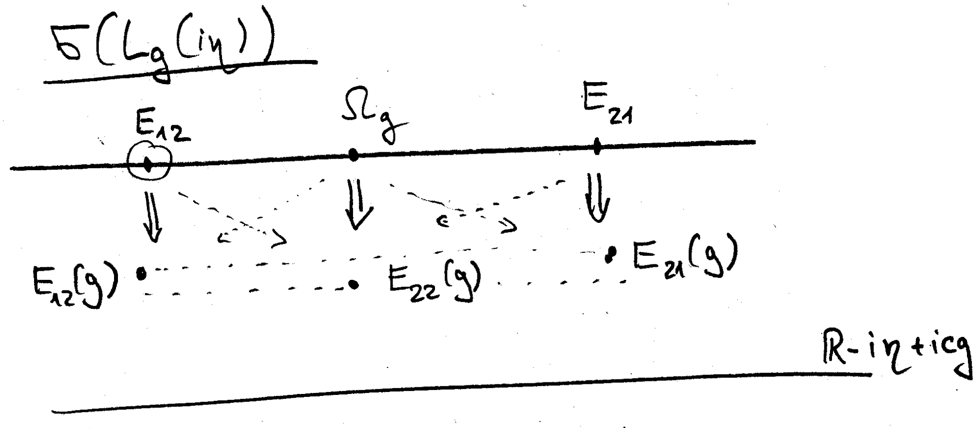
$$\begin{aligned}\langle \varphi_{ij} | \, P_{mn}(g, \eta) \varphi_{ij} \rangle &= \langle \varphi_{ij} | \, P_{mn}(0, \eta) \varphi_{ij} \rangle + \mathcal{O}(g^2) \\ &= |\langle \varphi_{ij} | \, \varphi_{mn} \rangle|^2 + \mathcal{O}(g^2) = \delta_{im} \delta jn + \mathcal{O}(g^2). \end{aligned} \tag{IV.42}$$

Inserting these estimates into (IV.33), we conclude that

$$\begin{aligned}\rho_{11/22}(t) - \rho_{11/22}(\infty) &= \left(\frac{e^{-\beta E_{1/2}}}{e^{-\beta E_1} + e^{-\beta E_2}} \right) \cdot e^{-iE_{22}(g) \cdot t} \left[1 + \mathcal{O}(g^2) \right] \\ &\quad + \mathcal{O}(g^2) \cdot e^{-iE_{12}(g) \cdot t},\end{aligned}$$

$$\rho_{12}(t) - \rho_{12}(\infty) = e^{-iE_{12}(g) \cdot t} \left[1 + \mathcal{O}(g^2) \right] + \mathcal{O}(g^2) \cdot e^{-iE_{22}(g) \cdot t},$$

i.e., the dominating contributions to the decoherence, i.e., the decay of $\rho_{ij}(t) - \rho_{ij}(\infty)$, come from the local part of the spectrum



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